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. Åas et al. (2021); 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 E.

Consider a supervised learning task characterised by a set of $M$ features $x_i$ and corresponding univariate responses $y_i$, for $i = 1, \ldots, N$, and a fitted model that is a mapping from feature values to response values, i.e. $x_i \rightarrow \hat{y}(x_i)$. 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 $\mathcal{M} = \{1, \ldots, M\}$, 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, $\phi_{\text{SHAP}}(x, \hat{y})$, introduced by Lundberg and Lee (2017), for a feature with index $k$ with respect to feature values $x$ and a corresponding fitted model $\hat{y}$, is defined as

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

1The procedures described in this paper can be generalised to multivariate responses, but this renders the derivations more convoluted.
Here, the value function \( v_{x, \hat{y}}(S) \) is defined as the expected output of a prediction model conditioned that only a subset \( S \) of all features are included in the model,

\[
v_{x, \hat{y}}(S) = E_{X_S}[\hat{y}(X|X_S = x_S)]. \tag{2}
\]

For instance, if \( x_S \) is continuous and we assume all features to be mutually independent, we have

\[
E_{X_S}[\hat{y}(X|X_S = x_S)] = \int_{x_S} \hat{y}(X_S = x_S, X_S = x_S) p(X_S = x_S|X_S = x_S) dx_S
\]

\[
= \int_{x_S} \hat{y}(X_S = x_S, X_S = x_S) p(X_S = x_S) dx_S. \tag{3}
\]

The stochastic behaviour in \( \hat{y}(X|X_S = x_S) \) is due to the random vector \( X_S \) of unknown feature values. We can think of the difference \( v_{x, \hat{y}}(S \cup \{k\}) - v_{x, \hat{y}}(S) \) 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 \( \ell(y_i, \hat{y}(x_i)) \) as a measure of how well the fitted model \( \hat{y}(x_i) \) maps the features to a response, compared to the true response value \( y_i \). As defined in [Covert et al. (2020b)](covert2020interpreting), we take the SAGE value function \( w(S) \) as the expected difference in the observed value of the loss function when the features in \( S \) are included in the model compared to excluding all features,

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

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

\[
E_{X,Y}[\ell(Y, V_{X,\hat{y}}(S))] = \int_y \int_{X_S} \ell(y(x), E_{X_S}[\hat{y}(X|X_S = x_S)]) p(y|x_S)p(x_S)dx_Sdy. \tag{5}
\]
Notice that the computation of $v_{x,\hat{y}}(S) = E_{X_S}[\hat{y}(X|X_S = x_S)]$ happens inside the loss function, which is usually non-linear. Also notice that in eq. (5), we integrate over all possible values of $X_S$.

The SAGE value for a feature $k$ is defined as

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

(6)

We can think of the difference $w_{X, Y, \hat{y}}(S \cup \{k\}) - w_{X, Y, \hat{y}}(S)$ as the expected difference in the loss function when including feature $k$ in the model compared to excluding feature $k$ with respect to the subset $S$ of known feature values. 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 be 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 feature 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 $f_\tau(x_i)$ with predicted response $\hat{y}(x_i)$, such that $\hat{y}(x_i) = \sum_{\tau=1}^T f_\tau(x_i)$ for $T$ trees. By the linearity property of the expected value, we have

$$v_{x,\hat{y}}(S) = E_{X_S} \left[ \sum_{\tau=1}^T f_\tau(X|X_S = x_S) \right] = \sum_{\tau=1}^T E_{X_S}[f_\tau(X|X_S = x_S)].$$

(7)

The computation of $E_{X_S}[f_\tau(X|X_S = x_S)]$ 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
mutually independent. The regression tree has parameters such as splitting points, $t_j$, for branch nodes, and leaf values $v_j$, for leaf nodes. Assume that $x_2 = 3$ is observed. We then have

$$E_{X_S}[f_\tau(X|X_S = x_S)] = E_{X_1}[f_\tau(X_1|X_2 = 3)] = P(X_1 \geq 20)v_3 + P(X_1 < 20)v_2. \tag{8}$$

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

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

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 $E_{X_S}[f_\tau(X|X_S = x_S)]$ for any regression tree can be achieved by a recursive algorithm (Lundberg et al., 2020) with running time $O(L^2 M)$, where $L$ is the number of leaves, see algorithm 1.

2.4. SAGE in practice

In practice, as the expressions in eq. (2) and eq. (4) 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 $S \subseteq M \setminus \{k\}$, for each
Algorithm 1 Recursive algorithm for computation of $E_{X_S}[f_\tau(X|X_S = x_S)]$.

1: Input: Tree $f_\tau$ with depth $d$, leaf values $v = (v_1, \ldots, v_{2^d})$, feature used for splitting $f = (f_1, \ldots, f_{2^d-1})$ and corresponding splitting points $t = (t_1, \ldots, t_{2^d-1})$. Estimated probabilities of ending at a node $j$ given previous information, for all nodes in the tree, $p = (p_1, \ldots, p_{2^d-1})$, by using some data $(x_1, y_1), \ldots, (x_N, y_N)$ of size $N$. The subset of features $S$ with corresponding known values $x_S$. The left and right descendant node for each internal node $l = (l_1, \ldots, l_{2^d-1})$ and $r = (r_1, \ldots, r_{2^d-1})$. The index of a node $j$ in the tree $f_\tau$.

