

Relative Feature Importance

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Abstract—Interpretable Machine Learning (IML) methods are used to gain insight into the relevance of a feature of interest for the performance of a model. Commonly used IML methods differ in whether they consider features of interest in isolation, e.g., Permutation Feature Importance (PFI), or in relation to all remaining feature variables, e.g., Conditional Feature Importance (CFI). As such, the perturbation mechanisms inherent to PFI and CFI represent extreme reference points. We introduce Relative Feature Importance (RFI), a generalization of PFI and CFI that allows for a more nuanced feature importance computation beyond the PFI versus CFI dichotomy. With RFI, the importance of a feature relative to any other subset of features can be assessed, including variables that were not available at training time. We derive general interpretation rules for RFI based on a detailed theoretical analysis of the implications of relative feature relevance, and demonstrate the method’s usefulness on simulated examples.

Index Terms—feature importance, interpretable machine learning, explainable artificial intelligence, causality

I. INTRODUCTION

Predictive modelling is increasingly deployed in high-stakes environments, e.g., in the criminal justice system [11], loan approval [32], recruiting [9] and medicine [27]. Due to legal regulations [10], [29] and ethical considerations, ML methods need not only perform robustly in such environments but also be able to justify their recommendations in a human-intelligible fashion. This development has given rise to the field of interpretable machine learning (IML) that involves studying methods that provide insight into the relevance of features for model performance, referred to as feature importance. Prominent feature importance techniques include permutation feature importance (PFI) [5], [12] and conditional feature importance (CFI) [12], [19], [25]. PFI is based on replacing the feature of interest X_j with a perturbed version sampled from the marginal distribution $P(X_j)$ while CFI perturbs X_j such that the conditional distribution with respect to the set R of remaining features $P(X_j|X_R)$ is preserved. The sampling strategy defines the method’s reference point and therefore affects the method’s implicit notion of relevance. While PFI quantifies the overall reliance of the model on the feature of interest, CFI quantifies its unique contribution given

all remaining features.

While both PFI and CFI are useful, they fail to answer more nuanced questions of feature importance. For instance, a stakeholder may be interested in the importance of a feature relative to a subset of features. Also, the user may want to know how important a feature is relative to variables that had not been available at training time. We suggest relative feature importance (RFI) as a generalization of PFI and CFI that moves beyond the dichotomy between PFI, which breaks all dependencies with features, and CFI, which preserves all dependencies with features. In contrast to PFI and CFI, RFI is based on a perturbation that is restricted to preserve the relationships with a set of variables G that can be chosen arbitrarily. We show that RFI is (1) semantically meaningful and (2) practically useful.

We demonstrate the semantical meaning of RFI in Section IV. In particular, we derive general interpretation rules that link nonzero RFI to (1) the conditional dependence of the feature of interest with the target and non-conditioned features X_R given the conditioned variables X_G in the data and (2) the conditional dependence of the input to the feature of interest X_j with the model’s prediction \hat{Y} given fixed inputs to the remaining features X_R (Theorem 1). Furthermore, we show that a nonzero difference between RFI_j^G and $\text{RFI}_j^{G \cup N}$, with N being an arbitrary set disjoint with G , implies the conditional dependence $X_j \not\perp\!\!\!\perp X_N|X_G$ (Theorem 2).

In Section V, we provide an implementation of RFI estimation that is based on recent results from the related knockoff research field [7], [23]. Furthermore, we translate the testing framework developed for conditional feature importance [30] to RFI. We support our theoretical analysis and findings by various simulation studies in Section VI. In particular, we show that RFI can expose the indirect contribution of variables that are not directly used by the model but provide information via dependent variables (Section VI-A). Similarly, we show how RFI can be used to assess feature importance with respect to variables not included at training time (Section VI-B).

A. Contributions and Related Work

While conditioning on subsets of variables has been suggested before [12], [25], the implications of this generalized variant of CFI have not yet been rigorously analyzed. Some IML methods perturb or hide subsets

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of features, e.g., in the context of multiple regression relative importance analysis is a model-specific technique that averages over all importances of models trained on feature subsets [6], [16]. Model-agnostic, local approximations to the respective feature effect that avoid retraining and instead perturb subsets of features have also been proposed [17], [33]. A very recent global, model-agnostic feature importance proposal called SAGE quantifies feature importance by perturbing multiple features [8].

While the aforementioned approaches are all based on removing several features to provide more nuanced insight into the model, our proposal only modifies the feature of interest. Our approach is model-agnostic and global, while most aforementioned approaches are model-specific or local. The exception is the global, model-agnostic SAGE [8], however the approaches are not only computationally but also semantically different. E.g. our method assigns an importance of zero for features that are not used by the model¹, which is not the case for SAGE. While our approach aims to provide nuanced insights into variable importance relative to a specific set, SAGE aims to quantify the overall importance of variables for the model.

