Inferring feature importance with uncertainties in high-dimensional data

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Abstract

Estimating feature importance is a significant aspect of explaining data-based models. Besides explaining the model itself, an equally relevant question is which features are important in the underlying data generating process. We present a Shapley value based framework for inferring the importance of individual features, including uncertainty in the estimator. We build upon the recently published feature importance measure of SAGE (Shapley additive global importance) and introduce sub-SAGE which can be estimated without resampling for tree-based models. We argue that the uncertainties can be estimated from bootstrapping and demonstrate the approach for tree ensemble methods. The framework is exemplified on synthetic data as well as high-dimensional genomics data.

1. Introduction

With the strong improvement of black-box machine learning models such as gradient boosting models and deep neural networks, the question of how

to infer feature importance in these types of models has become increasingly important. The Shapley decomposition, a solution concept from cooperative game theory (Shapley, 1953), has enjoyed a surge of interest in the literature on explainable artificial intelligence in recent years, (cf. Aas et al. (2020); Lundberg et al. (2020); Sellereite and Jullum (2019); Lundberg and Lee (2017); Strumbelj and Kononenko (2013, 2010); Lundberg et al. (2019); Redelmeier et al. (2020); Kwon et al. (2021); Song et al. (2016); Moehle et al. (2021); Covert et al. (2020a); Keinan et al. (2003); Fryer et al. (2021b)). A widely used Shapley based framework for deriving feature importances in a fitted machine learning model is Shapley additive explanations (SHAP) (Lundberg and Lee, 2017; Lundberg et al., 2020), which explains single predictions' deviations from the average model prediction. As such, SHAP attributes feature importances as they are perceived by the model. The more recently introduced Shapley additive global importance (SAGE) is also based on the Shapley decomposition, but attributes feature importances by a global decomposition of the model loss across a whole data set (Covert et al., 2020b). The SAGE framework thus provides an explanation of the influence of the features taking into account not only the model, but also implicitly the data via the loss function, thus encapsulating that the model might not be – and most likely isn't – a perfect description of the data (see Fryer et al., 2021a, for a discussion and comparison between SHAP and SAGE as feature performance measures).

The SAGE value needs to be estimated, and the SAGE estimator is itself a random variable as the corresponding SAGE estimate is based on data of finite size generated from some unknown probability distribution. As is the case for any feature importance measure, we argue that the uncertainty in the estimate is equally important as the estimate itself for drawing conclusions. However, even computation of the SAGE-estimate is infeasible for high-dimensional data, and thus further approximations are needed (Covert et al., 2020b). To this end, we introduce sub-SAGE, which is motivated by SAGE but can be estimated exactly for tree-ensemble models, by using a reduced subset of coalitions. Additionally, we describe how to estimate a confidence interval of the sub-SAGE value. No calculation of such uncertainty exists in the SAGE package or the literature. We do this using paired bootstrapping, and demonstrate its calculation on simulated as well as observed high-dimensional data. We argue that this procedure provides a way to infer the true importance of a feature in the underlying data. We restrict

ourselves to tree ensemble models. The remainder of this paper is structured as follows. In section 2 we introduce background concepts such as the Shapley value, SHAP and SAGE, before moving on to sub-SAGE in section 3 and its uncertainty in section 4. The method is exemplified in section 5 and section 6 before we discuss the results in section 7.

2. Background

In this section, we provide a brief introduction to the Shapley decomposition-based SHAP and SAGE frameworks, and how to apply these to tree ensemble models. The Shapley decomposition is a solution concept from cooperative game theory (Shapley, 1953). It provides a decomposition of any value function v(S) that characterises the game, and produces a single real number, or payoff, per set of players in the game. The resulting decomposition satisfies the three properties of efficiency, monotonicity and symmetry, and is provably the only method to satisfy all three (Young, 1985; Huettner and Sunder, 2012, Thm. 2). For details see appendix Appendix D.

Consider a supervised learning task characterised by a set of M features \mathbf{x}_i and corresponding univariate¹ responses y_i , for $i=1,\ldots,N$, and a fitted model that is a mapping from feature values to response values, i.e. $\mathbf{x}_i \to \hat{y}(\mathbf{x}_i)$. As usual, uppercase letters denote random variables while lowercase letters denote observed data values. In this work, we assume independent features, meaning $E[X_j|X_k=x_k]=E[X_j] \ \forall \ j\neq k$.

2.1. The SHAP value

Let $S \subseteq \mathcal{M} \setminus \{k\}$, with $\mathcal{M} = \{1, ..., M\}$, denote a subset of all features not including feature k. Denote \bar{S} the corresponding complement subset of excluded features $(S \cup \bar{S} = \mathcal{M})$. The SHAP value, $\phi_k^{\text{SHAP}}(\mathbf{x}, \hat{y})$, introduced by Lundberg and Lee (2017), for a feature with index k with respect to features \mathbf{x} and a corresponding fitted model \hat{y} , is defined as

$$\phi_k^{\text{SHAP}}(\mathbf{x}, \hat{y}) = \sum_{\mathcal{S} \subseteq \mathcal{M} \setminus \{k\}} \frac{|\mathcal{S}|!(M - |\mathcal{S}| - 1)!}{M!} \left[v_{\mathbf{x}, \hat{y}}(\mathcal{S} \cup \{k\}) - v_{\mathbf{x}, \hat{y}}(\mathcal{S}) \right]. \tag{1}$$

¹The procedures described in this paper can be generalised to multivariate responses, but this renders the derivations more convoluted.

Here, the value function $v_{\mathbf{x},\hat{y}}(\mathcal{S})$ is defined as the expected output of a prediction model conditioned that only a subset \mathcal{S} of all features are included in the model,

$$v_{\mathbf{x},\hat{y}}(\mathcal{S}) = E_{\mathbf{X}_{\overline{S}}}[\hat{y}(\mathbf{X}|\mathbf{X}_{\mathcal{S}} = \mathbf{x}_{\mathcal{S}})].$$
 (2)

For instance, if $\mathbf{x}_{\overline{S}}$ is continuous and we assume all features to be mutually independent, we have

$$E_{\mathbf{X}_{\overline{S}}}[\hat{y}(\mathbf{X}|\mathbf{X}_{S} = \mathbf{x}_{S})] = \int_{\mathbf{x}_{\overline{S}}} \hat{y} \left(\mathbf{X}_{S} = \mathbf{x}_{S}, \mathbf{X}_{\overline{S}} = \mathbf{x}_{\overline{S}}\right) p\left(\mathbf{X}_{\overline{S}} = \mathbf{x}_{\overline{S}}|\mathbf{X}_{S} = \mathbf{x}_{S}\right) d\mathbf{x}_{\overline{S}}$$

$$= \int_{\mathbf{x}_{\overline{S}}} \hat{y} \left(\mathbf{X}_{S} = \mathbf{x}_{S}, \mathbf{X}_{\overline{S}} = \mathbf{x}_{\overline{S}}\right) p\left(\mathbf{X}_{\overline{S}} = \mathbf{x}_{\overline{S}}\right) d\mathbf{x}_{\overline{S}}.$$
(3)

The stochastic behaviour in $v_{\mathbf{x},\hat{y}}(\mathcal{S})$ is due to the random vector $\mathbf{X}_{\bar{\mathcal{S}}}$ of unknown feature values. We can think of the difference $v_{\mathbf{x},\hat{y}}(\mathcal{S} \cup \{k\}) - v_{\mathbf{x},\hat{y}}(\mathcal{S})$ as the mean difference in a single model prediction when using feature k in the model compared to when the value of feature k is absent. Therefore, the SHAP value can be interpreted as a feature importance measure for each single model prediction. The larger absolute SHAP value a feature k has in a single prediction, the more influence the feature is regarded to have.