2: Function CondExpTree($j, f_\tau, v, t, f, l, r, p$)
3:  if IsLeaf($j$) then
4:      return $v_j$
5:  else
6:    if $f_j \in S$ then
7:      if $x_j \leq t_j$ then
8:        return CondExpTree($l_j, f_\tau, v, t, f, l, r, p$)
9:      else
10:     return CondExpTree($r_j, f_\tau, v, t, f, l, r, p$)
11:     end if
12:  else
13:    return CondExpTree($l_j, f_\tau, v, t, f, l, r, p$) $p_{l_j} +$
14:    CondExpTree($r_j, f_\tau, v, t, f, l, r, p$) $p_{r_j}$
15:  end if
16: end if
17: End Function
18: CondExpTree($1, f_\tau, v, t, f, l, r, p$) \Comment{Start at root node.}
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 $S$ is randomly sampled with replacement in each iteration out of $I$ iterations in total. The differences $w_{X,Y,\hat{g}}(S \cup \{k\}) - w_{X,Y,\hat{g}}(S)$ for each $S$ 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. 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 for all features in the model and selecting the most interesting looking ones. The reduced subset of promising features can 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 $S = \{0\}$ and $S = \{m\}$ for $m = 1, \ldots, k-1, k+1, \ldots, M$ is sufficient. In addition, by including $S = \{1, \ldots, k-1, k+1, \ldots, M\}$, 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 $Q_k$ denote the set of subsets $S$ chosen above. We define the sub-SAGE value, $\psi_k$, for feature $k$ as

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

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 E). 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 $w_{X,Y,\hat{y}}(S \cup \{k\}) - w_{X,Y,\hat{y}}(S)$. 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 $S$, 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 test data, \((X^0_1, Y^0_1), \ldots, (X^0_{N_I}, Y^0_{N_I})\), with \(N_I\) samples in total.

Consider a fitted linear regression model \(\hat{y}_i = \hat{\beta}^T x_i\). By using test data independent of the data used for constructing the linear regression model, and using the squared error loss, one can show that for a feature \(k\), and any \(S \in Q_k\) (see Appendix C):

\[
w_{X,Y,\hat{y}}(S \cup \{k\}) - w_{X,Y,\hat{y}}(S) = 2\hat{\beta}_k \text{Cov}(Y, X_k) - \hat{\beta}_k^2 \text{Var}(X_k).
\] (11)

As the expression is independent of the subset \(S\), this is also equal to the sub-SAGE value of feature \(k\).

The first term in eq. (11) can be interpreted as the extent to which the influence of feature \(k\) based on the model, constructed using training data, is reflected in the independent test data. If the signs of \(\hat{\beta}_k\) and \(\text{Cov}(Y, X_k)\) are identical, the first term is positive. If they differ, the sub-SAGE value will always be negative since the second term in eq. (11) is always negative.

The second term \(\hat{\beta}_k^2 \text{Var}(X_k)\) is equal to the increased variance in the model by including feature \(k\). So, if the model regards the feature as important (resulting in non-zero \(\hat{\beta}_k\)), while the covariance between \(X_k\) and \(Y\) from the independent test data goes in the same direction (same sign as \(\hat{\beta}_k\)), however small, then the benefit of including feature \(k\) in the model is smaller, the larger the variance of the feature, and at some point disadvantageous for sufficiently large variance.

### 3.2. sub-SAGE applied on tree ensemble models

SHAP values can be shown to be estimated efficiently for tree ensemble models, even with hundreds of thousands of features (e.g. Johnsen et al., 2021), by improving algorithm \[\pi\] to get a significantly reduced running time of \(O(TLD^2)\), for \(T\) trees each of tree depth \(D\) (see Lundberg et al., 2020 for details). Unfortunately, there is no similar way to reduce the running time for estimation of SAGE values, as well as sub-SAGE values, for tree ensemble models with non-linear choices of loss functions (Lundberg et al., 2020).

