Inherent Inconsistencies of Feature Importance

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Abstract

The black-box nature of modern machine learning techniques invokes a practical and ethical need for explainability. Feature importance aims to meet this need by assigning scores to features, so humans can understand their influence on predictions. Feature importance can be used to explain predictions under different settings: of the entire sample space or a specific instance; of model behavior, or the dependencies in the data themselves. However, in most cases thus far, each of these settings was studied in isolation.

We attempt to develop a sound feature importance score framework by defining a small set of desired properties. Surprisingly, we prove an inconsistency theorem, showing that the expected properties cannot hold simultaneously. To overcome this difficulty, we propose the novel notion of re-partitioning the feature space into separable sets. Such sets are constructed to contain features that exhibit inter-set independence with respect to the target variable. We show that there exists a unique maximal partitioning into separable sets. Moreover, assigning scores to separable sets, instead of single features, unifies the results of commonly used feature importance scores and annihilates the inconsistencies we demonstrated.

1 Introduction

Many feature importance scores are inspired by, or derived from, Shapley’s work on fair allocation in coalition games (1). In these, and other common methods, the importance score is computed in a two-step process. First, a value-function is computed, assigning a value to every subset of the features. Different metrics can be used to define the value-function, such as mutual information, classification accuracy, or the coefficient of determination. Second, the importance score is computed of the values assigned to these subsets. This two step process allows for a discussion about the expected behavior
Table 1: Examples of common feature importance functions

| Name | Feature importance score: $\phi(\nu, f)$ |
|------|------------------------------------------|
| Bivariate | $\nu(\{f\})$ |
| Ablation | $\nu(F) - \nu(F \setminus \{f\})$ |
| Shapley | $\sum_{S \subseteq F \setminus \{f\}} \frac{|S|!(|F|-|S|-1)!}{|F|!} \cdot (\nu(S \cup \{f\}) - \nu(S))$ |
| MCI | $\max_{S \subseteq F \setminus \{f\}} (\nu(S \cup \{f\}) - \nu(S))$ |

of the value-function and of the feature importance score in relation to the value-function. Here, we focus on several such feature importance scores: ablation-studies (2, 3, 4), bivariate-association (5), SHAP (6) and MCI (7). The definitions of these feature importance functions can be found in Table 1.

The study of feature importance can be divided into four different settings, across two axes: local and global, as well as data and model. Studies focusing on local interpretations seek to explain individual predictions (e.g., the role of each feature in a patient’s diagnosis (8)). On the other hand, studies focusing on global interpretation try to understand how each feature affects a phenomenon (e.g., the role of each gene in a particular disease (9, 10)). Along the second axis, the data and the model are distinguished by the type of conclusion required. The scientist seeks an explanation of the data, to infer conclusions about the world that are encoded in the data (11, 12, 13). The engineer, however, uses an explanation to monitor and debug a man-made system, to ensure it is working as intended, e.g., for security purposes (14, 15). Table 2 maps feature importance research according to the local vs. global and data vs. model settings.

Several studies have examined the relations between the different settings. For example, Lundberg et al. (16) presented a global score that is computed by combining local scores, hence indicating that at least the local and the global settings are not independent. Nevertheless, most studies focus solely on one setting. The studies that do consider multiple settings, often do not present an explicit set of expectations from the relations between importance scores under the different settings.

In this work, we define the expected behaviors of feature importance scores under different settings, and the expected relations between the settings. In Section 2 we define, using formal language, the value-function, the feature importance function, and the expected properties of these functions. For example, the Triviality property (Definition 2.3) requires that if the value of a set of features is non-zero, then it contains a feature with non-zero importance. We also add consistency requirements between the settings. The Importance Consistency property (Definition 2.4) requires that the global importance score is the expected value of the local importance scores. The Data-Model Equivalence property (Definition 2.5) requires that a model that perfectly predicts the entire sample space will generate the same feature importance scores as those calculated on the data.