2.2. The SAGE value

Define a loss function $\ell(y_i, \hat{y}(\mathbf{x}_i))$ as a measure of how well the fitted model $\hat{y}(\mathbf{x}_i)$ maps the features to a response, compared to the true response value y_i . As defined in Covert et al. (2020b), we take the SAGE value function $w(\mathcal{S})$ as the expected difference in the observed value of the loss function when the features in \mathcal{S} are included in the model compared to excluding all features,

$$w_{\mathbf{X},Y,\hat{y}}(\mathcal{S}) = E_{\mathbf{X},Y}[\ell(Y, V_{\mathbf{X},\hat{y}}(\emptyset))] - E_{\mathbf{X},Y}[\ell(Y, V_{\mathbf{X},\hat{y}}(\mathcal{S}))]. \tag{4}$$

Here, \emptyset denotes the empty set, while $V_{\mathbf{X},\hat{y}}(\mathcal{S})$ is the stochastic version of eq. (2). Specifically, $V_{\mathbf{X},\hat{y}}(\mathcal{S})$ is a random variable since its observed value varies depending on the random vector $X_{\mathcal{S}}$, while $v_{\mathbf{x},\hat{y}}(\mathcal{S})$ is a constant as we condition on the *observed* vector $\mathbf{x}_{\mathcal{S}}$. For instance, for the case where \mathbf{x} and y are continuous, the expected value of the loss function when only a subset \mathcal{S} of feature values are known is

$$E_{\mathbf{X},Y}[\ell(Y,V_{\mathbf{X},\hat{y}}(\mathcal{S}))] = \int_{y} \int_{\mathbf{x}_{\mathcal{S}}} \ell\left(y(\mathbf{x}), E_{\mathbf{X}_{\mathcal{S}}}\left[\hat{y}\left(\mathbf{X}|\mathbf{X}_{\mathcal{S}} = \mathbf{x}_{\mathcal{S}}\right)\right]\right) p(y|\mathbf{x}_{\mathcal{S}}) p(\mathbf{x}_{\mathcal{S}}) d\mathbf{x}_{\mathcal{S}} dy . \quad (5)$$

Notice that the computation of $v_{\mathbf{x},\hat{y}}(\mathcal{S}) = E_{\mathbf{X}_{\bar{\mathcal{S}}}}[\hat{y}(\mathbf{X}|\mathbf{X}_{\mathcal{S}} = \mathbf{x}_{\mathcal{S}})]$ happens inside the loss function, which is usually non-linear. Also notice that in eq. (5), we integrate over *all* possible values of $X_{\mathcal{S}}$.

The SAGE value for a feature k is defined as

$$\phi_k^{\text{SAGE}}(\mathbf{X}, Y, \hat{y}) = \sum_{\mathcal{S} \subseteq \mathcal{M} \setminus \{k\}} \frac{|\mathcal{S}|!(M - |\mathcal{S}| - 1)!}{M!} \left[w_{\mathbf{X}, Y, \hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X}, Y, \hat{y}}(\mathcal{S}) \right].$$
(6)

We can think of the difference $w_{\mathbf{X},Y,\hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X},Y,\hat{y}}(\mathcal{S})$ as the expected difference in the loss function when including feature k in the model compared to excluding feature k. SAGE is therefore a global feature importance measure, as opposed to the SHAP value, as it does not evaluate a single prediction, but rather the impact feature k has across all predictions. The use of the loss function in the SAGE definition also makes sure that the feature importance is not only based on the model, as for the SHAP value, but also on the data itself.

The features and response can be both continuous and discrete. In the discrete case, integrals must replaced by sums and vice versa in eqs. (3) and (5). The expressions in eqs. (2) and (4) are in general unknown and need to be estimated for each choice of model and loss function. Consequently, the SHAP and SAGE values become estimates as well.

An interpretation of SAGE is that a positive SAGE value for a features implies that including this feature in the model reduces the expected model loss compared to when not including the feature.

2.3. Tree ensemble models

Consider a tree ensemble model consisting of several regression trees $f_{\tau}(\mathbf{x}_i)$ with predicted response $\hat{y}(\mathbf{x}_i)$, such that $\hat{y}(\mathbf{x}_i) = \sum_{\tau=1}^{T} f_{\tau}(\mathbf{x}_i)$ for T trees. By the linearity property of the expected value, we have

$$v_{\mathbf{x},\hat{y}}(\mathcal{S}) = E_{\mathbf{X}_{\bar{\mathcal{S}}}} \left[\sum_{\tau=1}^{T} f_{\tau}(\mathbf{X}|\mathbf{X}_{\mathcal{S}} = \mathbf{x}_{\mathcal{S}}) \right] = \sum_{\tau=1}^{T} E_{\mathbf{X}_{\bar{\mathcal{S}}}} [f_{\tau}(\mathbf{X}|\mathbf{X}_{\mathcal{S}} = \mathbf{x}_{\mathcal{S}})].$$
 (7)

The computation of $E_{\mathbf{X}_{\bar{S}}}[f_{\tau}(\mathbf{X}|\mathbf{X}_{\bar{S}}=\mathbf{x}_{\bar{S}})]$ can be understood through a simple example: Consider the regression tree illustrated in fig. 1. It has depth two and splits on the two features indexed 1 and 2, which are continuous and

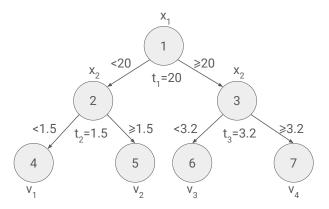


Figure 1: A regression tree including two features X_1 and X_2 .

mutually independent. The regression tree has parameters such as *splitting* points, s_j , for branch nodes, and *leaf values* v_j , for leaf nodes. Assume that $x_2 = 3$ is observed. We then have

$$E_{\mathbf{X}_{\bar{S}}}[f_{\tau}(\mathbf{X}|\mathbf{X}_{\bar{S}} = \mathbf{x}_{\bar{S}})] = E_{X_1}[f_{\tau}(X_1|X_2 = 3)]$$

$$= P(X_1 \ge 20)v_3 + P(X_1 < 20)v_2.$$
(8)

In general, we do not know the value of $P(X_1 \leq 20)$, and need to estimate it. Consider N data instances with recorded feature values from feature k. An unbiased estimate of $P(X_k \leq t)$ is then

$$\hat{P}(X_k \le t) = \frac{1}{N} \sum_{i=1}^{N} I(x_{i,k} \le t),$$
(9)

where $x_{i,k}$ is the observed value of feature k for data instance i. Using this estimate, we can also get an unbiased estimate for eq. (8). An unbiased estimate of $E_{\mathbf{X}_{\bar{S}}}[f_{\tau}(\mathbf{X}|\mathbf{X}_{\mathcal{S}}=\mathbf{x}_{\mathcal{S}})]$ for any regression tree can be achieved by a recursive algorithm (Lundberg et al., 2020), however it must be adjusted with respect to the estimation of the probabilities $\hat{P}(X_k \leq t)$ for every feature k and splitting point t in the tree ensemble model, see algorithm 1. In Lundberg et al. (2020), the estimate of a particular probability $\hat{P}(X_k \leq t)$ in a regression tree is estimated based on the training data used to construct the regression tree. We discuss this practice in section 5.