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 \(S \in Q_k\). We separate the trees in the model into two groups \(\tau_k\) and the complement
group \((\mathcal{T}_k)\) where \(\tau_k\) 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. \(\ell = (\hat{y}(x) - \hat{y}(x))^2\). Then one can show that (see Appendix B for the derivation),

\[
\begin{align*}
\hat{w}_{X,Y,\hat{g}}(S \cup \{k\}) - \hat{w}_{X,Y,\hat{g}}(S) \\
= E_{X,Y} \left[ (Y(X) - V_{X,\hat{g}}(S))^2 \right] - E_{X,Y}[(Y(X) - V_{X,\hat{g}}(S \cup \{k\}))^2] \\
= E_{X,Y} \left[ 2Y(X) \left( \sum_{j \in \tau_k} V_{X,f,j}(S \cup \{k\}) - V_{X,f,j}(S) \right) + \left( \sum_{j \in \tau_k} V_{X,f,j}(S) \right)^2 \right] \\
- \left( \sum_{j \in \tau_k} V_{X,f,j}(S \cup \{k\}) \right)^2 + 2 \left( \sum_{j \in \tau_k} V_{X,f,j}(S) \right) \left( \sum_{j \in \tau_k} V_{X,f,j}(S \cup \{k\}) - V_{X,f,j}(S) \right). \tag{12}
\end{align*}
\]

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

\[
\begin{align*}
\hat{w}_{X,Y,\hat{g}}(S \cup \{k\}) - \hat{w}_{X,Y,\hat{g}}(S) \\
= E_{X,Y} \left[ (1 - Y(X)) \sum_{j=1}^{T} V_{X,f,j}(S) + \log \left( 1 + \exp \left( - \sum_{j=1}^{T} V_{X,f,j}(S) \right) \right) \right] \\
- E_{X,Y} \left[ (1 - Y(X)) \sum_{j=1}^{T} V_{X,f,j}(S \cup \{k\}) + \log \left( 1 + \exp \left( - \sum_{j=1}^{T} V_{X,f,j}(S \cup \{k\}) \right) \right) \right] \\
= E_{X,Y} \left[ (1 - Y(X)) \left( \sum_{j \in \tau_k} V_{X,f,j}(S) - V_{X,f,j}(S \cup \{k\}) \right) \right] \\
+ \log \left( \frac{1 + \exp \left( - \sum_{j \in \tau_k} V_{X,f,j}(S) - \sum_{j \notin \tau_k} V_{X,f,j}(S) \right) \right) \\
\right) \left( \frac{1 + \exp \left( - \sum_{j \in \tau_k} V_{X,f,j}(S \cup \{k\}) - \sum_{j \notin \tau_k} V_{X,f,j}(S \cup \{k\}) \right) \right). \tag{13}
\end{align*}
\]

3.2.1. Plug-in estimates

As discussed earlier, the expression \(w_{X,Y,\hat{g}}(S \cup \{k\}) - w_{X,Y,\hat{g}}(S)\) needs to be estimated for each \(S \in \mathcal{Q}_k\), and based on data, \((x_1^o,y_1^o), \ldots, (x_{N_f}^o,y_{N_f}^o)\), never used during training of the model. Let \(\hat{w}_{X,Y,\hat{g}}(S)\) for a particular observation \((x^o, y^o)\) and regression tree \(f_r\) denote the estimate of \(w_{X,Y,\hat{g}}(S) = \)
\[E_{X_S}[f_\tau(X^0|X^0_S = x^0_S)]\] as described in algorithm [1]. A plug-in estimate of \(\psi_k\), denoted \(\hat{\psi}_k\), for a regression problem with continuous response, for a tree ensemble model using the squared error loss is given by

\[
\hat{\psi}_k = \sum_{S \in Q} \frac{|S|!(M - |S| - 1)!}{3(M - 1)!} \left[ \frac{2}{N_f} \sum_{i=1}^{N_I} \hat{y}^0_i \left( \sum_{j \in \tau_k} \hat{v}_{x_0^i,f_j}(S \cup \{k\}) - \hat{v}_{x_0^i,f_j}(S) \right) \right. \\
+ \frac{1}{N_f} \sum_{i=1}^{N_I} \left( \sum_{j \in \tau_k} \hat{v}_{x_0^i,f_j}(S) \right)^2 - \frac{1}{N_f} \sum_{i=1}^{N_I} \left( \sum_{j \in \tau_k} \hat{v}_{x_0^i,f_j}(S \cup \{k\}) \right)^2 \\
\left. + \frac{2}{N_f} \sum_{i=1}^{N_I} \left( \sum_{j \notin \tau_k} \hat{v}_{x_0^i,f_j}(S) \right) \left( \sum_{j \in \tau_k} \hat{v}_{x_0^i,f_j}(S \cup \{k\}) - \hat{v}_{x_0^i,f_j}(S) \right) \right]. \tag{14}
\]

The corresponding plug-in estimate for the binary cross-entropy loss given in eq. [13] 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 [14] is further reduced and can be expressed as sample variance and covariance terms, see Appendix D.

### 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 \(k\) indicates that including the feature in the model is expected, based on the subsets \(S \in Q_k\), to reduce the loss function. However, the corresponding sub-SAGE plug-in estimator given the data generating process \((X^0_1,Y^0_1), \ldots, (X^0_{N_I},Y^0_{N_I})\) 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 \((x^0_1,y^0_1), \ldots, (x^0_{N_I},y^0_{N_I})\), resample the data points with replacement to get a new bootstrapped sample \((x^*_1,y^*_1), \ldots, (x^*_{N_I},y^*_{N_I})\). For each bootstrapped sample, a corresponding plug-in estimate, \(\hat{\psi}^*_k\), can be computed, and after \(B\) iterations, the sample \((\hat{\psi}^*_1, \ldots, \hat{\psi}^*_B)\) 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 100\(\alpha\) empirical percentile, meaning the \(B \cdot \alpha\)th least value in the ordered list of the samples.
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, first introduced in Efron (1987), may give even more accurate confidence intervals at the cost of considerable increase in computational efforts.