Feature importance relative to variables that have not been included in the training set has not been studied before. The indirect influence of variables that the model does not computationally rely but statistically depend on has been studied e.g. in [1].

II. BACKGROUND AND NOTATION

A. Notation

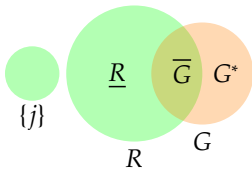


Fig. 1. Overview of our notation.

We denote the target variable, i.e., the variable the model predicts, as Y and feature variables by $X_{(\cdot)}$. We refer to the variables as features to emphasize when they were used in model training. Their observations are denoted by y and $x_{(\cdot)}$. We use $D := \{1, \dots, p\}$ for the index set of all features included in model training and j for the index of our feature of interest, X_j . The index set of the remaining variables is denoted as $R := D \setminus \{j\}$ (rest, remainder). The index set of features, relative to which the importance of X_j is considered, is denoted as G . As G can refer to any index set of variables, we denote its intersection with R as $\bar{G} = R \cap G$ and its complement as $\underline{R} = R \setminus G$. We denote the index set of

conditioning variables that were not made available to the model during training as $G^* = G \setminus R$.

In case we add new elements to the conditioning set G , we will denote this set as N . The set may include variables within and outside D . The respective components are denoted as $N^* = N \setminus R$ and as $\bar{N} = R \cap N$. The remainder of R without G and N is denoted as $\underline{R} = R \setminus N$. We denote perturbed variables of interest relative to G as \tilde{X}_j^G . We refer to the original and perturbed probability distribution of X_j as the observational and interventional distribution $P(X_j, \dots)$ and $P(\tilde{X}_j^G, \dots)$. The inspected model is denoted as f , its prediction as \hat{Y} . Independence of Y and X conditional on Z is denoted using $X \perp\!\!\!\perp Y|Z$, the respective conditional dependence as $X \not\perp\!\!\!\perp Y|Z$.

B. Feature Importance

Performance-based feature importance methods assess the relevance of a feature of interest X_j by assessing the impact of a perturbation of X_j on the model's performance. Local feature importance methods focus on the importance of features for specific data points, whereas global feature importance methods assess the impact over the whole domain. In the following, we focus on global methods.

Global feature importance is computed according to the following general schemata:

$$FI_j = \tilde{\mathcal{R}}^j - \mathcal{R} \text{ or } FI_j = \frac{\tilde{\mathcal{R}}^j}{\mathcal{R}}$$

where we denote the original risk of the model and the risk after perturbing X_j as \mathcal{R} and $\tilde{\mathcal{R}}^j$, respectively. For estimation, the true risk \mathcal{R} is replaced with the empirical risk \mathcal{R}_{emp} .

Feature importance methods furthermore differ in how they perturb and whether they rely on retraining the model. While some methods retrain the model after the perturbation (e.g. LOCO, [15]), others evaluate the impact of the perturbation on the same original model (e.g. [5], [25]). In this work, we focus on methods that avoid retraining.

For methods that avoid retraining, we observe a dichotomy between two general perturbation approaches: resampling that preserves the *marginal* and resampling that preserves the *conditional* distribution. Marginal resampling was originally proposed to compute perturbed versions of X_j by permuting the observations $x_j^{(i)}$ within the sample [5]. The respective sample breaks the dependence between X_j and (Y, X_R) while preserving the marginal distribution $P(X_j)$. More recently, Model Reliance was proposed [12], which takes the expectation over all possible permutations. Resampling from the marginal distribution has been criticized to introduce bias, in particular because it overestimates the importance of correlated variables

¹A proof of this property is given in Lemma 2.

[25], resulting in incorrect feature rankings [26]. It also leads to extrapolation under dependent features [14], [19], i.e. conclusions about the model are being drawn using unrealistic data points on which the model was not trained. CFI, on the other hand, samples from the conditional distribution $P(X_j|X_R)$ [2], [7], [12], [14], [19], [25], [28]. A large variety of model-specific methods exist [13], [31]. Conditional variants quantify the importance of a feature given the information that all remaining features R contain about X_j [20], thereby avoiding evaluation of the model on unrealistic datapoints [19].

III. RELATIVE FEATURE IMPORTANCE

Relative Feature Importance is a general framework that assesses feature importance relative to arbitrary variable sets G . The framework subsumes PFI and CFI as two extreme special cases.

In PFI, X_j is replaced with a perturbed version that preserves the marginal distribution $P(X_j)$ while breaking the dependencies with Y and all features. In CFI, a perturbed version of X_j is used that preserves the conditional distribution $P(X_j|X_R)$, thereby only breaking conditional dependence between X_j and Y given all features. As our analysis in Section IV establishes, the replacement strategies of PFI and CFI define extreme reference points. CFI quantifies the contribution relative to *all* remaining features R , whereas PFI regards a feature in isolation.