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used for splitting \mathbf{f} = (f_1, \dots, f_{2^d-1}) and corresponding splitting points
   \mathbf{t} = (t_1, \dots, t_{2^d-1}). Estimated probabilities of ending at a node j given
   previous information, for all nodes in the tree, \mathbf{p} = (p_1, \dots, p_{2^d-1}), by
   using some data (\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N) of size N. The subset of features
   \mathcal{S} with corresponding known values x_{\mathcal{S}}. The left and right descendant
   node for each internal node \mathbf{l} = (l_1, \dots, l_{2^d-1}) and \mathbf{r} = (r_1, \dots, r_{2^d-1}).
   The index of a node j in the tree f_{\tau}.
2: Function CondExpTree(j, f_{\tau}, \mathbf{v}, \mathbf{t}, \mathbf{f}, \mathbf{l}, \mathbf{r}, \mathbf{p})
3: if IsLeaf(j) then
4:
        return v_i
5: else
        if f_j \in \mathcal{S} then
6:
            if x_j \leq t_j then
7:
```

return CondExpTree $(l_j, f_\tau, \mathbf{v}, \mathbf{t}, \mathbf{f}, \mathbf{l}, \mathbf{r}, \mathbf{p})$

return CondExpTree $(r_i, f_\tau, \mathbf{v}, \mathbf{t}, \mathbf{f}, \mathbf{l}, \mathbf{r}, \mathbf{p})$

return CondExpTree $(l_j, f_\tau, \mathbf{v}, \mathbf{t}, \mathbf{f}, \mathbf{l}, \mathbf{r}, \mathbf{p}) p_{l_j} +$

CondExpTree $(r_i, f_\tau, \mathbf{v}, \mathbf{t}, \mathbf{f}, \mathbf{l}, \mathbf{r}, \mathbf{p}) p_{r_i}$

8: 9:

10:

11:

12:

13:

14:

15:

else

else

end if

end if

Algorithm 1 Recursive algorithm for computation of $E_{\mathbf{X}_{\bar{S}}}[f_{\tau}(\mathbf{X}|\mathbf{X}_{\bar{S}}=\mathbf{x}_{\bar{S}})]$. 1: Input: Tree f_{τ} with depth d, leaf values $\mathbf{v}=(v_1,\ldots,v_{2^d})$, feature

16: **end if** 17: **End Function** 18: CondExpTree $(1, f_{\tau}, \mathbf{v}, \mathbf{t}, \mathbf{f}, \mathbf{l}, \mathbf{r}, \mathbf{p})$ \triangleright Start at root node.

2.4. SAGE in practice

In practice, as the expressions in eq. (2) and eq. (5) must be estimated, we get a SAGE estimator rather than a SAGE value. However, since the SAGE estimator requires summing over all 2^{M-1} subsets $\mathcal{S} \subseteq \mathcal{M} \setminus \{k\}$, for each feature, computing the SAGE estimator for observed data with many features becomes infeasible. In Covert et al. (2020b), the SAGE estimate is approximated through a Monte Carlo simulation process. Specifically, instead of iterating over all 2^{M-1} subsets, a subset \mathcal{S} is randomly sampled with replacement in each iteration out of I iterations in total. The differences $w_{\mathbf{X},Y,\hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X},Y,\hat{y}}(\mathcal{S})$ for each \mathcal{S} are estimated by sampling data instances with replacement and computing sample means (see Covert et al., 2020b, Appendix D for details). For an arbitrarily large data set, the authors show convergence to the true SAGE estimate as $I \to \infty$. Among other things, both the accuracy and convergence speed of the algorithm naturally depends on the number of features in the prediction model.

Keeping in mind that the SAGE estimator is a random variable, we argue that its uncertainty is equally important as the estimate itself. No calculation of this inherent uncertainty exists in the SAGE package or the literature 2 . To this end, we introduce sub-SAGE, which is inspired by the SAGE framework, but consisting of a reduced number of subsets $S \in Q$. While applicable to any number of features, it is best suited for interpreting a small number of features, or a small subset of features in a large feature set.

3. Sub-SAGE

Given hundreds or thousands of features in a model, the computation time required to get a satisfactory accurate estimate of SAGE (Covert et al., 2020b), for each feature, quickly becomes unacceptable. A hybrid approach is to select a reduced subset of features of particular interest to investigate. Such a subset can for instance be selected by computing a model-based feature importance score, like SHAP, for all features in the model and selecting the most interesting looking ones. The reduced subset of promising features can

 $^{^2{\}rm The}$ SAGE code provides the degree of convergence of the approximation procedure; not the uncertainty.

then by more thoroughly investigated in order to infer whether their model-based importance is also reflected in the underlying data generating process. For this purpose, we introduce sub-SAGE, where only a selection of the in total 2^{M-1} subsets are involved in the computation of each feature.

If we want to measure the importance of a feature k based on its marginal effect, as well as potential pairwise interactions it may be involved in, computing $S = \{\emptyset\}$ and $S = \{m\}$ for m = 1, ..., k-1, k+1, ..., M is sufficient. In addition, by including $S = \{1, ..., k-1, k+1, ..., M\}$, the set of all features except feature k, this can be used to measure the importance of feature k in the presence of all features at the same time. Let Q denote the set of subsets S chosen above. We define the sub-SAGE value, ψ_k , for feature k as

$$\psi_k(\mathbf{X}, Y, \hat{y}) = \sum_{S \in \mathcal{Q}} \frac{|S|!(M - |S| - 1)!}{3(M - 1)!} \left[w_{\mathbf{X}, Y, \hat{y}}(S \cup \{k\}) - w_{\mathbf{X}, Y, \hat{y}}(S) \right], \quad (10)$$

Each subset is weighted such that the sum of the weights of all subsets with equal size is the same for each subset size. In addition, the sum of all weights is equal to one. Hence, the construction is similar to the weights defined for Shapley values. See Appendix A for details. In this particular case, there are three possible subset sizes, and so the sum of the weights for each subset size is $\frac{1}{3}$. Shapley properties such as symmetry, dummy property and monotonicity still holds for sub-SAGE. However, as the sum is not over all possible subsets, the sub-SAGE values do no longer satisfy the efficiency axiom of the Shapley decomposition, which SHAP and SAGE do (see Appendix D) However, we regard the efficiency property as not necessary in this particular setting, as we still consider the sub-SAGE to be informative with respect to feature importance via the computed differences $w_{\mathbf{X},Y,\hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X},Y,\hat{y}}(\mathcal{S})$. In addition, the purpose is only to evaluate a small fraction of all features, not all of them. By only considering a reduced number of subsets \mathcal{S} , compared to SAGE, and only considering a reduced number of features to evaluate, both computing the sub-SAGE estimate as well as the uncertainty in the corresponding sub-SAGE estimator become feasible for black-box models, such as for tree ensemble models as discussed in section 4.

3.1. Using sub-SAGE to infer true relationships in the data

As the goal is to infer feature importance from a black-box model using sub-SAGE values, similar to calculating p-values without taking into account the

effect of model selection, we must be extra careful. Any model selection procedure using training data is likely to overfit, resulting in a model containing false relationships that are not a general property of the population from which the data was sampled. It is therefore essential that the sub-SAGE value is calculated using independent data the model was not fitted on. We denote such independent data as $(\mathbf{X}_1^0, Y_1^0), \ldots, (\mathbf{X}_{n_I}^0, Y_{n_I}^0)$, with n_I samples in total.

3.2. sub-SAGE applied on tree ensemble models