Naturally, the next step in our inquiry is to seek feature importance scores that satisfy the required properties and are consistent between the settings. However, in Section 3 we show that it is impossible to define such importance scores. That is, properties of feature importance scores within and between setting contradict each other. Hence, there are inherent inconsistencies between the expected behaviors of feature importance scores in the different settings.

We further exemplify practical gaps in feature importance scores when applied to specific dependency structures. We show that the presence of highly correlated features and collider variables yield inconsistent and misleading interpretations of feature importance. Therefore, the use of feature importance to study phenomena in the world might be deceiving even in the presence of unlimited data and perfect models.

The inconsistencies of feature importance scores and their misleading behavior jeopardize their use as valid explanations (17). In an attempt to find a remedy for these inherent inconsistencies, we propose that scores can be assigned to sets of features that are inter-set independent with respect to the target variable. We term these separable sets and prove that there exists a unique maximal partition of the feature space into separable sets. We consider these separable sets as “meta-features” and extend the feature importance scores to them. We show that the commonly used importance scores
mentioned above consolidate when applied on separable sets. Finally, scores applied to separable sets do not suffer from the inconsistencies of scores assigned to individual features.

1.1 Related Work

Many feature importance scores have been proposed in the literature. Table 2 lists several popular feature importance scores and their mapping to the different settings, according to the global-local and data-model divisions. Most feature importance scores thus far focused on explaining models, although the data setting has also been gaining increased attention in recent years. However, the quadrant of the data-local setting is still unexplored in the field of explainable AI. Perhaps this is due to the challenge of providing an accurate explanation as to why a specific outcome (rather than average result) came into being (rather than was calculated by a model). For example, which characteristic of John Doe is responsible for the fact that he did, or did not, suffer a stroke? These types of questions pertain to individual causal effects, that are notoriously difficult to estimate [18, 19].

There is an ongoing discussion regarding the formulations and interpretations of feature importance scores. Several studies attempted to link the scores under different settings. Covert et al. [5] proposed a method of assigning global importance to features, which draws a connection with the local feature importance score of SHAP [6]. Chen et al. [20] defined distinctions between the data and the model and argued that the nature of an explanation depends on what one seeks to explain – the data or the model. Furthermore, despite their popularity, the interpretation of Shapely value based methods has been questioned by recent studies. Shapley based values can be invalid under co-linearity between features [21, 22, 7], or when interpreting modification of features as an intervention [23]. These discussions motivate our attempt to define expected properties of importance scores, which will allow us to gauge the suitability of different solutions.

1.2 Our Contribution

The contributions of this work are:

1. We propose a unified framework for the desired properties of different settings of feature importance: global-data, local-data, global-model, and local-model.

2. We present intrinsic problems of inconsistency in feature importance scores across the various settings:
   - We show that the requirement that global feature importance is the expected value of local feature importance is inconsistent with results in the data setting.
   - We show that results in the data setting and results in the model setting are inconsistent, even in the case where the data and the model agree everywhere.
   - We show concrete examples in which feature importance scores fail to provide the explanation we would have expected.

3. Based on our results, we define a method of calculating importance scores for sets of features that are inter-set independent with respect to the target variable. We show that there exists a unique maximal partition to such independent (separable) sets. This partition overcomes the aforementioned difficulties and unifies the results of different feature importance score. Therefore, we propose considering these separable sets as “meta-features” and assigning scores to them.

The paper is structured as follows: The second section contains notations and framework properties. The third section contains the inconsistency theorems for the two axes we have presented earlier, as well as examples of internal causal problems that appear in the feature importance method. The fourth section contains our proposal for the limited case in which consistency is maintained, as well as overcoming the problems we have presented.
Table 2: Examples of feature importance scores and their categorization according to the global/local and data/model settings

| Model                  | Global                                                                 | Local                                                                 |
|-----------------------|------------------------------------------------------------------------|-----------------------------------------------------------------------|
| Additive-Importance-  | SHAP ([8] Lime ([25]                                                |
| Measures ([5])        | Gradient-Based-Localization ([26]                                      |
| Bivariate-Association | Relevance-Propagation ([27])                                           |
| ([5])                 |                                                                        |
| Ablation-Studies ([2];[3];[4]) | Tree-Shap ([16])                                                                |
| FIRM ([24])           |                                                                        |
| TreeExplainer ([16])  |                                                                        |
|                       |                                                                        |
| Data                  | True-To-Data ([20] MCI ([7]                                  |
| UMFI ([28])           |                                                                        |
Definition 2.3 (Triviality) The triviality requirement holds if