Algorithm 2 Paired bootstrap of sub-SAGE value with percentile interval
1: Given independent test data $(x_0^1, y_0^1), \ldots, (x_0^N, y_0^N)$, model $\hat{y}(x) = \sum_{\tau=1}^T f_{\tau}(x)$, feature $k$, a loss function and $\alpha$ to estimate $1 - 2\alpha$ confidence interval:
2: Preallocate vector BootVec of length $B$, the total number of bootstrap iterations.
3: for $b = 1, 2, \ldots, B$ do
4: Resample data $N_I$ times with replacement to get $(x_1^*, y_1^*), \ldots, (x_{N_I}^*, y_{N_I}^*)$
5: Update probabilities estimates in all the trees in $\hat{y}(x)$ to get $p^*$
6: BootVec$[b] = \hat{\psi}_k^*$
7: end for
8: Percentile interval given by $[ \hat{\psi}_k^{*(\alpha)}, \hat{\psi}_k^{*(1-\alpha)}]$

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

$$f(X_i) = a_0 + a_1 X_{i,1} + a_2 X_{i,2} + a_{21} X_{i,1} e^{X_{i,2}} + a_3 X_{i,3}^2 + a_4 \sin(X_{i,4})$$
$$+ a_5 \log(1 + X_{i,5}) - X_{i,5} I(X_{i,6} > 7) + \epsilon_i,$$

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

$$X_1 \sim \text{Binom}(\text{size} = 2, p = 0.4)$$
$$X_2 \sim \text{Binom}(\text{size} = 2, p = 0.04)$$
$$X_3 \sim \Gamma(\text{shape} = 10, \text{rate} = 2)$$
$$X_4 \sim \text{Unif}(0, \pi)$$
$$X_5 \sim \text{Poisson}(\lambda = 15)$$
$$X_6 \sim \text{N}(\mu = 0, \sigma = 10)$$
$$\epsilon_i \sim \text{N}(\mu = 0, \sigma = 2).$$

(16)

In addition, we generate 94 noise variables, $j = 7, \ldots, 47$ with a normal distribution $X_j \sim \text{N}(\mu_j, \sigma_j)$ and $j = 48, \ldots, 100$ with a binomial distribution $X_j \sim \text{Binom}(2, p_j)$ where $\mu_j, \sigma_j$ 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,

$$r_k = \sum_{i=1}^{N} \frac{|\phi_{i,k}^{\text{SHAP}}(x_i, \hat{y})|}{|\phi_0^{\text{SHAP}}| + \sum_{j=1}^{K} |\phi_{i,j}^{\text{SHAP}}(x_i, \hat{y})|},$$

(17)

with $\phi_0^{\text{SHAP}} = v_{x, \hat{y}}(\emptyset)$. 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
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|

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 XGBoost 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 $f(x_i)$ in eq. (15). 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 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 esti-
mated 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

![](image1.png)

![](image2.png)

![](image3.png)

![](image4.png)

Figure 2: The estimate of the sub-SAGE, and the corresponding bootstrap distribution for the synthetic data for features $x_6$, $x_2$, $x_1$ and $x_{12}$, when applying data used during training (orange), and independent test data (blue).
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 give more accurate bootstrap confidence intervals [Efron 1987]. 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.

Figure 3: Comparison of true SHAP value for each data point with the estimated SHAP value from the model fitted on the synthetic data, eq. (15). The deviations explain the reasons behind under- and overestimation of feature importance.
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. See Appendix F for derivations.

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 $5 \times 10^{-8}$ 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 $\eta = 0.05$, $colsample = subsample =$
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|

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 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 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 genome-wide association 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 based on UK Biobank data (Gagliano Taliun et al. 2020). The SNPs mentioned above are explored further by computing sub-SAGE estimates.
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.

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.

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. We emphasize the importance of using test data, independent of data used to construct the model, to compute sub-SAGE estimates.

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)].

It seems reasonable to apply the same loss function in the sub-SAGE estimate as the loss function that was used to construct the model. However, there may be situations where it is meaningful to compute the sub-SAGE values for a different
loss function than the loss function used during training in order to make more objective interpretations. This may e.g. be the case when the model is provided ‘as is’ and you do not know the training loss function, or when using adapted loss functions, e.g. weighted binary cross-entropy, but the interpretation is relevant for a standard cross-entropy.

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., 2021]). 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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9. Code availability

Source code is available at [https://github.com/palVJ/subSAGE](https://github.com/palVJ/subSAGE).