SHAP values can be computed efficiently Lundberg et al. (2020) for tree ensemble models even with hundreds of thousands of features (Johnsen et al., 2021, e.g.). However, the SAGE value function defined in eq. (4) does not share the same property for tree ensemble models with non-linear choices of loss functions (Lundberg et al., 2020). This motivates the idea of using fast calculated SHAP values to select features for which to compute the more expensive SAGE values.

We consider a tree ensemble model consisting of T trees. Consider a particular feature k to compute the sub-SAGE value as well as a subset $S \in Q$. We separate the trees in the model into two groups τ_k and the complement group $(\bar{\tau}_k)$ where τ_k is the set of trees including feature k as a splitting feature. The loss function is taken to be the squared error between the response and prediction per sample, i.e. $\ell = (y(\mathbf{x}) - \hat{y}(\mathbf{x}))^2$. Then one can show that (see Appendix B for the derivation),

$$w_{\mathbf{X},Y,\hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X},Y,\hat{y}}(\mathcal{S})$$

$$= E_{\mathbf{X},Y} \left[(Y(\mathbf{X}) - V_{\mathbf{X},\hat{y}}(\mathcal{S}))^{2} \right] - E_{\mathbf{X},Y} \left[(Y(\mathbf{X}) - V_{\mathbf{X},\hat{y}}(\mathcal{S} \cup \{k\}))^{2} \right]$$

$$= E_{\mathbf{X},Y} \left[2Y(\mathbf{X}) \left(\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) - V_{\mathbf{X},f_{j}}(\mathcal{S}) \right) + \left(\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) \right)^{2} \right]$$

$$- \left(\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) \right)^{2} + 2 \left(\sum_{j \notin \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) \right) \left(\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) - V_{\mathbf{X},f_{j}}(\mathcal{S}) \right) \right].$$

$$(11)$$

A commonly used loss function for binary classification problems is binary cross-entropy, $\ell = -y(\mathbf{x}) \log \hat{y}(\mathbf{x}) - (1-y(\mathbf{x})) \log (1-\hat{y}(\mathbf{x})) = (1-y(\mathbf{x})) \sum_{j=1}^{T} f_j(\mathbf{x}) + \log \left(1 + e^{-\sum_{j=1}^{T} f_j(\mathbf{x})}\right)$. For this loss function, one can show that (see Ap-

pendix B)

$$w_{\mathbf{X},Y,\hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X},Y,\hat{y}}(\mathcal{S})$$

$$= E_{\mathbf{X},Y} \left[(1 - Y(\mathbf{X})) \sum_{j=1}^{T} V_{\mathbf{X},f_{j}}(\mathcal{S}) + \log \left(1 + \exp \left(-\sum_{j=1}^{T} V_{\mathbf{X},f_{j}}(\mathcal{S}) \right) \right) \right]$$

$$- E_{\mathbf{X},Y} \left[(1 - Y(\mathbf{X})) \sum_{j=1}^{T} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) + \log \left(1 + \exp \left(-\sum_{j=1}^{T} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) \right) \right) \right]$$

$$= E_{\mathbf{X},Y} \left[(1 - Y(\mathbf{X})) \left(\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) - V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) \right) + \log \left(\frac{1 + \exp \left(-\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) - \sum_{j \notin \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) \right)}{1 + \exp \left(-\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) - \sum_{j \notin \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) \right) \right].$$

$$(12)$$

3.2.1. Plug-in estimates

As discussed earlier, the expression $w_{\mathbf{X},Y,\hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X},Y,\hat{y}}(\mathcal{S})$ needs to be estimated for each $\mathcal{S} \in \mathcal{Q}$, and based on data, $(\mathbf{x}_1^0, y_1^0), \dots, (\mathbf{x}_{N_I}^0, y_{N_I}^0)$, never used during training of the model. Let $\hat{v}_{\mathbf{x}^0,y^0,f_{\tau}}(\mathcal{S})$ for a particular observation (\mathbf{x}^0,y^0) and regression tree f_{τ} denote the estimate of $v_{\mathbf{x}^0,f_{\tau}}(\mathcal{S}) = E_{\mathbf{X}_{\bar{\mathcal{S}}}}[f_{\tau}(\mathbf{X}^0|\mathbf{X}_{\mathcal{S}}^0 = \mathbf{x}_{\mathcal{S}}^0)]$ as described in algorithm 1. A plug-in estimate of ψ_k , denoted $\hat{\psi}_k$, for a regression problem with continuous response, for a tree ensemble model using the squared error loss is given by

$$\hat{\psi}_{k} = \sum_{\mathcal{S} \in \mathcal{Q}} \frac{|\mathcal{S}|! (M - |\mathcal{S}| - 1)!}{3(M - 1)!} \left[\frac{2}{N_{I}} \sum_{i=1}^{N_{I}} y_{i}^{0} \left(\sum_{j \in \tau_{k}} \hat{v}_{\mathbf{x}_{i}^{0}, f_{j}} (\mathcal{S} \cup \{k\}) - \hat{v}_{\mathbf{x}_{i}^{0}, f_{j}} (\mathcal{S}) \right) + \frac{1}{N_{I}} \sum_{i=1}^{N_{I}} \left(\sum_{j \in \tau_{k}} \hat{v}_{\mathbf{x}_{i}^{0}, f_{j}} (\mathcal{S}) \right)^{2} - \frac{1}{N_{I}} \sum_{i=1}^{N_{I}} \left(\sum_{j \in \tau_{k}} \hat{v}_{\mathbf{x}_{i}^{0}, f_{j}} (\mathcal{S} \cup \{k\}) \right)^{2} + \frac{2}{N_{I}} \sum_{i=1}^{N_{I}} \left(\sum_{j \notin \tau_{k}} \hat{v}_{\mathbf{x}_{i}^{0}, f_{j}} (\mathcal{S}) \right) \left(\sum_{j \in \tau_{k}} \hat{v}_{\mathbf{x}_{i}^{0}, f_{j}} (\mathcal{S} \cup \{k\}) - \hat{v}_{\mathbf{x}_{i}^{0}, f_{j}} (\mathcal{S}) \right) \right].$$
(13)

The corresponding plug-in estimate for the binary cross-entropy loss given in eq. (12) can be found in a similar fashion, basically by estimating expected values as their corresponding sample means. For tree ensemble models with tree stumps

(maximum depth of one for each tree), the estimate in (13) is further reduced and can be expressed as sample variance and covariance terms, see Appendix C.

4. Inference of sub-SAGE via bootstrapping

The importance of any feature may be evaluated by estimating sub-SAGE values. Similar to SAGE, a positive sub-SAGE value for a feature indicates that including the feature in the model is expected, based on the subsets $S \in \mathcal{Q}$, to reduce the loss function. However, the corresponding sub-SAGE plug-in estimator given the data generating process $(\mathbf{X}_1^0, Y_1^0), \dots, (\mathbf{X}_{N_I}^0, Y_{N_I}^0)$ from some unknown probability distribution includes uncertainty, and this should be evaluated before making any assumptions about feature importance. The complexity of the sub-SAGE plug-in estimators makes paired bootstrapping a tempting approach. Specifically, the procedure is to iteratively, given independent data points at hand $(\mathbf{x}_1^0, y_1^0), \dots, (\mathbf{x}_{N_I}^0, y_{N_I}^0)$, resample the data points with replacement to get a new bootstrapped sample $(\mathbf{x}_1^*, y_1^*), \dots, (\mathbf{x}_n^*, y_n^*)$. For each bootstrapped sample, a corresponding plug-in estimate, $\hat{\psi}_b^*$, can be computed, and after B iterations, the sample $(\hat{\psi}_1^*, \dots, \hat{\psi}_B^*)$ can approximate B realizations arising from the true distribution of the plug-in estimator. A $1-2\alpha$ confidence interval can be approximated by the percentile interval given by $[\hat{\psi}^{*(\alpha)}, \hat{\psi}^{*(1-\alpha)}]$, where $\hat{\psi}^{*(\alpha)}$ is the 100α empirical percentile, meaning the $B \cdot \alpha$ th least value in the ordered list of the samples $(\hat{\psi}_1^*, \dots, \hat{\psi}_R^*)^3$. The accuracy in the percentile interval increases for larger number of bootstrap iterations. A typical number is B = 1000 regarded to be sufficient in most cases. The algorithm of the paired bootstrap applied specifically to tree ensemble models is given in algorithm 2. Notice that for each bootstrap sample, the probability estimates in the trees need to be updated according to eq. (9). In situations where the plug-in estimator is biased, or there is skewness in the corresponding distribution, the bias-corrected and accelerated bootstrap yields even more accurate confidence intervals (Efron and Tibshirani, 1994).

 $^{^3 \}text{Assuming } B \cdot \alpha$ is an integer. See for instance Efron and Tibshirani (1994) for conventions.