1. \( \forall S \subseteq F, \) if \( \nu(S) \neq 0 \) then \( \exists f \in S \) s.t. \( \phi(\nu, f) \neq 0 \)

2. If \( \phi(\nu, f) \neq 0 \) then \( \exists S \subseteq F \) s.t. \( \nu(S \cup \{ f \}) \neq \nu(S) \)

The triviality requirement establishes a non-trivial relationship between the value and the importance functions. Simply said, it requires that if a subset of features has any value, it will be expressed in the importance of at least one feature from this subset. In the other direction, it requires that if any feature is important (i.e., has non-zero importance) so this feature must be included in some valuable subset. Note that it also holds that if a feature \( f \) is such that for any subset of features, \( \nu(S) = \nu(S \cup \{ f \}) \) then \( f \) has zero importance.

Definition 2.4 (Null Feature) If for \( f \subseteq F, \forall x, x' \in X, \) s.t. \( x \) differs from \( x' \) only at the \( f \)'th feature, it holds that \( M(x) = M(x') \), then

\[
\phi(\nu^M, f) = 0
\]

The null feature property states that if changing the value of a feature has no effect on a model, then its importance is zero.

Definition 2.5 (Data-Model Equivalence) \( \phi \) is data-model consistent, if \( \forall M, D \) s.t. \( \forall (x, y) \in (X, Y), M(x) = y \) it holds that \( \forall f \in F \),

\[
\phi(\nu^M, f) = \phi(\nu^D, f)
\]

The data-model equivalence property states that if a model predicts the target perfectly, then the data and model importance scores of each feature will be identical.

Definitions 2.1 and 2.2 define the expected relation between explanations of single case and explanations of the model or the data. Therefore, when they both hold, we say that \( (\phi, \nu) \) is local-global consistent. The later definitions, namely Definitions 2.4 and 2.5, focus on the relation between explaining the data and explaining a model. Therefore, when these three definitions hold, we say that \( (\phi, \nu) \) is data-model consistent.

The goal of stating these definition is to find consistent families of feature importance scores. However, in the next section we show that such families do not exist.

3 Feature importance inconsistencies

3.1 The local-global inconsistency

We begin by studying the local-global consistency in the data setting. In addition to Definitions 2.1 and 2.2 we assume a set of properties, defined in Catav et al. (7), that a feature importance score in the data-global setting is expected to have. The properties described therein are the Marginal Contribution property, which states that \( \phi^g(\nu, f) \geq \nu(F) - \nu(F \setminus \{ f \}) \); the Elimination property, which states that if \( f \in F \subseteq F' \), then the importance of \( f \) in the context of \( F' \) is not smaller then its importance in the context of \( F \); and the Minimalism property, which requires that a feature importance score is the minimal score function that satisfies the Marginal Contribution and Elimination properties. Formal definitions of the properties are attached in the Supplementary Material.

Theorem 1 The assumptions of the data-global setting (the Marginal Contribution property, the Elimination property, and the Minimalism property) cannot hold simultaneously with the local-global consistency of \( (\phi, \nu) \) (Definitions 2.1,2.2).

The proof uses the following two lemmas, which proofs are attached in the Supplementary Material.

Lemma 1 If \( (\nu, \phi) \) is local-global consistent, then \( \forall x \in X \), it holds that

\[
\phi^g(\nu_x) = \phi_l(\nu_x)
\]

Note that we did not require the feature importance function to be identical in the local and global case. The lemma states that under these assumptions, the global and local feature importance functions are identical.
Lemma 2 If \((\nu, \phi)\) is local-global consistent, then \(\phi_g\) is a linear function of \(\nu_g\).