We go beyond the PFI versus CFI dichotomy. We argue that it is (1) meaningful (Section IV) and (2) practically useful (Section VI) to replace X_j with perturbed versions that preserve the conditional distribution $P(X_j|X_G)$ with respect to *arbitrary* sets G while requiring $\tilde{X}_j^G \perp\!\!\!\perp (X_R, Y)|X_G$. G can be a subset of R , but can also include variables not available at training time such that $G \setminus R \neq \emptyset$. We term the resulting method Relative Feature Importance (RFI):

Definition 1 (Relative Feature Importance – RFI): We define Relative Feature Importance with respect to a feature set G with $Y \notin G$ and a fixed model f as

$$\text{RFI}_j^G := \tilde{\mathcal{R}}^{jG} - \mathcal{R},$$

where $\tilde{\mathcal{R}}^{jG} := \mathcal{R}(Y, f(X_R, \tilde{X}_j^G))$ is the risk w.r.t. to a replacement variable \tilde{X}_j^G and $\mathcal{R} = \mathcal{R}(Y, f(X_j, X_R))$ refers to the original risk. The replacement variable has to satisfy

- $\tilde{X}_j^G \sim P(X_j|X_G)$ and
- $\tilde{X}_j^G \perp\!\!\!\perp (X_R, Y)|X_G$.

In the following section, we discuss the semantic meaning of RFI. The estimation of RFI is discussed in Section V.

IV. INTERPRETING RELATIVE FEATURE IMPORTANCE

IML techniques aim to provide insight into the model and, possibly, into the underlying data generating mechanism. However, IML techniques themselves are subject to interpretation. The characterization of an IML method by its mathematical definition is computationally precise, but has limited aid in guiding users to make conclusions about the underlying model and data. In this section we provide a (non-comprehensive) list of interpretation rules for RFI, that *characterize the method by how it behaves in its context*. This context includes *both the model and the underlying data generating mechanism*. More specifically, we link RFI to (conditional) independence in the underlying data set as well as to whether the model's prediction \hat{Y} is constant in the argument x_j for a fixed x_R . While RFI can be used for quantification of feature importance, we focus our analysis on relevance as a binary property and characterize relative feature relevance (RFI $\neq 0$). We show that the implicit notion of relevance of RFI is defined by the choice of G . By modifying the conditioning set G beyond the PFI versus CFI dichotomy, we are able to gain insight into more nuanced aspects of the model and the data generating mechanism. The main results are given in Theorem 1 and Theorem 2. Furthermore, we highlight limitations stemming from the choice of the loss function L and the model fit for the interpretation, which are, in our humble opinion, underrepresented in the current discussion.

We structure our analysis by taking the user's perspective and asking "What can we infer from relative feature relevance?".

A. Implications of Relative Feature Relevance

In the following, we analyze the implications of RFI without further assumptions about model and data. We thereby distinguish between two levels of explanation. Relative feature relevance provides insight, both into *model* and *data*.

Theorem 1: If $\text{RFI}_j^G \neq 0$ then

- $X_j \not\perp\!\!\!\perp (Y, X_R)|X_G$ in the underlying distribution (data level)
- $\tilde{X}_j \not\perp\!\!\!\perp \hat{Y}|X_R$ w.r.t. the interventional distribution $P(X_j|X_G)P(X_G, X_R) > 0$ (model level)

We prove Theorem 1 in two steps. First, we assess the implications of the respective independence for the underlying data set (Lemma 1). Then, we assess the implications of the respective independence for the model (Lemma 2). The contrapositions yield Theorem 1.

Lemma 1: If $X_j \perp\!\!\!\perp (Y, X_R)|X_G$ for any G with $Y \notin G$ then $\text{RFI}_j^G = 0$.

We base the proof of Lemma 1 on the insight that (because the model f is fixed) an equivalence in distribution implies an equivalence in risk (Proposition 1). Therefore conditions under which the interventional distribution $P(\tilde{X}_j^G, X_R, Y)$ coincides with the original distribution $P(X_j, X_R, Y)$ are sufficient for $RFI = 0$.

Proposition 1: If observational and interventional distribution coincide, then risks with and without perturbation are equal:

$$P(Y, X_j, X_R) = P(Y, \tilde{X}_j^G, X_R) \Rightarrow \mathcal{R}(f) = \tilde{\mathcal{R}}^{jG}(f)$$

Proof of Proposition 1: Given that $P(Y, X_j, X_R) = P(Y, \tilde{X}_j^G, X_R)$ we can write

$$\begin{aligned} \mathcal{R}(f) &= \mathbb{E}_{Y, X_j, X_R}[L(Y, f(X_j, X_R))] \\ &= \mathbb{E}_{Y, \tilde{X}_j^G, X_R}[L(Y, f(\tilde{X}_j^G, X_R))] = \tilde{\mathcal{R}}(f). \end{aligned}$$

We show next that the conditional independence $X_j \perp\!\!\!\perp (X_R, Y) | X_G$ is a sufficient condition for identity of both distributions.