Algorithm 2 Paired bootstrap of sub-SAGE value with percentile interval

- 1: Given independent test data $(\mathbf{x}_1^0, y_1^0), \dots, (\mathbf{x}_{N_I}^0, y_{N_I}^0)$, model $\hat{y}(\mathbf{x}) = \sum_{\tau=1}^T f_{\tau}(\mathbf{x})$, feature k, a loss function and α to estimate $1 2\alpha$ confidence interval:
- 2: Preallocate vector BootVec of length B, the total number of bootstrap iterations.
- 3: **for** b = 1, 2, ..., B **do**
- 4: Resample data N_I times with replacement to get
- 5: $(\mathbf{x}_1^*, y_1^*), \dots, (\mathbf{x}_{N_I}^*, y_{N_I}^*)$
- 6: Update probabilities estimates in all the trees in $\hat{y}(\mathbf{x})$ to get \mathbf{p}^*
- 7: BootVec[b] = ψ_k^*
- 8: end for
- 9: Percentile interval given by $[\hat{\psi}^{*(\alpha)}, \hat{\psi}^{*(1-\alpha)}]$

5. Proof of concept - With known underlying data generating process

In this section, we exemplify the sub-SAGE method on synthetic data with a known relationship defined as

$$f(\mathbf{X}_{i}) = a_{0} + a_{1}X_{i,1} + a_{2}X_{i,2} + a_{21}X_{i,1}e^{X_{i,2}} + a_{3}X_{i,3}^{2} + a_{4}\sin(X_{i,4})$$

$$a_{5}\log(1 + X_{i,5}) - X_{i,5}I(X_{i,6} > 7) + \epsilon_{i},$$
(14)

with $a_0 = -0.5$, $a_1 = 0.03$, $a_2 = -0.05$, $a_{21} = 0.3$, $a_3 = 0.02$, $a_4 = 0.35$, $a_5 = -0.2$, and where the features are sampled from the following distributions

$$X_{1} \sim \text{Binom(size} = 2, p = 0.4)$$

$$X_{2} \sim \text{Binom(size} = 2, p = 0.04)$$

$$X_{3} \sim \Gamma(\text{shape} = 10, \text{rate} = 2)$$

$$X_{4} \sim \text{Unif}(0, \pi)$$

$$X_{5} \sim \text{Poisson}(\lambda = 15)$$

$$X_{6} \sim \text{N}(\mu = 0, \sigma^{2} = 10)$$

$$\epsilon_{i} \sim \text{N}(\mu = 0, \sigma^{2} = 2).$$

$$(15)$$

In addition, we generate 94 noise variables. $j=7,\ldots,47$ with a normal distribution $X_j \sim \mathrm{N}(\mu_j,\sigma_j^2)$ and $j=48,\ldots,100$ with a binomial distribution $X_j \sim \mathrm{Binom}(2,p_j)$ where μ_j,σ_j^2 and p_j are sampled from a uniform distribution. Data is generated to give a total of 16000 samples, and then separated randomly in

three disjoint subsets: Data for training (50%), data for evaluation during training (30%) and independent test data (20%) used for estimating sub-SAGE values. We fit an ensemble tree model using XGBoost (Chen and Guestrin, 2016) to the true influential features $1, \ldots, 6$ together with the noise variables $7, \ldots, 100$.

The hyperparameters are fixed to max_depth = 2, learning rate $\eta = 0.05$, subsample = 0.7, regularization parameters $\lambda = 1$, $\gamma = 0$ and colsample_bytree = 0.8 with early_stopping_rounds = 20 using training data (n = 8000) and validation data (n = 4800). See (Chen and Guestrin, 2016) for details about the hyperparameters. We apply the squared error loss during training. This results in a final model including a total of 230 trees and 62 unique features out of the 100 input-features.

From the trained model, each feature is given a score to evaluate its feature importance based on the model. We apply the expected relative feature contribution (ERFC), given N data points, introduced in Johnsen et al. (2021), which is basically a summary score from the corresponding SHAP values for each feature and individual data point,

$$\kappa_k = \sum_{i=1}^{N} \frac{|\phi_{i,k}^{\text{SHAP}}(\mathbf{x}_i, \hat{y})|}{|\phi_0^{\text{SHAP}}| + \sum_{j=1}^{K} |\phi_{i,j}^{\text{SHAP}}(\mathbf{x}_i, \hat{y})|},$$
(16)

with $\phi_0^{\text{SHAP}} = v_{\mathbf{x},\hat{y}}(\emptyset)$. The ERFCs scores can be computed based on the data used to construct the model, as we only need to measure what the model considers important. The features with the largest ERFC-values are then considered the most promising ones based on the model. Depending on your hypothesis of interest, one can evaluate the uncertainty in the feature importance by computing sub-SAGE estimates with corresponding bootstrap-derived percentile intervals. However, it is important that the sub-SAGE estimates are calculated based on independent test data never used during training. From the trained model, we compute the ERFC based on the training data and validation data together (n = 12800), and table 1 shows the top 10 features with the largest ERFC-values. This shows that the XG-Boost model has accurately ranked the most influential features among the top 10 list, for this rather simple relationship. These scores, based on SHAP values, are only with respect to what the *model* considers important. The sub-SAGE can now be applied to infer whether the importance of any feature from the model is also reflected in the data. As an example, let us consider features 6, 1, 2 and 12 where feature 6 has a strong influence, feature 1 has a weaker influence, and feature 2 has the weakest influence, while feature 12 has no influence with respect to $f(\mathbf{x}_i)$ in eq. (14). Their sub-SAGE estimate along with histograms to estimate the corresponding distribution of the sub-SAGE estimators are shown in fig. 2 for training plus validation data as well as for independent test data. We see that sub-SAGE values inferred using training data overestimates the false influence of

Table 1: The resulting ranking based on the expected relative feature contribution (ERFC) after having trained an XGBoost model consisting of 6 influential features and 94 noise features.

Feature	ERFC
x_6	0.48
x_5	0.060
x_3	0.026
x_1	0.022
x_4	0.0036
x_2	0.0030
x_{12}	0.0028
x_{30}	0.0022
x_{40}	0.0019

feature 12, while using the test data correctly indicates that feature 12 has a weak or no influence. We also see from the other histograms that using the training data underestimates the uncertainty in the sub-SAGE estimate.

By using the test data for computation of the sub-SAGE estimates, the estimated 95% percentile intervals of the sub-SAGE values for each feature are $6:(39.45,\ 44.15),\ 1:(-0.038,\ 0.14),\ 2:(-0.043,\ 0.040)$ and $12:(-0.030,\ 0.0050)$. These ranges allow us to conclude that feature 6, correctly, is highly influential, while feature 12 is highly unlikely to have any influence. The added benefit of the estimated confidence intervals is to prevent us from concluding that features 1 and 2 are influential but rather concluding that feature 1 is highly likely to be influential, as its average is above zero.

To correct for a potential bias in the plug-in estimator of the sub-SAGE as well as potential changes in the standard deviation of the estimator at different levels, the bias-corrected and accelerated bootstrap confidence interval may be applied. This results in the following intervals $6:(39.45,\ 44.13),\ 1:(-0.034,\ 0.14),\ 2:(-0.047,\ 0.037)$ and $12:(-0.031,\ 0.0040)$, with only negligible changes from the percentile confidence intervals. The sub-SAGE underestimation of the influence of both features 1 and 2, but particularly feature 2, can be explained by looking at fig. 3. As the data generating process is known, we can compare the true SHAP

value at each point with the corresponding SHAP value from the fitted model. It shows that the influence of feature 6 is quite accurately modelled, while the effect of feature 1 and particularly feature 2 is highly underestimated when $x_1 = 1$ and $x_2 = 2$. As features 1 and 2 interact, the SHAP value of feature 1 depends on the value of feature 2. It also becomes clear that feature 12, according to the model, has a negative trend in the SHAP value, but the true SHAP value is equal to zero (no importance), regardless of the value of feature 12.

6. Application on genetic data using the UK Biobank resource