Proof. [of Theorem 1]

Assume in contradiction that \((\nu, \phi)\) is local-global consistent in the data setting. From Lemma 1 it holds that \(\phi_g \equiv \phi_l\), and from Lemma 2 we have the \(\phi_g\) is a linear function. However, Catav et al. proved that the only function that satisfies the Marginal Contribution property, the Elimination property, and the Minimalism property is MCI which is not a linear function.

A numeric example showing that MCI is not linear can be found in the Supplementary Material.

3.2 The data-model inconsistency

Models are often used as a proxy to represent the world. In cases where the model is perfect, i.e., the model predictions are identical to the data, we would expect the data and the model to also agree on each feature’s importance. However, this expectation implies a degenerate case, where the value-function is the zero function.

Theorem 2 If Triviality holds and \((\nu, \phi)\) is data-model consistent (Definitions 2.3, 2.4, 2.5), then \(\nu \equiv 0\).

Proof. Let \(\rho\) be a random variable, and let \(f_0, f_1\) be two features s.t \(f_0 = f_1 = \rho\). Let \((\nu, \phi)\) be data-model consistent, and let \(\mathcal{M}^0, \mathcal{M}^1\) be two models s.t each model focuses on one feature and neglects the other: for \(i \in \{0, 1\}, \mathcal{M}^i(x) = f_i(x)\).

Assume in contradiction that \(\forall i \in \{0, 1\}, \nu^{\mathcal{M}^i} \neq 0\). Let \(\mathcal{M}^0, \mathcal{M}^1\) be identical to the data \(\rho\), and therefore \(\forall f \in \mathcal{F}, \phi(\nu^{\mathcal{M}^i}, f) = \phi(\nu^D, f)\) by the Data-Model Equivalence property.

By the Null Feature property, we get that \(\phi(\nu^{\mathcal{M}^i}, f_{1-i}) = 0\). We assumed that the value-function is not the zero function, hence by Triviality it holds that \(\exists S \subseteq \mathcal{F} \text{ s.t } \nu^{\mathcal{M}^i}(S \cup \{f\}) - \nu^{\mathcal{M}^i}(S) \neq 0\). Combining the last two statements with Triviality, we get that \(\phi(\nu^{\mathcal{M}^i}, f_i) \neq 0\).

To conclude, \(\forall i \in \{0, 1\}, \phi(\nu^{\mathcal{M}^0}, f_i) \neq \phi(\nu^{\mathcal{M}^1}, f_i)\), in contradiction to the Data-Model Equivalence property.

3.3 Reasoning for feature importance

Feature importance is often used, even if not stated explicitly, as a proxy for the causal analysis. Unfortunately, known difficulties from the field of causality also arise when calculating feature importance. The example we used to prove the inconsistency of the data-model often appears in real-world problems. Two features can be highly similar because a common, unobserved factor, caused them, or one of them caused the other. In other cases, features may be highly correlated because they are both proxies for another variable. For example, when continuously measuring a variable of interest but recording only its mean or maximum values in discretized time points. This problem of lacking information to disentangle the effect of two variables, is known as non-identifiability.

To illustrate this in our context, consider two penalized regression models that are trained on two identical features. The first model employs an L1 regularization, also known as lasso regression; and the second model employs an L2 regularization, also known as ridge regression. The predictions of the two models are identical. However, the calculation of commonly used feature important methods will lead to different results - lasso regression will result in assigning all the importance to one of the features, whereas ridge regression will result in assigning equal importance to both features.

Another situation that may lead to unexpected outcomes from feature importance scores is when a collider (also known as an inverted fork) exists in the data. As an example, assume that the following relationships hold in the real world (illustrated in Figure 1): Smoking cigarettes (Smoking) causes cancer (Cancer), but also increases chewing gum consumption (Gum). Assume also that doctors recommend people with earaches (Earache) to chew gum. Now, imagine a researcher developing a model to predict Cancer using different subsets of the features Gum and Earache, but lacks information on Smoking.
In a first setting, the researcher uses only the *Earache* feature. Since earache and cancer are independent, any value-based feature importance score will assign zero importance to *Earache*. In a second setting, where only the *Gum* feature is present, the researcher will conclude that *Gum* is an important feature, since it is correlated with *Cancer*. In a third setting, where a model that contains both *Earache* and *Gum* is considered, the researcher will infer that *Earache* has a non-zero importance. This results from conditioning on *Gum*, creating an association between *Earache* and *Cancer* due to presence of a collider. Intuitively, a person who chews gum and does not have an earache is more likely to be a smoker, and hence at high risk of cancer. Therefore, the feature importance score might mislead a naïve researcher into thinking that earaches are predictive of cancer.