Proof of Lemma 1: It holds that

$$\begin{aligned} P(Y, X_j, X_R, X_G) &= P(X_j | Y, X_R, X_G) P(Y, X_R, X_G) \\ &\stackrel{X_j \perp\!\!\!\perp (X_R, Y) | X_G}{=} P(X_j | X_G) P(Y, X_R, X_G) \\ &\stackrel{(\text{def})}{=} P(\tilde{X}_j^G | X_G) P(Y, X_R, X_G) \\ &= P(\tilde{X}_j^G, Y, X_R, X_G). \end{aligned}$$

Using Proposition 1 we can infer that $RFI_j^G = 0$. ■

So far, we have assessed implications for the underlying data generating mechanism. Next, we assess implications for the inspected model f .

Lemma 2: If $\tilde{X}_j^G \perp\!\!\!\perp \hat{Y} | X_R$ w.r.t. the interventional distribution $P(\tilde{X}_j^G, X_G, X_R)$ then $RFI_j^G = 0$ for any G .

Proof of Lemma 2: If the prediction for an observation (x_1, \dots, x_p) is independent of the value x_j' w.r.t. the interventional distribution, the prediction is unaffected when replacing x_j with any value x_j' with $P(x_j' | X_G = x_G) P(X_G = x_G, X_R = x_R) > 0$. Consequently, any sample from \tilde{X}_j^G yields the same prediction.

Furthermore values x_j' with nonzero probability over the interventional distribution also have nonzero probability over the observational distribution. The interventional distribution can be rewritten as

$$\begin{aligned} P(\tilde{X}_j^G, X_G, X_R) &= P(\tilde{X}_j^G | X_G, X_R) P(X_G, X_R) \\ &= P(\tilde{X}_j^G | X_G) P(X_G, X_R) \\ &= P(X_j | X_G) P(X_G, X_R). \end{aligned}$$

Similarly, the observational distribution can be factorized into $P(X_j | X_G, X_R) P(X_G, X_R)$. As $P(X_j | X_G, X_R) > 0 \Rightarrow P(X_j | X_G) > 0$ (which can be derived from, e.g., the law of total probability) it follows that $P(\tilde{X}_j^G, X_G, X_R) > 0 \Rightarrow P(X_j, X_G, X_R) > 0$.

Consequently the prediction \hat{y} for any value x_j with positive probability $P(X_j = x_j | X_R = x_R)$ is identical given unchanged x_R .

As the conditional distributions of X_j and \tilde{X}_j^G overlap and the distribution of X_R is unaffected, the prediction \hat{Y} is identical with and without perturbation. Therefore $\mathcal{R} = \tilde{\mathcal{R}}^{jG}$ and $RFI_j^G = 0$. ■

To summarize, we have shown that independence on the dataset and on the model level respectively imply $RFI_j^G = 0$ and can thereby prove Theorem 1.

Proof of Theorem 1: The result follows from contraposition of Lemma 1 and contraposition of Lemma 2. ■

Theorem 1 shows that nonzero RFI_j^G implies dependencies between sets of variables on the model level as well as on the data level. Which dependencies are relevant for RFI_j^G can be controlled with the conditioning set G . Consequently, the conditioning set G determines the method's implicit definition of relevance. I.e., on the data level, if $X_j \perp\!\!\!\perp (X_R, Y) | X_G$ holds, RFI_j^G is zero irrespective of any other dependencies that may hold, e.g. with X_G (Lemma 1). Nonzero RFI, a difference in performance on interventional and observational distribution, can only be caused by dependencies that have been destroyed in the interventional distribution, the dependencies with and via X_G are preserved by the replacement \tilde{X}_j^G and can therefore not be responsible for $RFI_j^G \neq 0$. Similarly, on the model level, $\tilde{X}_j^G \perp\!\!\!\perp \hat{Y} | X_R$ over the interventional distribution $P(X_j | X_G) P(X_G, X_R)$ yields zero RFI (Lemma 2). The behavior of the model outside the domain in which it is evaluated is irrelevant for RFI_j^G . What domain the model is evaluated over depends on the choice of G .