Appendix A. The weights in sub-SAGE

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

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

(A.1)

with \( Q_k \) 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 \( M \). 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 \( S = \{ \phi \} \) and \( S = \{ 1, 2, \ldots, k-1, k+1, \ldots, M \} \) to be 1/3, while the sum of the weights for \( S = \{ m \} \) for \( m = 1, \ldots, k-1, k+1, \ldots, M \) needs to be 1/3. For \( S = \{ \phi \} \), we see that the weight is \( 0!(M-1)!/3(M-1)! = 1/3 \) and for \( S = \{ 1, 2, \ldots, k-1, k+1, \ldots, M \} \) 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: \( \tau_k \), being the set of trees including feature \( k \) as a splitting point, and its complement group (\( \bar{\tau}_k \)). Then, for any \( S \in \mathcal{Q}_k \),

\[
w_{X,Y,\hat{y}}(S \cup \{k\}) - w_{X,Y,\hat{y}}(S) \\
= E_{X,Y} \left[ (Y(X) - V_{X,\hat{y}}(S))^2 \right] - E_{X,Y} \left[ (Y(X) - V_{X,\hat{y}}(S \cup \{k\}))^2 \right] \\
= E_{X,Y} \left[ \left( Y - \sum_{j \in \tau_k} V_{X,f_j}(S) - \sum_{j \notin \tau_k} V_{X,f_j}(S) \right)^2 - \left( Y - \sum_{j \in \tau_k} V_{X,f_j}(S \cup \{k\}) - \sum_{j \notin \tau_k} V_{X,f_j}(S \cup \{k\}) \right)^2 \right] \\
= E_{X,Y} \left[ \left( Y - \sum_{j \in \tau_k} V_{X,f_j}(S) - \sum_{j \notin \tau_k} V_{X,f_j}(S) \right)^2 - \left( Y - \sum_{j \in \tau_k} V_{X,f_j}(S \cup \{k\}) - \sum_{j \notin \tau_k} V_{X,f_j}(S \cup \{k\}) \right)^2 \right] \\
= E_{X,Y} \left[ 2Y \left( \sum_{j \in \tau_k} V_{X,f_j}(S \cup \{k\}) - V_{X,f_j}(S) \right) + \left( \sum_{j \in \tau_k} V_{X,f_j}(S) \right)^2 - \left( \sum_{j \in \tau_k} V_{X,f_j}(S \cup \{k\}) \right)^2 \right] \\
+ 2 \left( \sum_{j \notin \tau_k} V_{X,f_j}(S) \right) \left( \sum_{j \in \tau_k} V_{X,f_j}(S \cup \{k\}) - V_{X,f_j}(S) \right)
\]

(B.1)

having used that the two random variables \( V_{X,f_j}(S \cup \{k\}) \) and \( V_{X,f_j}(S) \) are equivalent, or equal in distribution, for \( j \notin \tau_k \). Note that the corresponding observed value \( v_{X,f_j}(S \cup \{k\}) = E_{X,S} [f_j(X|X_S = x_{S \cup \{k\}})] = E_{X,S} [f_j(X|X_S = x_S)] = \)
\(v_{x,f_j}(S)\) for all \(S \in \mathcal{Q}_k\) 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
\[
w_{X,Y,\hat{y}}(S \cup \{k\}) - w_{X,Y,\hat{y}}(S)
= E_{X,Y} \left[(1 - Y(X)) \sum_{\tau \in \tau_k} V_{X,f_j}(S) + \log \left(1 + \exp \left(- \sum_{\tau \in \tau_k} V_{X,f_j}(S)\right)\right)\right]
- E_{X,Y} \left[(1 - Y(X)) \sum_{\tau \notin \tau_h} V_{X,f_j}(S \cup \{k\}) + \log \left(1 + \exp \left(- \sum_{\tau \notin \tau_h} V_{X,f_j}(S \cup \{k\})\right)\right)\right]
= E_{X,Y} \left[(1 - Y(X)) \left(\sum_{j \in \tau_k} V_{X,f_j}(S) + \sum_{j \notin \tau_k} V_{X,f_j}(S)\right)\right]
+ E_{X,Y} \left[\log \left(1 + \exp \left(- \sum_{j \in \tau_k} V_{X,f_j}(S) - \sum_{j \notin \tau_k} V_{X,f_j}(S)\right)\right)\right]
- E_{X,Y} \left[(1 - Y(X)) \sum_{j \notin \tau_k} V_{X,f_j}(S \cup \{k\}) + \sum_{j \in \tau_h} V_{X,f_j}(S \cup \{k\})\right]
= E_{X,Y} \left[(1 - Y(X)) \left(\sum_{j \in \tau_k} V_{X,f_j}(S) - V_{X,f_j}(S \cup \{k\})\right)\right]
+ \log \left(\frac{1}{1 + \exp \left(- \sum_{j \in \tau_k} V_{X,f_j}(S) - \sum_{j \notin \tau_k} V_{X,f_j}(S)\right)}\right)\right].
\]