The situations described here have been studied in the causality literature and there is no recipe for overcoming them that does not involve additional information about the world (18; 19).

### 4 Separable sets

In the previous section we presented several inherent inconsistencies and limitations of feature importance scores. In this section, we present a special scenario where these problems do not apply. The main observation is that problems emerged when the data contained dependencies between features with respect to the target.

Therefore, we propose a feature importance framework that assigns scores to sets of features, rather than to single features. We will demonstrate that for sets that have inter-set independence, this feature importance framework manages to overcome the previously described obstacles. We note, moreover, that when applied to inter-independent sets, many popular methods for calculating feature importance, including those presented in Table 1, merge.

Inspired by the notion of inessential games (29; 30; 31), we propose the following definitions to partition the feature space into separable sets:

**Definition 4.1 (Separable set)** $S \subseteq F$ is separable with respect to $\nu$, if:

$$\forall T \subseteq F, \quad \nu(T) = \nu(T \cap S) + \nu(T \setminus S)$$

A set $S$ is separable with respect to $\nu$ if the value of any set $T$ is the sum of the value of its intersection with $S$ and the value of the part of $T$ that is complementary to $S$. Next, we define a partition of the feature space into separable sets.

![Figure 1: An example of a directed acyclic graph with a collider variable *Gum*.](image-url)

Figure 1: An example of a directed acyclic graph with a collider variable *Gum*. 

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Definition 4.2 (Partitioning to separable sets) \( \mathcal{G} \) is a partition of \( \mathcal{F} \) to separable sets w.r.t \( \nu \) if \( \mathcal{G} \) is a collection of disjoint subsets of \( \mathcal{F} \) which are separable w.r.t \( \nu \), and \( \bigcup_{g \in \mathcal{G}} g = \mathcal{F} \).

For a partition of \( \mathcal{F} \) to separable sets \( \mathcal{G} \), we consider every set \( g \in \mathcal{G} \) as a meta-feature. For a subset of meta-features \( G \subseteq \mathcal{G} \) we can denote a subset of feature \( S \subseteq \mathcal{F} \) s.t \( S = \bigcup_{g \in G} \bigcup_{f \in g} f \).

The separable set property implies that \( \nu(S) = \sum_{g \in G} \nu(g) \). Hence, we can extend \( \nu \) to operate on subsets of meta-features, by defining, for \( G \subseteq \mathcal{G} \), that \( \nu(G) = \sum_{g \in G} \nu(g) \). Using the terminology of Kumar et al. \((3)\), \( \nu \) induces an inessential game with respect to \( \mathcal{G} \).

A useful property of a separable partitioning is that there exists a unique maximal partition.

Theorem 3 There exists a maximal unique partition to separable sets \( \mathcal{G}^* \) such that for any other partition to separable sets \( \mathcal{G} \), \( |G| < |G^*| \). Moreover, for every separable set \( S \subseteq \mathcal{F} \) there exists \( G \subseteq \mathcal{G}^* \) such that \( S = \bigcup_{g \in G} \bigcup_{f \in g} f \).

The proof uses the following three lemmas, the proofs of which are attached in the supplementary material section.

Lemma 3 If \( S \subseteq \mathcal{F} \) is a separable set, then \( \mathcal{F} \setminus S \) is also a separable set.

Lemma 4 If \( S_1, S_2 \subseteq \mathcal{F} \) are separable sets, then \( S_1 \cup S_2 \) is a separable set.

Lemma 5 If \( S_1, S_2 \subseteq \mathcal{F} \) are separable sets, then \( S_1 \cap S_2 \) is a separable set.