Because we can control RFI's implicit definition of relevance with G , RFI allows more nuanced insights into model and data than PFI or CFI alone. In Theorem 1, we aim to make the implicit definition of relevance explicit. On the data level, nonzero RFI implies the dependence of X_j with the tuple (Y, X_R) given X_G ($X_j \not\perp\!\!\!\perp (Y, X_R) | X_G$). In order to understand the aforementioned dependence, using the graphoid axioms contraction and weak union [22], the equivalent formulation below can be added:

$$(X_j \not\perp\!\!\!\perp Y | X_G) \vee (X_j \not\perp\!\!\!\perp X_R | X_G, Y).$$

At least one of the two conditional dependencies has to hold for nonzero RFI_j^G . The first dependence can be rephrased as: X_j is informative of Y , even if we already know X_G . It is more difficult to make sense of the second

dependence. Under dependent features ($X_j \not\perp\!\!\!\perp X_R | X_G, Y$), the distribution of X_j with X_R is not preserved under perturbation \tilde{X}_j^G . In the interventional distribution $P(\tilde{X}_j^G, X_R)$ observations that are improbable or impossible w.r.t. the observational distribution $P(X_j, X_R)$ can be possible and probable (and vice versa). Consequently, in the interventional distribution the feature distribution differs from the observation feature distribution. Even if $X_j \perp\!\!\!\perp Y | X_G$ holds, the model may perform suboptimally due to this distribution shift and cause RFI_j^G nonzero². If the conditioning set is a superset of R ($G \supseteq R$), such that set of remaining variables X_R is empty, it holds that ($X_j \perp\!\!\!\perp X_R | X_G, Y$). Therefore nonzero RFI must be attributed to ($X_j \not\perp\!\!\!\perp Y | X_G$) for $G \supseteq R$.

On the model level, nonzero RFI implies that the model's predictions are conditionally dependent on \tilde{X}_j^G given the remaining features R are fixed. E.g. for a linear model that has coefficient zero for all terms involving X_j , this dependence would not be fulfilled, and RFI_j^G would be zero (Lemma 2). The model is evaluated over the interventional distribution $P(X_j | X_G)P(X_G, X_R) > 0$, which varies depending on G . If G contains a nearly perfect correlate of X_j , X_j can be reconstructed well. In contrast, if $G = \emptyset$, for every possible x_R the model is evaluated over the whole marginal distribution of X_j . Although choosing a smaller set $G \subset R$ leads to extrapolation under dependent features, it allows more insight into the model's mechanism. For interpretation purposes like safety, this is highly desirable.

In the preceding paragraphs we have highlighted the importance of the conditioning set G for the method's implicit notion of relevance and illustrated the results from Theorem 1. We have argued that the conditioning set controls which potential dependencies can be responsible for nonzero RFI_j^G . The insights lead to a further, interesting application of RFI. By assessing the difference $\Delta \text{RFI}_j^{G \rightarrow GUN} = \text{RFI}_j^G - \text{RFI}_j^{GUN}$ when modifying the conditioning set G by adding new elements N , we are able to assess the role of the dependencies with variables in N relative to a baseline G . While for RFI_j^G only dependencies of X_j with and via G are preserved, for RFI_j^{GUN} also dependencies with and via N are maintained. If $\Delta \text{RFI}_j^{G \rightarrow GUN}$ is nonzero, this change has to be due to dependencies involving N , but not G . We substantiate this claim with Theorem 2. In order for $\Delta \text{RFI}_j^{G \rightarrow GUN}$ to be positive, the dependence $X_j \not\perp\!\!\!\perp X_N | X_G$ has to hold.

Theorem 2: If the difference $\Delta \text{RFI}_j^{G \rightarrow GUN} = \text{RFI}_j^G - \text{RFI}_j^{GUN} \neq 0$, then $X_j \not\perp\!\!\!\perp X_N | X_G$.

²Let e.g. X_1, X_2 be perfectly correlated and independent of Y . Then adding $X_1 - X_2$ does not alter its prediction performance, unless the dependence between the variables is broken. Also see [14] for a discussion in PFI.

Proof of Theorem 2: Under independence $X_j \perp\!\!\!\perp X_N | X_G$ it holds that

$$\begin{aligned} P(\tilde{X}_j^G, Y, X_R, X_G, X_N) &= P(\tilde{X}_j^G | Y, X_R, X_G, X_N) P(Y, X_R, X_G, X_N) \\ &\stackrel{(\text{def } \tilde{X}_j^G)}{=} P(X_j | X_G) P(Y, X_R, X_G, X_N) \\ &\stackrel{X_j \perp\!\!\!\perp X_N | X_G}{=} P(X_j | X_G, X_N) P(Y, X_R, X_G, X_N) \\ &\stackrel{(\text{def } \tilde{X}_j^{GUN})}{=} P(\tilde{X}_j^{GUN} | X_G, X_N) P(Y, X_R, X_G, X_N) \\ &\stackrel{(\text{def } \tilde{X}_j^{GUN})}{=} P(\tilde{X}_j^{GUN} | Y, X_G, X_N, X_R) P(Y, X_R, X_G, X_N) \\ &= P(\tilde{X}_j^{GUN}, Y, X_R, X_G, X_N) \end{aligned}$$