**Appendix C. (Sub-)SAGE with multiple linear regression**

Consider a fitted linear regression model \(\hat{y}_i = \hat{\beta}^T x_i\), with uncorrelated features. By applying the squared error loss, and by considering \(\hat{\beta}\) as a constant (by using
data not used to estimate \( \hat{\beta} \), we have for a feature \( k \), and a subset \( S \in Q_k \) that
\[
w_{X,Y,\hat{g}}(S \cup \{k\}) - w_{X,Y,\hat{g}}(S) = E_{X,Y}[(Y - V_{X,\hat{g}}(S))^2] - E_{X,Y}[(Y - V_{X,\hat{g}}(S \cup \{k\}))^2]
\]
\[= E_{X,Y}[2\hat{\beta}_k(X_k - E[X_k]) + V_{X,\hat{g}}(S)^2 - V_{X,\hat{g}}(S \cup \{k\})^2]
\]
\[= 2\hat{\beta}_k E_{X,Y}[Y(X_k - E[X_k])] + 2E_{X,Y}\left[\hat{\beta}_k(\hat{\beta}_S X_S + \hat{\beta}_{S \cup \{k\}} X_{S \cup \{k\}})\right](E[X_k] - X_k)
\]
\[= 2\hat{\beta}_k Cov(Y, X_k) - \hat{\beta}_k^2 \text{Var}(X_k),
\]
(C.1)

with
\[
V_{X,\hat{g}}(S) = \hat{\beta}_k E[X_k] + \hat{\beta}_S X_S + \hat{\beta}_{S \cup \{k\}} E[X_{S \cup \{k\}}],
\]
the stochastic version of \( v_{x,\hat{g}}(S) = E[\hat{g}(X)|X_S = x_S] = \hat{\beta}_k E[X_k] + \hat{\beta}_S x_S + \hat{\beta}_{S \cup \{k\}} E[X_{S \cup \{k\}}] \), and
\[
V_{X,\hat{g}}(S \cup \{k\}) = \hat{\beta}_k X_k + \hat{\beta}_S X_S + \hat{\beta}_{S \cup \{k\}} E[X_{S \cup \{k\}}],
\]
the stochastic version of \( v_{x,\hat{g}}(S \cup \{k\}) \). See Appendix B in [Aas et al. (2021)] for proof of \( v_{x,\hat{g}}(S) \) in linear regression. The second term in the third line of eq. (C.1) is equal to zero since the features are independent, and \( \hat{\beta} \) is considered a constant. Notice therefore that the sub-SAGE value, as well as the SAGE-value, is independent of the subset \( S \) used, and equal to eq. (C.1).

The second term \( \hat{\beta}_k^2 \text{Var}(X_k) \) is in fact equal to the increased variance in the model by including feature \( k \) actively in the model since
\[
E[V_{X,\hat{g}}(S)^2] - V_{X,\hat{g}}(S \cup \{k\})^2]
\]
\[= E[V_{X,\hat{g}}(S)^2] - E[V_{X,\hat{g}}(S)^2] - (E[V_{X,\hat{g}}(S \cup \{k\})^2] - E[V_{X,\hat{g}}(S \cup \{k\})^2])^2
\]
\[= \text{Var}(V_{X,\hat{g}}(S)) - \text{Var}(V_{X,\hat{g}}(S \cup \{k\})),
\]
(C.2)

because \( E[V_{X,\hat{g}}(S)] = E[V_{X,\hat{g}}(S \cup \{k\})] \).

For linear regression models, this shows that the sub-SAGE value is only positive if the agreement between the model and the independent test data (first term in eq. (C.1)) upweights the increased variance in the model (second term in eq. (C.1)) by including feature \( k \).

We neither know the variance of \( X_k \) nor the correlation between \( X_k \) and \( Y \), and so these must also be estimated from the data. The sample mean and sample covariance are unbiased and consistent estimators. Therefore, by using independent
test data \((x_0^0, y_0^0), \ldots, (x_{N_I}^0, y_{N_I}^0)\) of size \(N_I\), the estimator of \(\hat{\beta}_k\), denote it \(T(\hat{\beta}_k)\), is statistically independent from the test data, and by applying the sample mean and covariance we get the following unbiased estimate of eq. (C.1)

\[
\hat{w}_{X,Y,\hat{g}(S \cup \{k\})} - \hat{w}_{X,Y,\hat{g}(S)} = 2 \beta_j \text{Cov} \left( X, \sum_{j \in \tau_k} f_j(X_k) \right) - \beta_k^2 \text{Var} \left( \sum_{j \in \tau_k} f_j(X_k) \right).
\]

If we did not use training data separately for constructing the model, and test data to compute sub-SAGE values, the second term in the third line of eq. (C.1) would no longer become zero since the estimator \(T(\hat{\beta})\) naturally is correlated with the training data itself. It may seem confusing to treat \(\hat{\beta}_k\) in eq. (C.1) as a constant when the corresponding estimator \(T(\hat{\beta}_k)\) indeed has a distribution based on the training data. However, one may look at the procedure of sub-SAGE as objectively observing the properties of the raw model itself without taking into account the data used for training the model.