To demonstrate the ability of sub-SAGE on observed data, we consider a realistic high-dimensional machine learning problem that often occurs when using genetic data, namely the influence of specific features on a given trait.

We use both genetic and non-genetic data from UK Biobank, a large prospective cohort study in the United Kingdom that began in 2006 consisting of about 500'000 participants (Sudlow et al., 2015; Bycroft et al., 2018), and attempt to infer the influence of specific features with respect to obesity (BMI \geq 30), by training an XGBoost model and computing sub-SAGE values.

We treat this as a classification problem between the categories obese and non-obese (see Johnsen et al., 2021, for details). Of particular interest is whether any genetic markers are important. The most used method in this setting is a so-called genome-wide association study (GWAS), where each genetic variant is tested individually in a general linear (mixed-effects) regression model (Visscher et al., 2017; Zhou et al., 2018). A corresponding p-value less than 5×10^{-8} is often considered statistically significant, a tiny significance level due to the multiple comparison problem (Goeman and Solari, 2014). When the same association is replicated in an independent data set, the association is considered to be robust.

We study the XGBoost model constructed in Johnsen et al. (2021) based on 3000 features both genetic (single nucleotide polymorphism (SNP)) and non-genetic, for 64'000 unrelated White-British participants from UK Biobank. The genetic data consists of so-called minor allele counts or genotype values from SNPs (see e.g. Visscher et al., 2017) filtered to ensure independence without significant loss of information (Johnsen et al., 2021). Non-genetic features included are sex, age, physical activity frequency, intake of saturated fate, sleep duration, stress and alcohol consumption (see Johnsen et al., 2021, for definitions). The model is trained with hyperparameters: learning rate $\eta = 0.05$, $colsample = subsample = colsample_by_tree = 0.8$, $max_depth = 2$, $\lambda = 1$, $\gamma = 1$, $early_stopping_rounds = 20$, and binary cross-entropy loss. The trained model included only 532 features

Table 2: The resulting ranking based on the expected relative feature contribution (ERFC) after having trained an XGBoost model consisting of 3000 features and 64'000 individuals from UK Biobank.

Feature	ERFC
Alcohol intake frequency	0.088
Genetic sex	0.086
Physical activity frequency	0.073
Intake of saturated fat	0.044
Sleep duration	0.036
Stress	0.034
Age at recruitment	0.033
rs17817449	0.017
rs489693	0.012
rs1488830	0.011
rs13393304	0.010
rs10913469	0.01
rs2820312	0.0086

among the 3000 input features spread along a total of 607 trees. The features with the largest ERFC-scores, based on the training data, and therefore considered the most promising features, are given in table 2.

While the non-genetic features are unsurprisingly considered the most important, the most important SNP according to the model is rs17817449, a SNP connected to the FTO gene at chromosome 16, previously associated (statistically significant) with obesity in a large number of studies including different independent data sets (Locke et al., 2015). The SNP rs13393304 at chromosome 2 has previously been associated with obesity using UK Biobank data Karlsson et al. (2019). The SNP rs2820312 has not previously been associated with obesity, but with hypertension closely connected to obesity based on UK Biobank data, closely connected to obesity (Gagliano Taliun et al., 2020). The SNPs mentioned above are explored further by computing sub-SAGE estimates including paired bootstrap-derived percentile intervals by using 20'000 (unrelated White-British) participants from UK

Biobank not used while training the model. We also compute sub-SAGE for the randomly selected SNP rs7318381, which has never been associated with obesity, and with a small ERFCs in the XGBoost model (0.0016). The result is given in fig. 4.

The sub-SAGE values do indicate that both rs17817449 and rs13393304 are highly likely to be associated with obesity. The 95% percentile interval of the sub-SAGE value for rs17817449 is (0.0006, 0.0016), and (0.00014, 0.00073) for rs13393304. The SNPs rs2820312 and rs7318381 are less likely to be associated with obesity, and if they are true associations, the uncertainties in the estimates indicate that the effects are microscopic. The 95% percentile intervals for rs2820312 is $(-7.08 \cdot 10^{-5}, 2.95 \cdot 10^{-4})$, and $(-1.13 \cdot 10^{-5}, 6.32 \cdot 10^{-5})$ for rs7318381.

When dealing with relatively large data sizes such as for the genetic example above, the bias-corrected and accelerated bootstrap interval can become infeasible due to the estimation of the acceleration parameter. However, as the acceleration parameter is proportional to the skewness of the bootstrap distribution, and if the bootstrap distribution indeed has a small skewness, as is the case here, it is often sufficient to set the acceleration parameter equal to zero. This gives no change in the percentile intervals of rs17817449 and rs13393304, but the bias-corrected 95% bootstrap intervals of rs2820312 and rs7318381 become $(-6.10 \cdot 10^{-5}, 0.00030)$ and $(-1.18 \cdot 10^{-5}, 6.19 \cdot 10^{-5})$ respectively. These are negligible changes, indicating that the plug-in estimates are low-biased.

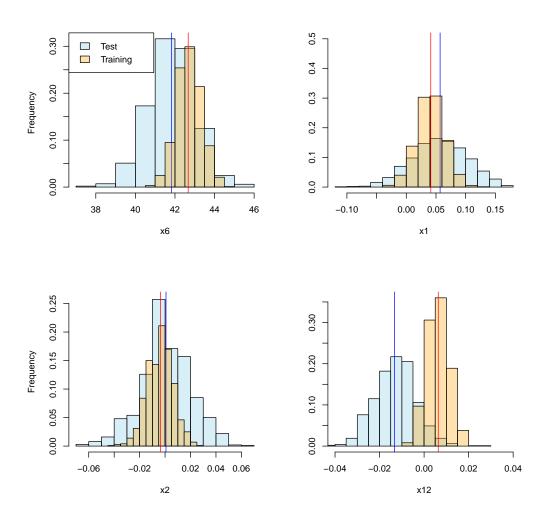


Figure 2: The estimate of the sub-SAGE and corresponding distribution from the bootstrap samples for features x_6 , x_2 , x_1 and x_{12} when using data used during training (orange), and independent test data (blue).

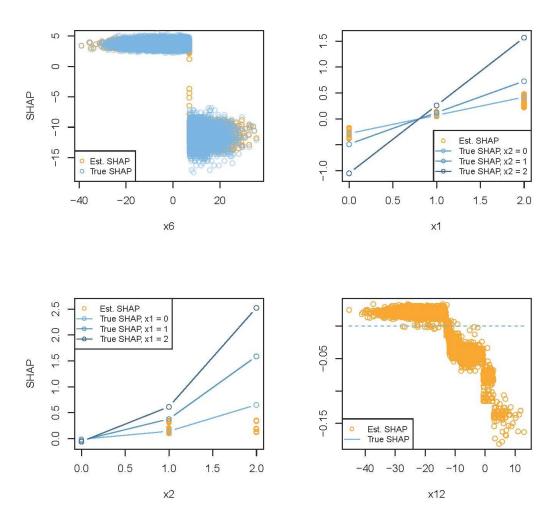


Figure 3: Comparison of true SHAP value for each data point with the estimated SHAP value from the fitted model. The deviations explain the reasons behind under- and over-estimation of feature importance.

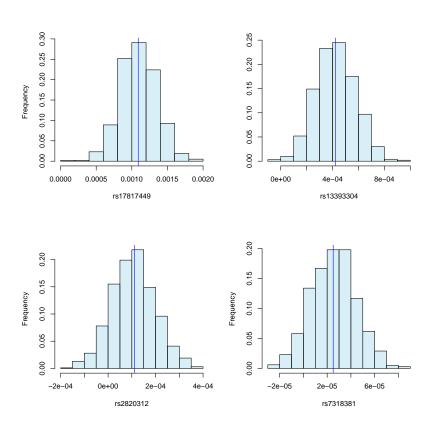


Figure 4: The estimates and corresponding uncertainties in the sub-SAGE values for the four SNPs agree with previous studies (GWAS) regarding SNP-association with obesity.

7. Discussion and conclusion

We present a Shapley value based framework for inferring the importance of individual features, including uncertainty in the estimator. We demonstrate how to infer feature influence for a tree ensemble model with high-dimensional data using sub-SAGE and paired bootstrapping. As an example, we use XGBoost, a gradient tree-boosting model, applied to both a known data generating process, as well as realistic high-dimensional data.

It is important to notice that the percentile intervals, constructed to evaluate the uncertainty in the sub-SAGE estimate, themselves include uncertainty. The uncertainty of the percentile intervals depends on the number of bootstraps, B, as well as the size n of data. However, in addition, the uncertainty also depends on the ratio p/n, where p is the total number of features used in the model (not necessarily the number of input-features for constructing the model). This fact is particularly important in high-dimensional problems, and it has been discussed for instance in Karoui and Purdom (2018). When applied to linear models, one observation from a simulation is for instance that the paired bootstrap becomes more conservative (loss of power) the larger the ratio p/n is. Observe that for the simulation example above, p/n = 62/3200 = 0.019, while for the genetic data, the ratio is p/n = 533/20000 = 0.027, deliberately chosen to be small in order to account for the problems arising when p/n becomes too large. For the genetic data, a filtering process is first needed as the data from UK Biobank originally includes around 530'000 SNPs and 207'000 individuals (p/n = 2.56). The applied filtering method and potential pitfalls are described in Johnsen et al. (2021).