The equality $P(\tilde{X}_j^G, Y, X_R, X_G, X_N) = P(\tilde{X}_j^{GUN}, Y, X_R, X_G, X_N)$ implies $P(\tilde{X}_j^G, Y, X_R) = P(\tilde{X}_j^{GUN}, Y, X_R)$. Invoking Proposition 1 it holds that the corresponding risks \mathcal{R}^{jG} and \mathcal{R}^{jGUN} are equal. As $\text{RFI}_j^G - \text{RFI}_j^{GUN} = \mathcal{R}^{jG} - \mathcal{R}^{jGUN}$ it holds that $X_j \not\perp\!\!\!\perp X_N | X_G \Rightarrow \Delta \text{RFI}_j^{G \rightarrow GUN} = 0$. Contraposition proves Theorem 2. ■

While nonzero RFI_j^G as well as nonzero $\Delta \text{RFI}_j^{G \rightarrow GUN}$ have clear implications, interpreting zero RFI_j^G or zero $\Delta \text{RFI}_j^{G \rightarrow GUN}$ is difficult. For example, we may be tempted to interpret $\text{RFI}_j^G = 0$ as conditional independence in the data. However, the general principle that absence of evidence is no evidence for absence also applies in the context of RFI. A dependence in the data may not be captured by the model when it has a poor fit and does not rely on the respective variable. Similarly, although f may be optimal, a dependence in higher moments may simply not be modeled by f or captured by the loss L . As all aforementioned causes of nonzero RFI are potentially sufficient, but not necessary, it is unclear which of the causes nonzero RFI can be attributed to. Furthermore, the related problem of conditional independence testing is provably hard [24]. The theoretical insights that we derive in this Section (Theorem 1 and 2) are applied and illustrated in a simulation study in Section VI.

V. ESTIMATION AND TESTING

Estimating and sampling from the conditional distribution is in general difficult, especially in high-dimensional continuous settings. Various approaches for replacing X_j with samples from its conditional distribution exist, e.g., knockoff approaches [2], [7], [23], imputation and weighting [12] or permutation within decision tree leaves [18]. We used Model-X knockoffs [7] in this work, but note that the RFI approach is agnostic to its algorithmic implementation.

Using (standard) empirical risk estimates, our RFI estimate is

$$\widehat{\text{RFI}}_j^G = \frac{1}{n} \sum_{i=1}^n L(y^{(i)}, f(\tilde{x}_j^{(i)}, x_R^{(i)})) - \frac{1}{n} \sum_{i=1}^n L(y^{(i)}, f(x_j^{(i)}, x_R^{(i)}))$$

where $\tilde{x}_j^{(i)}$ is a sample from \tilde{X}_j^G . We can then test for nonzero $\widehat{\text{RFI}}_j^G$ using procedures for conditional independence tests, e.g., [30], thereby quantifying the uncertainty coming from empirical risk minimization. Because of the central limit theorem, the empirical risk converges (in probability) to a Gaussian distribution with increasing number of observations. Therefore, one-sided, paired t-tests can be used to infer tests and confidence intervals [30]. The test procedures proposed in [30] are agnostic to the conditioning set for the perturbation \tilde{X}_j^G . For smaller samples, the Exact Test by Fisher may be used.

The t-test and Fisher Exact Test ignore uncertainty and bias of the estimation procedures, i.e. the ML model and the knockoff-sampler are treated as “fixed”. E.g. misspecified, suboptimal models may not capture dependencies. Or dependencies are in higher moments that are not captured by the loss. Consequently, without further assumptions, the framework does not provide a test for conditional independence in the dataset.

The popular testing procedures for knockoffs proposed by [7] provide FDR over all features, but does not test the significance of the importance of individual features.

VI. SIMULATION STUDIES

In the following, we demonstrate the usefulness of RFI on two simulation studies. In the first example, we use RFI to expose indirect influence of variables that are not computationally used by the model. In the second example, we assess feature importance relative to a confounder that was unavailable at training time. In both examples, we represent the underlying data generating mechanism, that gives rise to the dependencies in the data, with a causal directed acyclic graph (DAG). The code for the examples is available online³.

A. Indirect Influence

A prominent application of interpretable machine learning is auditing models regarding its reliance on protected attributes A like age or sex. A reliance on the respective attributes may result in unfair discrimination and requires further inspection. With approaches like fairness through unawareness [3], the model does not rely on protected attributes directly. However, by implicitly reconstructing the sensitive attributes using seemingly harmless correlates, the model can indirectly make use of the protected attribute resulting in potentially harmful, unfair discrimination [3].

PFI and CFI cannot expose such indirect influence. As Lemma 2 proves, RFI_A^G is zero for a model that does not (directly) use the feature of interest A for the prediction for any conditioning set G . Furthermore, from PFI and CFI alone, we cannot infer whether the importance of a variable can be attributed to its dependence with an indirect influence. Using RFI_j^G with $G = A$ we preserve the influence of A on the prediction and can thereby restrict the attribution of importance to contributions stemming from dependencies not involving A (Theorem 1, Lemma 1). The difference to $\Delta \text{RFI}_j^{G \rightarrow G \cup N}$ with $G = \emptyset$ and $N = A$ exposes the indirect influence.