Appendix D. 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 \(M\) of all \(M\) features. In accordance with earlier notation, let \(\tau_k\) denote the set of tree stumps that include feature \(k\). Then, eq. (B.1) reduces to

\[
\hat{w}_{X,Y,\hat{g}(S \cup \{k\})} - \hat{w}_{X,Y,\hat{g}(S)} = \text{Cov} \left( Y, \sum_{j \in \tau_k} f_j(X) \right) - \text{Var} \left( \sum_{j \in \tau_k} f_j(X) \right),
\]

because all random variables \(V_{X,f_j}(S)\) for \(j \notin \tau_k\), for every \(S\) are now independent of all \(V_{X,f_j}(S)\) and \(V_{X,f_j}(S \cup \{k\})\) for \(j \in \tau_k\). Further, for every \(j \in \tau_k\), \(V_{X,f_j}(S) = \)
\(E_X[f_j(X)]\), a constant equal to the expected value of the output of the regression tree \(f_j\), and \(E_X[V_{X,f_j}(S \cup \{k\})] = E_X[f_j(X)]\), 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 tree stumps,

\[
E_{X,Y} \left[ Y \left( \sum_{j \in \tau_k} V_{X,f_j}(S \cup \{k\}) - V_{X,f_j}(S) \right) \right] = E_X \left[ Y \left( \sum_{j \in \tau_k} f_j(X_k) \right) \right] - E_Y[Y]E_X \left[ \sum_{j \in \tau_k} f_j(X_k) \right] = \text{Cov} \left( Y, \sum_{j \in \tau_k} f_j(X_k) \right).
\]

Likewise,

\[
E_{X,Y} \left[ \left( \sum_{j \in \tau_k} V_{X,f_j}(S \cup \{k\}) \right)^2 - \left( \sum_{j \in \tau_k} V_{X,f_j}(S) \right)^2 \right] = E_X \left[ \left( \sum_{j \in \tau_k} f_j(X_k) \right)^2 \right] - E_X \left[ \sum_{j \in \tau_k} f_j(X_k) \right]^2 = \text{Var} \left( \sum_{j \in \tau_k} f_j(X_k) \right).
\]

Hence, the expression given in eq. (D.1) independent of the subset \(S\). The expression in eq. (D.1) is therefore also equal to the sub-SAGE value, \(\hat{\psi}_k\) (or SAGE value). Both the covariance and the variance need to be estimated in practice. Given independent test data \((x_0^0, y_0^0), \ldots, (x_{N_I}^0, y_{N_I}^0)\), an unbiased estimate is given by

\[
\hat{\psi}_k = \frac{1}{N_I - 1} \sum_{i=1}^{N_I} \left( y_i^0 - \sum_{i=1}^{N_I} y_i^0 \right) \left( \sum_{j \in \tau_k} f_j(x_{i,k}^0) - \sum_{j \in \tau_k} v_{x_{i,k},f_j}(\emptyset) \right) - \frac{1}{N_I - 1} \sum_{i=1}^{N_I} \left( \sum_{j \in \tau_k} f_j(x_{i,k}^0) - \sum_{j \in \tau_k} v_{x_{i,k},f_j}(\emptyset) \right)^2. \tag{D.2}
\]

Appendix E. Sub-SAGE properties related to Shapley values

Symmetry, null player, linearity, monotonicity and efficiency are all properties of Shapley values. Below we investigate whether the same properties apply for sub-SAGE values.
Appendix E.1. Symmetry

Given two features \( j \) and \( k \) such that \( v(S \cup \{ j \}) = v(S \cup \{ k \}) \) for all \( S \in \{ Q_j, Q_k \} \) in which \( \{ j, k \} \notin S \). Then their sub-SAGE values indeed are identical, \( \psi_j = \psi_k \), and so the symmetry property follows by definition. This means in practice that two perfectly correlated features have equal sub-SAGE values.

Appendix E.2. Dummy property (null player)

Given a feature \( k \) where \( v(S \cup \{ k \}) = v(S) \) for all \( S \in Q_k \). Then \( \psi_k = 0 \), and so the dummy property follows by definition.

Appendix E.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,

\[ \psi_k(v + w) = \psi_k(v) + \psi_k(w). \] (E.1)

Appendix E.4. Monotonicity

Consider two models \( \hat{f}_1 \) and \( \hat{f}_2 \) used to predict the same relationship \( y = f(x) \), for the same features \( x \). If for any feature \( k \) we have \( v_{\hat{f}_1}(S \cup \{ k \}) - v_{\hat{f}_1}(S) \geq v_{\hat{f}_2}(S \cup \{ k \}) - v_{\hat{f}_2}(S) \) for all \( S \in Q_k \), then by definition, \( \psi_{\hat{f}_1}^k \geq \psi_{\hat{f}_2}^k \), with \( \psi_{\hat{f}_1}^k \) the sub-SAGE value of feature \( k \) when applying model \( \hat{f}_1 \) and \( \psi_{\hat{f}_2}^k \) 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 \( k \)'s importance increases also increases its sub-SAGE value. Therefore, the monotonicity property follows by definition.