In this work we have assumed all features to be mutually statistically independent, an unrealistic scenario in most cases, except for situations such as with genetic data where one can make sure that the genetic distance between the SNPs is sufficiently large to minimize the correlation. If many features are statistically dependent, one is required to estimate conditional expected values (see e.g. Aas et al., 2020). In a high-dimensional setting, this often becomes very tedious and even infeasible in most cases. An important line of future research to allow for easy evaluation of feature influence in a high-dimensional setting, is dimensionality reduction of the features with reduced loss of interpretation of the cluster variables created.

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Appendix A. The weights in sub-SAGE

The sub-SAGE, ψ_k , is defined as eq. (10) and repeated here for convenience,

$$\psi_k(\mathbf{X}, Y, \hat{y}) = \sum_{S \in \mathcal{O}} \frac{|\mathcal{S}|! (M - |\mathcal{S}| - 1)!}{3(M - 1)!} \left[w_{\mathbf{X}, Y, \hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X}, Y, \hat{y}}(\mathcal{S}) \right], \quad (A.1)$$

with \mathcal{Q} consisting of the subsets $\{\emptyset\}$, $\{m\}$ for $m=1,\ldots,k-1,k+1,\ldots,M$ and $\{1,2,\ldots,k-1,k+1,\ldots,M\}$. In other words, there are three different achievable subset sizes, namely of size zero, one and M-1. As we want the sum of all weights to be equal to one, and that the sum of the weights of equal subset size is the same for all subset sizes, we need the corresponding weight for $\mathcal{S}=\{\phi\}$ and $\mathcal{S}=\{1,2,\ldots,k-1,k+1,\ldots,M\}$ to be 1/3, while the sum of the weights for $\mathcal{S}=\{m\}$ for $m=1,\ldots,k-1,k+1,\ldots,M$ needs to be 1/3. For $\mathcal{S}=\{\phi\}$, we see that the weight is 0!(M-1)!/3(M-1)!=1/3 and for $\mathcal{S}=\{1,2,\ldots,k-1,k+1,\ldots,M\}$ the weight is (M-1)!0!/3(M-1)!=1/3, just as we wanted. For the subsets of size one, the weight is 1!(M-2)!/3(M-1)!=1/3(M-1). There are M-1 subsets of size one in total, and so the sum of the weights are also 1/3. In other words, the definition of the weights in sub-SAGE makes sure that the sum of all weights is equal to one, and that the sum of the weights of equal subset size is the same for all subset sizes.

Appendix B. Derivation of Sub-SAGE for squared error and binary cross-entropy

Using as loss function the squared error loss, the loss per sample is $\ell = (y - \hat{y})^2$. Considering a feature k for which to compute the sub-SAGE value, we separate the trees in our ensemble model into two groups: τ_k , being the set of trees including

feature k as a splitting point, and its complement group $(\bar{\tau}_k)$. Then, for any $S \in \mathcal{Q}$,

$$w_{\mathbf{X},Y,\hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X},Y,\hat{y}}(\mathcal{S})$$

$$= E_{\mathbf{X},Y} \left[\left(Y(\mathbf{X}) - V_{\mathbf{X},\hat{y}}(\mathcal{S}) \right)^{2} \right] - E_{\mathbf{X},Y} \left[\left(Y(\mathbf{X}) - V_{\mathbf{X},\hat{y}}(\mathcal{S} \cup \{k\}) \right)^{2} \right]$$

$$= E_{\mathbf{X},Y} \left[\left(Y - \sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) - \sum_{j \notin \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) \right)^{2} - \left(Y - \sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) - \sum_{j \notin \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) \right)^{2} \right]$$

$$= E_{\mathbf{X},Y} \left[\left(Y - \sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) - \sum_{j \notin \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) \right)^{2} - \left(Y - \sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) - \sum_{j \notin \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) \right)^{2} \right]$$

$$= E_{\mathbf{X},Y} \left[2Y \left(\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) - V_{\mathbf{X},f_{j}}(\mathcal{S}) \right) + \left(\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) \right)^{2} - \left(\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) \right)^{2} \right]$$

$$+ 2 \left(\sum_{j \notin \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S}) \right) \left(\sum_{j \in \tau_{k}} V_{\mathbf{X},f_{j}}(\mathcal{S} \cup \{k\}) - V_{\mathbf{X},f_{j}}(\mathcal{S}) \right) \right],$$
(B.1)

having used that the two random variables $V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\})$ and $V_{\mathbf{X},f_j}(\mathcal{S})$ are equivalent, or equal in distribution, for $j \notin \tau_k$. Note that the corresponding observed value $v_{\mathbf{x},f_j}(\mathcal{S} \cup \{k\}) = E_{\mathbf{X}_{\overline{\mathcal{S}}}}[f_j(\mathbf{X}|\mathbf{X}_{\mathcal{S}} = \mathbf{x}_{\mathcal{S} \cup \{k\}})] = E_{\mathbf{X}_{\overline{\mathcal{S}}}}[f_j(\mathbf{X}|\mathbf{X}_{\mathcal{S}} = \mathbf{x}_{\mathcal{S}})] = v_{\mathbf{x},f_j}(\mathcal{S})$ for all $\mathcal{S} \in \mathcal{Q}$ since the regression tree f_j does not include feature k, and the features are assumed mutually independent.

Using as loss function the binary cross-entropy, the loss function per sample is $\ell = -y \log \hat{y} - (1-y) \log (1-\hat{y}) = (1-y) \sum_{\tau=1}^{T} f_{\tau} + \log \left(1 + e^{-\sum_{\tau=1}^{T} f_{\tau}}\right)$. Then,

we have

$$\begin{split} &w_{\mathbf{X},Y,\hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X},Y,\hat{y}}(\mathcal{S}) \\ &= E_{\mathbf{X},Y} \left[(1 - Y(\mathbf{X})) \sum_{\tau=1}^{T} V_{\mathbf{X},f_{\tau}}(\mathcal{S}) + \log \left(1 + \exp \left(- \sum_{\tau=1}^{T} V_{\mathbf{X},f_{\tau}}(\mathcal{S}) \right) \right) \right] \\ &- E_{\mathbf{X},Y} \left[(1 - Y(\mathbf{X})) \sum_{\tau=1}^{T} V_{\mathbf{X},f_{\tau}}(\mathcal{S} \cup \{k\}) + \log \left(1 + \exp \left(- \sum_{\tau=1}^{T} V_{\mathbf{X},f_{\tau}}(\mathcal{S} \cup \{k\}) \right) \right) \right] \\ &= E_{\mathbf{X},Y} \left[(1 - Y(\mathbf{X})) \left(\sum_{j \in \tau_k} V_{\mathbf{X},f_j}(\mathcal{S}) + \sum_{j \notin \tau_k} V_{\mathbf{X},f_j}(\mathcal{S}) \right) \right] \\ &+ E_{\mathbf{X},Y} \left[\log \left(1 + \exp \left(- \sum_{j \in \tau_k} V_{\mathbf{X},f_j}(\mathcal{S}) - \sum_{j \notin \tau_k} V_{\mathbf{X},f_j}(\mathcal{S}) \right) \right) \right] \\ &- E_{\mathbf{X},Y} \left[(1 - Y(\mathbf{X})) \left(\sum_{j \in \tau_k} V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\}) + \sum_{j \notin \tau_k} V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\}) \right) \right] \\ &- E_{\mathbf{X},Y} \left[\log \left(1 + \exp \left(- \sum_{j \in \tau_k} V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\}) - \sum_{j \notin \tau_k} V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\}) \right) \right) \right] \\ &= E_{\mathbf{X},Y} \left[(1 - Y(\mathbf{X})) \left(\sum_{j \in \tau_k} V_{\mathbf{X},f_j}(\mathcal{S}) - V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\}) \right) \right] \\ &+ \log \left(\frac{1 + \exp \left(- \sum_{j \in \tau_k} V_{\mathbf{X},f_j}(\mathcal{S}) - \sum_{j \notin \tau_k} V_{\mathbf{X},f_j}(\mathcal{S}) \right)}{1 + \exp \left(- \sum_{j \in \tau_k} V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\}) - \sum_{j \notin \tau} V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\}) \right)} \right]. \end{split}$$