Not every indirect influence from a sensitive attribute is considered undesirable. Certain correlates of A may indeed be valid criteria for a decision (e.g. [4]). Importance stemming from dependencies with A via such resolving variables Z would be considered acceptable. We can assess the indirect influence beyond contributions stemming from dependence via Z by comparing to a baseline $G = Z$. In this baseline, contributions via Z are preserved and therefore irrelevant for RFI. Consequently, when setting $N = A$, the difference $\Delta \text{RFI}_j^{G \rightarrow G \cup N}$ only quantifies indirect influence that is not resolved by Z .

We demonstrate the usefulness of RFI to expose indirect influence in a simulation study. The dataset is a sample drawn from the distribution induced by a structural causal model (SCM) depicted in Figure 2. All relationships are additive linear with coefficients 1 and Gaussian noise terms ($\sigma_1 = \sigma_2 = \sigma_4 = 1$, $\sigma_3 = 0.3$ and $\sigma_y = 0.5$). An ordinary least squares linear regression model was fit to predict Y from X_1, \dots, X_4 ($\text{MSE} = 0.25$, $f(x_1, x_2, x_3, x_4) = 0.00x_1 - 0.01x_2 + 1.01x_3 + 1.00x_4$). We trained model-X knockoffs [7] on the training data and evaluated RFI on test data. Sample size is 10^5 with 10% test data.

In order to quantify the direct influence of the features we compute PFI. As we can see in Figure 3, X_1 and X_2 are considered irrelevant. In order to expose their indirect influence, we additionally compute RFI with respect to $G = \{X_1\}$ and $G = \{X_2\}$ respectively. For both variables we observe a drop in importance of X_3 and X_4 . Consequently both X_1 and X_2 have an indirect influence on the target (Theorem 2).

Furthermore we are interested in whether the indirect influence of X_1 can be resolved by X_2 . We therefore compute $\text{RFI}_j^{G \cup N}$ with $G = \{X_2\}$ and $N = \{X_1\}$. We see that for X_3 no change in importance can be observed. This is due to the independence $X_1 \perp\!\!\!\perp X_3 | X_2$ ⁴ (Theorem 2). The indirect influence is resolved. However, for X_4 the importance decreases further and is therefore not resolved by X_2 . This is in alignment with the dependence $X_1 \not\perp\!\!\!\perp X_4 | X_2$ implied by the graph (Figure 2).

⁴As faithfulness and causal markov condition hold, d -separation in the graph and (conditional) independence coincide [21]. We can therefore read the independence structures off Figures 2 and 4.

³Link to Code: <https://github.com/gcskoenig/icpr2020-rfi>

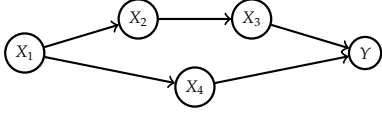


Fig. 2. Variable X_1 influences Y both via the chain $X_2 \rightarrow X_3$ and via X_4 . X_1 may be some undesired influence, and X_2 a variable resolving the undesired influence. We find that the prediction can nevertheless be influenced via X_4 by comparing $RFI_4^{X_2}$ with $RFI_4^{X_2, X_1}$ (Figure 3). All relationships are additive linear Gaussian with all coefficients being equal to 1 and $\sigma_1 = \sigma_2 = \sigma_4 = 1$, $\sigma_3 = 0.3$ and $\sigma_y = 0.5$.

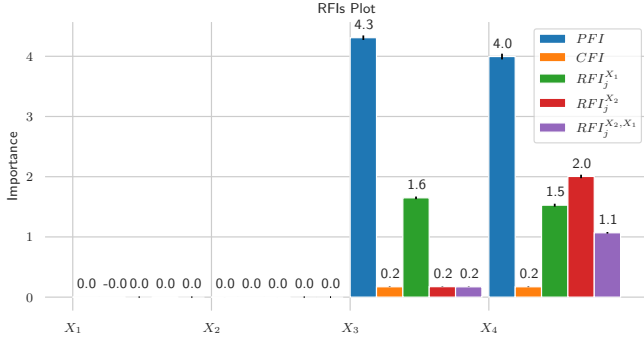


Fig. 3. RFI's for a linear regression model fitted on the dataset illustrated in Figure 2. Feature importance values are averaged over 30 runs and rounded. Feature importance values are averaged over 30 runs and rounded. We evaluated significance using a t-test for the first run. All positive features were significant at $\alpha = 0.01$, whereas for all zero RFI values the null could not be rejected. For X_1 and X_2 all RFIs are zero, whereas for X_3 and X_4 RFIs are positive. We see that X_1 and X_2 both have an indirect influence on X_3 and X_4 , but that X_2 can resolve the influence of X_1 on X_3 .

B. Variables Outside Training Set

When designing a model f , a practitioner may have decided to exclude a variable from the feature set, e.g., because it was then considered irrelevant, it belongs to a different modality or would have required further preprocessing. Furthermore, when auditing a machine learning model f , variables that have not been available for the training of the model may be accessible.