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

Consider the definition of the Shapley value, \( \phi_k \), applied on a specific value function \( v \):

\[ \phi_k = \sum_{S \subseteq M \setminus \{ k \}} \frac{|S|!(M - |S| - 1)!}{M!} [v(S \cup \{ k \}) - v(S)]. \] (E.2)

The efficiency property for the Shapley value reads

\[ \sum_{k=1}^{M} \phi_k = v(M) - v(\emptyset), \] (E.3)
for $M$ "players". This can be observed more easily by using instead the following formulation of the Shapley value

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

(E.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 $M = \{1, 2, 3\}$, one possible ordering is $R = (2, 3, 1)$ with $s_1(R) = (2, 3)$. We then have

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

(E.5)

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

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

$$
\psi_k(y, \hat{y}) = \sum_{S \in Q_k} \frac{|S|!(M - |S| - 1)!}{M!(M - 1)!} \left[ v(S \cup \{k\}) - v(S) \right],
$$

(E.6)

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

**Appendix F. SHAP computations for fig. 3**

Consider this time the SHAP value of a given data generating process, $f$, with known relationship:

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

(F.1)
By applying the data generating process, $f$, explained in Section 5, the exact SHAP value of feature 1 can be computed by partitioning in the subsets $S$ not including feature 2, as well as those including feature 2. For all $S$ not including feature 2, and by using the result in Appendix B in [Aas et al. (2021)]:

$$v_{x_i, f}(S \cup \{k\}) - v_{x_i, f}(S) = a_1(x_{i,1} - E[X_1]) + a_{21}E[e^{X_2}](x_{i,1} - E[X_1]),$$

independent of the subset $S$ used. Of all $S \subseteq \mathcal{M} \setminus \{1\}$, a half of them will not include feature 2, and the sum of the corresponding Shapley weights are given by:

$$\sum_{|S|=0}^{M-2} \frac{|S|!(M-|S| - 1)(M-2)}{M!} = \sum_{|S|=0}^{M-2} \frac{|S|!(M-|S| - 1)(M-2)!}{|S|!(M-2 - |S|)!}$$

$$= \frac{1}{M(M-1)} \sum_{|S|=0}^{M-2} |S| = \frac{1}{2}.$$

For all $S$ including feature 2:

$$v_{x_i, f}(S \cup \{k\}) - v_{x_i, f}(S) = a_1(x_{i,1} - E[X_1]) + a_{21}e^{x_{i,2}}(x_{i,1} - E[X_1]).$$

As the sum of the Shapley weights are equal to one, the sum of the Shapley weights for these $S$ must also be $1/2$. Hence, the SHAP value of feature 1 is given by:

$$\phi_{i,1}(x_i) = \frac{1}{2}(a_1(x_{i,1} - E[X_1]) + a_{21}E[e^{X_2}](x_{i,1} - E[X_1]))$$

$$+ \frac{1}{2}(a_1(x_{i,1} - E[X_1]) + a_{21}e^{x_{i,2}}(x_{i,1} - E[X_1]))$$

$$= a_1(x_{i,1} - E[X_1]) + a_{21}E[e^{X_2}](x_{i,1} - E[X_1])$$

$$+ \frac{1}{2}a_{21}x_{i,1}(e^{x_{i,2}} - E[e^{X_2}]) - \frac{1}{2}a_{21}E[X_1](e^{x_{i,2}} - E[e^{X_2}]). \tag{F.2}$$

In the exact same manner one can show that:

$$\phi_{i,2}(x_i) = \frac{1}{2}(a_2(x_{i,2} - E[X_2]) + a_{21}E[X_1](e^{x_{i,2}} - E[e^{X_2}])$$

$$+ \frac{1}{2}(a_2(x_{i,2} - E[X_2]) + a_{21}x_{i,1}(e^{x_{i,2}} - E[e^{X_2}]))$$

$$= a_2(x_{i,2} - E[X_2]) + a_{21}E[X_1](e^{x_{i,2}} - E[e^{X_2}])$$

$$+ \frac{1}{2}a_{21}x_{i,1}(e^{x_{i,2}} - E[e^{X_2}]) - \frac{1}{2}a_{21}E[X_1](e^{x_{i,2}} - E[e^{X_2}]). \tag{F.3}$$
\[ \phi_{i,6} = \frac{1}{2}(a_6E[X_5|(I(x_{i,6} > 7) - E[I(X_6 > 7)])] \]
\[ \frac{1}{2}(a_6x_{i,5}(I(x_{i,6} > 7) - E[I(X_6 > 7)])] \]
\[ = a_6E[X_5|(I(x_{i,6} > 7) - E[I(X_6 > 7)])] \]
\[ + \frac{1}{2}a_6I(x_{i,6} > 7)(x_{i,5} - E[X_5]) - \frac{1}{2}a_6E[I(X_6 > 7)](x_{i,5} - E[X_5]). \]

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