Using these three lemmas we are proving the main theorem:

Proof. [of Theorem 3]

For every feature \( f \in \mathcal{F} \) let \( S_f \) be the intersection of all separable sets that contain \( f \). Note that since \( \mathcal{F} \) by itself is a separable set then this intersection is well defined.

From Lemma 5 it follows that \( S_f \) is a separable set. Moreover, from the definition of \( S_f \) it follows that for two features \( f_1, f_2 \in \mathcal{F} \) we have that either \( S_{f_1} \cap S_{f_2} = \emptyset \) or \( S_{f_1} = S_{f_2} \).

Let \( \mathcal{G}^* \) be the collection of unique \( S_f \)’s. \( \mathcal{G}^* \) is a partition of \( \mathcal{F} \) to separable sets since it is made of disjoint separable sets which cover \( \mathcal{F} \).

For any separable set \( S' \subseteq \mathcal{F} \) we have that \( S' = \bigcup_{f \in S'} S_f \) which completes the proof. \( \square \)

Theorem 4 For a partitioning of \( \mathcal{F} \) to separable sets \( \mathcal{G} \), the following properties hold:

1. The feature importance scores defined in Table 1 are identical
2. \( (\phi, \nu) \) is local global consistent (i.e. Definitions 2.1,2.2 hold)
3. The Triviality property holds (2.3) for any value-functions that satisfy \( \nu(\emptyset) = 0 \).

Proof. If \( \mathcal{G} \) is a partition of \( \mathcal{F} \) into separable sets, it holds that \( \forall g \in \mathcal{G} \)

1. MCI, Shapley and ablation are identical to the bivariate-association function.
   - Ablation:
     \[
     \phi(\nu, g) := \nu(\mathcal{G}) - \nu(\mathcal{G} \setminus \{g\}) = \nu(\mathcal{G} \cap g) + \nu(\mathcal{G} \setminus g) - \nu(\mathcal{G} \setminus g) = \nu(g)
     \]
   - Shapley:
     \[
     \phi(\nu, g) := \sum_{S \subseteq \mathcal{G} \setminus \{g\}} \Delta_S \cdot (\nu(S \cup \{g\}) - \nu(S))
     = \sum_{S \subseteq \mathcal{G} \setminus \{g\}} \Delta_S \cdot (\nu((S \cup \{g\}) \cap g) + (\nu((S \cup \{g\}) \setminus g) - \nu(S))
     = \nu(g) \cdot \sum_{S \subseteq \mathcal{G} \setminus \{g\}} \Delta_S = \nu(g)
     \]
     where \( \sum_{S \subseteq \mathcal{G} \setminus \{g\}} \Delta_S = 1 \) for \( \Delta_S := \frac{|S|!(|g| - |S| - 1)!}{|g|!} \).


- MCI:
  \[ \phi(\nu, g) := \max_{S \subseteq \emptyset \setminus \{g\}} (\nu(S \cup \{g\}) - \nu(S)) \]
  \[ = \max_{S \subseteq \emptyset \setminus \{g\}} (\nu((S \cup \{g\}) \cap g) + \nu((S \cup \{g\}) \setminus g) - \nu(S)) = \nu(g) \]

2. \((\phi, \nu)\) is local-global consistent:
  \[ \phi_{g}(\nu, g) = \nu_{g}(g) = \mathbb{E}[\nu_{x}(g)] = \mathbb{E}[\phi_{i}(\nu, g)] \]

3. • \(\forall S \subseteq \mathcal{G}, \nu(S) = \sum_{g \in S} \nu(g)\) (by definition).
   Hence, if \(\nu(S) \neq 0\) then \(\exists g \in S\) s.t. \(\nu(g) \neq 0\), and therefore by item (1) \(\phi(\nu, g) \neq 0\).
   • If \(\phi(\nu, g) \neq 0\) then again by item (1) \(\nu(g) \neq 0\) and \(\nu(\emptyset) \neq \nu(\emptyset \cup \{g\})\).