In this example, we demonstrate that variables outside the training set can be included in the conditioning set for RFI. Consequently, importance of the features relative to variables outside the training set and the indirect influence of such variables can be assessed. More specifically, we simulate a hypothetical situation where the influence of a previously unknown confounder C shall be evaluated. This variable C is available for the model audit. In particular, we wonder whether the features X_1 , X_2 and X_3 are only or partly important due to a dependence via C .

The dataset was sampled from a structural causal model (SCM) depicted in Figure 4. Assuming faithfulness and the causal Markov condition, this DAG implies the following (conditional) (in-)dependencies: X_1 is independent of C , X_3 is independent of Y conditional on C , and

X_2 is dependent on Y . Note that the dependence between X_2 and Y is due to the common cause C as well as due to a direct effect of X_2 on Y . All relationships are additive linear with coefficients 1 and additive Gaussian noise ($\sigma_1 = \sigma_2 = \sigma_C = 1.0$ and $\sigma_3 = \sigma_Y = 0.5$). We fit an ordinary least squares linear regression model on X_1 , X_2 and X_3 to predict Y ($MSE = 0.40$, $f(x_1, x_2, x_3) = 1.0x_1 + 1.17x_2 + 0.67x_3$). C was not available for model training. We trained Model-X knockoffs [7] on training data and sampled from \tilde{X}_j^G on test data. Sample size is 10^5 with 10% test data.

When computing RFI_j^C ($G = \{C\}$) for each variable, the different relationships with C become apparent. The respective results are depicted in Figure 5. For X_1 the feature importance relative to C remains unchanged as the variables are pairwise independent (Theorem 2). For X_3 , that is only dependent with Y via C , it completely vanishes (Lemma 1). For X_2 the feature importance decreases but remains nonzero, as X_2 is dependent with Y directly and via C .

Consequently, using RFI, we can (1) identify variables that are important due to a variable unavailable at training time and (2) distinguish between variables that only depend on Y via C from those that do not. With PFI ($G = \emptyset$) or CFI ($G = R$) such a distinction is in general not possible.

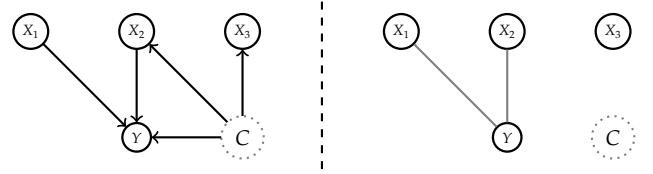


Fig. 4. Left: We see the causal graph \mathcal{G} corresponding to the Structural Causal Model that was used to generate the dataset used in Figure 5. All relationships are additive linear Gaussian with all coefficients equal to 1 and $\sigma_1 = \sigma_2 = \sigma_C = 1.0$ and $\sigma_3 = \sigma_Y = 0.5$. Right: Pairwise dependencies after conditioning on C .

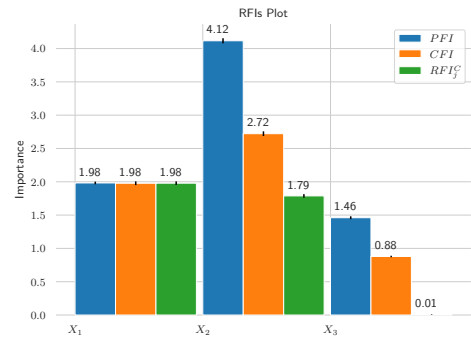


Fig. 5. Feature Importance results corresponding to the dataset depicted in Figure 4. We averaged RFI over 30 runs. RFI for X_1 is unaffected by changes in G , for X_2 RFI drops with C is added to G . For X_3 RFI vanishes relative to C . For all except for $RFI_{X_3}^C$ the null can be rejected at $\alpha = 0.01$ in the first run.

VII. DISCUSSION

We proposed relative feature importance (RFI), a general conditional feature importance framework which allows to condition on arbitrary sets of other features, including features outside the training set. We underpin the method with theoretical results allowing insight into both model and underlying dataset. In a simulation study, the usefulness of the method for the exposure of indirect influence is demonstrated.

Relative feature importance requires sampling from (unknown) conditional distributions. For continuous variables and in high-dimensional settings this task is challenging and an open area of research [7], [23]. Uncertainty stemming from inaccurate sampling may affect the interpretation. The quality of insight into the underlying dataset strongly depends on the training and evaluation of the model. Dependencies in higher moments are usually not modeled and not captured by standard loss functions and can therefore not be detected. Especially the interpretation of zero RFI requires careful assessment of the model specification. Further research is needed to assess necessary assumptions for the interpretation of RFI. These challenges are not unique to RFI, but apply more generally in the field of interpretable machine learning [20].

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