Appendix C. Sub-SAGE estimate for tree ensemble models with tree stumps

Consider a tree ensemble model with regression trees of depth one, so-called tree stumps. Each tree stump includes exactly one feature from the set \mathcal{M} of all M features. In accordance with earlier notation, let τ_k denote the set of tree stumps that include feature k. Then, eq. (B.1) reduces to

$$\begin{split} w_{\mathbf{X},Y,\hat{y}}(\mathcal{S} \cup \{k\}) &- w_{\mathbf{X},Y,\hat{y}}(\mathcal{S}) \\ &= E_{\mathbf{X},Y} \left[2Y \left(\sum_{j \in \tau_k} V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\}) - V_{\mathbf{X},f_j}(\mathcal{S}) \right) + \left(\sum_{j \in \tau_k} V_{\mathbf{X},f_j}(\mathcal{S}) \right)^2 - \left(\sum_{j \in \tau_k} V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\}) \right)^2 \right] \\ &= 2Cov \left(Y_i^0, \sum_{j \in \tau_k} f_j(X_{i,k}^0) \right) - Var \left(\sum_{j \in \tau_k} f_j(X_{i,k}^0) \right) + 2Cov \left(\sum_{j \in \tau_k} f_j(X_{i,k}^0), \sum_{j \notin \tau_k} f_{j,S}(\mathbf{X}_{i,S}^0) \right) \\ &= 2Cov \left(Y_i^0, \sum_{j \in \tau_k} f_j(X_{i,k}^0) \right) - Var \left(\sum_{j \in \tau_k} f_j(X_{i,k}^0) \right) , \end{split}$$

$$(C.1)$$

because all random variables $V_{\mathbf{X},f_j}(\mathcal{S})$ for $j \notin \tau_k$, and every \mathcal{S} are now independent of all $V_{\mathbf{X},f_j}(\mathcal{S})$ and $V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\})$ for $j \in \tau_k$. Further, for every $j \in \tau_k$, $V_{\mathbf{X},f_j}(\mathcal{S}) = E_{\mathbf{X}}[f_j(\mathbf{X})]$, a constant equal to the expected value of the regression tree f_j , and $E_{\mathbf{X}}[V_{\mathbf{X},f_j}(\mathcal{S} \cup \{k\})] = E_{\mathbf{X}}[f_j(\mathbf{X})]$, since the regression tree f_j only includes feature k. Therefore, the last term in eq. (B.1) vanishes. Observe that, in the case of regression trees,

$$E_{\mathbf{X},Y} \left[Y \left(\sum_{j \in \tau_k} V_{\mathbf{X},f_j} (\mathcal{S} \cup \{k\}) - V_{\mathbf{X},f_j} (\mathcal{S}) \right) \right]$$

$$= E_{\mathbf{X},Y} \left[Y \left(\sum_{j \in \tau_k} f_j(X_k) \right) \right] - E_Y[Y] E_{\mathbf{X}} \left[\sum_{j \in \tau_k} f_j(X_k) \right] = \operatorname{Cov} \left(Y, \sum_{j \in \tau_k} f_j(X_k) \right).$$

Likewise.

$$\left(\sum_{j\in\tau_k} V_{\mathbf{X},f_j}\left(\mathcal{S}\right)\right)^2 - \left(\sum_{j\in\tau_k} V_{\mathbf{X},f_j}\left(\mathcal{S}\cup\left\{k\right\}\right)\right)^2 = -\operatorname{Var}\left(\sum_{j\in\tau_k} f_j(X_k)\right).$$

Therefore, eq. (C.1) can be expressed as

$$w_{\mathbf{X},Y,\hat{y}}(\mathcal{S} \cup \{k\}) - w_{\mathbf{X},Y,\hat{y}}(\mathcal{S}) = 2\operatorname{Cov}\left(Y, \sum_{j \in \tau_k} f_j(X_k)\right) - \operatorname{Var}\left(\sum_{j \in \tau_k} f_j(X_k)\right),$$
(C.2)

independent of the subset \mathcal{S} . The expression in eq. (C.2) is therefore also equal to the sub-SAGE value, $\hat{\psi}_k$, as well (or SAGE value). Both the covariance and the variance needs to be must be estimated. Given independent test data $(\mathbf{x}_1^0, y_1^0), \ldots, (\mathbf{x}_{N_I}^0, y_{N_I}^0)$, an unbiased estimate is given by

$$\hat{\psi}_{k} = \frac{1}{N_{I}^{0} - 1} \sum_{i=1}^{N_{I}^{0}} \left(y_{i}^{0} - \sum_{i=1}^{N_{I}} y_{i}^{0} \right) \left(\sum_{j \in \tau_{k}} f_{j}(x_{i,k}^{0}) - \sum_{j \in \tau_{k}} v_{x_{i,k}^{0}, f_{j}}(\emptyset) \right) - \frac{1}{N_{I}^{0} - 1} \sum_{i=1}^{N_{I}^{0}} \left(\sum_{j \in \tau_{k}} f_{j}(x_{i,k}^{0}) - \sum_{j \in \tau_{k}} v_{x_{i,k}^{0}, f_{j}}(\emptyset) \right)^{2}.$$
(C.3)

Appendix D. Sub-SAGE properties related to Shapley values

Appendix D.1. Symmetry

Given two features j and k such that $v(S \cup \{j\}) = v(S \cup \{k\})$ for all $S \in \mathcal{Q}$ such that $\{j,k\} \notin S$, where \mathcal{Q} is the set of all subsets S included in the definition of

the sub-SAGE value given in Equation (9) in the main article. Then their sub-SAGE values are identical, $\psi_j = \psi_k$ by definition. This means in practice that two perfectly correlated features have equal sub-SAGE values.

Appendix D.2. Dummy property (null player)

Given a feature j where $v(S \cup \{j\}) = v(S)$ for all $S \in Q$. Then by definition $\psi_j = 0$, meaning that any feature j that is not included in the model used for computing the sub-SAGE value has $\psi_j = 0$.

Appendix D.3. Linearity

Given two value functions v(S) and w(S), the sub-SAGE value of the sum of the value functions v(S) + w(S) is equal to the sum of the sub-SAGE for each value function,

$$\psi_k(v+w) = \psi_k(v) + \psi_k(w). \tag{D.1}$$

Appendix D.4. Monotonicity property

Consider two models \hat{f}_1 and \hat{f}_2 used to predict the same relationship $y = f(\mathbf{x})$, for the same features \mathbf{x} . If for any feature j we have $v_{\hat{f}_1}(\mathcal{S} \cup \{j\}) - v_{\hat{f}_1}(\mathcal{S}) \geq v_{\hat{f}_2}(\mathcal{S} \cup \{j\}) - v_{\hat{f}_2}(\mathcal{S})$ for all $\mathcal{S} \in \mathcal{Q}$, then by definition, $\psi_j^{\hat{f}_1} \geq \psi_j^{\hat{f}_2}$, with $\psi_j^{\hat{f}_1}$ the sub-SAGE value of feature j when applying model \hat{f}_1 and $\psi_j^{\hat{f}_2}$ the corresponding sub-SAGE value when applying model \hat{f}_2 . This means that an adjustment of model \hat{f}_2 to \hat{f}_1 such that feature j's importance increases also increases its sub-SAGE value.

Appendix D.5. sub-SAGE does not share the efficiency property

Consider the definition of the Shapley value, ϕ_k , in this setting applied to a model $\hat{y}(\mathbf{x})$

$$\phi_k(\mathbf{x}, \hat{y}) = \sum_{\mathcal{S} \subset \mathcal{M} \setminus \{k\}} \frac{|\mathcal{S}|!(M - |\mathcal{S}| - 1)!}{M!} \left[v(\mathcal{S} \cup \{k\}) - v(\mathcal{S}) \right]. \tag{D.2}$$

The efficiency property for the Shapley value reads

$$\sum_{j=1}^{M} \phi_k = v(\mathcal{M}) - v(\emptyset), \qquad (D.3)$$

for M features. This can be observed more easily by using instead the following formulation of the Shapley value

$$\phi_k(\mathbf{x}, \hat{y}) = \frac{1}{M!} \sum_{R} \left[v(s_k(R) \cup \{k\}) - v(s_k(R)) \right],$$
 (D.4)

where the sum is over all orderings R of the M features, with a total of M! orders. The function $s_k(R)$ maps a given ordering R and a particular feature k to the corresponding subset of features preceding feature k in the specific ordering. For instance, for $\mathcal{M} = \{1, 2, 3\}$, one possible ordering is R = (2, 3, 1) with $s_1(R) = (2, 3)$. We then have

$$\sum_{k=1}^{M} \phi_k(\mathbf{x}, \hat{y}) = \sum_{k=1}^{M} \frac{1}{M!} \sum_{R} \left[v(s_k(R) \cup \{k\}) - v(s_k(R)) \right]$$

$$= \frac{1}{M!} \sum_{R} \sum_{k=1}^{M} \left[v(s_k(R) \cup \{k\}) - v(s_k(R)) \right]$$

$$= \frac{1}{M!} \sum_{R} \left(v(\mathcal{M}) - v(\emptyset) \right)$$

$$= \frac{1}{M!} M! \left(v(\mathcal{M}) - v(\emptyset) \right) = v(\mathcal{M}) - v(\emptyset),$$
(D.5)

since for a specific ordering R and feature k, in the sum $\sum_{k=1}^{M} [v(s_k(R) \cup \{k\}) - v(s_k(R))]$ all terms cancel each other, except $v(\mathcal{M})$ and $v(\emptyset)$.

The sub-SAGE value, ψ_k , for a feature k is not a sum over all subsets $S \subseteq \mathcal{M} \setminus \{k\}$, but limited to the sets in \mathcal{Q} ,

$$\psi_k(\mathbf{y}, \hat{\mathbf{y}}) = \sum_{\mathcal{S} \in \mathcal{Q}} \frac{|\mathcal{S}|!(M - |\mathcal{S}| - 1)!}{3(M - 1)!} \left[v\left(\mathcal{S} \cup \{k\}\right) - v\left(\mathcal{S}\right) \right], \tag{D.6}$$

and therefore, from the definition in eq. (D.4), is *not* the sum over all orderings R. The sub-SAGE value therefore does not share the efficiency property of the Shapley value.

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