We further notice several additional consequences of partitioning the feature space into separable sets. First, the Null Feature property \(2.3\) aligns with Triviality \(2.3\) and Theorem 4. If \(g \in \mathcal{G}\) is a Null Feature then \(\phi(\nu^{M}, g) = 0\). The contraposition of the first item of Triviality implies that \(\exists G \subseteq \mathcal{G}\) s.t. \(g \in G\) and \(\nu^{M}(G) = 0\). This aligns with the first item of Theorem 4, \(\phi(\nu^{M}, g) = 0 \Rightarrow \nu^{M}(g) = 0\).

Second, we notice that the proof that \((\phi, \nu)\) is data-model inconsistent breaks: co-linear features which are not null features, as in our example, will always be grouped into the same set since they are dependent and therefore they will not harm the data-model consistency.

Finally, the practical issues we raised in 3.3 no longer hold. Identical features, in any partition to separable sets, will always be in the same separable set, so assigning them different feature importance scores is impossible. As for the example of the collider / inverted fork, one of the two must occur: either both Earache and Gum will be in the same separable set, and Earache will not have a separate score. Or, they will be in different separable sets, which will cause the importance of Earache to be zero, as easily seen by its bivariate-association importance.

5 Conclusion

Feature importance can be categorized into four settings, along two main axes: global vs. local and model vs. data. In this work, we attempted to create a unified framework of feature importance, accounting for all four settings and their interactions. We defined expected properties of feature importance scores and the relations between them. Surprisingly, we found that it is impossible to define feature importance scores that will be consistent between the settings. Specifically, the expected behavior of local-global scores contradicts previous results of the data-global setting. Furthermore, there is no guarantee that feature importance scores of a model that perfectly predicts the data will reflect the data feature importance.

To overcome these limitations of feature importance scores, we proposed an alternative: assigning a single score to each set of features that has inter-set independence with respect to their values – termed separable sets. We showed that a unique maximal partition to separable sets exists, and that the demonstrated limitations of feature importance do not apply when using these sets as meta-features. We note that other methods previously proposed assigning a score to every set of features of size \(k\) \((31, 32)\). In contrast, our partition does not prespecify a set size, nor demands a constant size for each separable set. It relies on the data structure to create sets that yield a consistent feature importance score. Separable sets also possess the advantage that common feature importance scores unify on them, dismissing the need to select a certain score. The number of separable sets is bounded by the number of features, therefore avoiding the complexity associated with presenting \(\binom{|\mathcal{F}|}{k}\) scores to the user. However, we do not present an explicit way to re-partition the feature space into separable sets. Achieving such a re-partition, or at least the maximal partition, may prove to be of high computational complexity. Future work should explore methods of finding and optimizing the partition of the feature space into separable sets.

We do not argue that we have defined the only possible set of relevant properties for the various settings. We did, however, attempt to define a minimal set of properties that we believe are essential.
Yet, even these requirements led to inconsistencies. It could be argued that the inconsistencies we identified are invalid, because our assumptions are flawed. For example, the assumptions made by Catav et al. (7) may not be convincing. Or, the assumption that the global score matches the expectancy of the local score is not a proper way to establish consistency between the settings. Despite these potential pitfalls, we believe that our work contains theoretical developments that integrate previously isolated concepts of feature importance scores.

Our results show that feature importance scores should be used cautiously, responsibly and ethically, to prevent naive researchers and users from reaching incorrect conclusions. This is aligned with recent research that tries to measure the quality of explainability tools and their usefulness for different applications (33; 34; 35). A possible negative consequence of this study might be attenuating the trust in explainable AI. However, our work promotes substantive discussions and accurate definitions of explainability, as previously advocated (21; 17). We hope that our work will contribute to stimulating additional research that will result in solid foundations for explainable AI.

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A Appendix

A.1 Properties of the data setting

In this section we attach the settings from Catav et al. (7), which we followed in the definition of the data-global setting.

The properties use the Elimination operation, which is defined as follows:

Definition A.1 Let $\mathcal{F}$ be a set of features and $\nu$ be a value-function. Eliminating the set $T \subset \mathcal{F}$ creates a new set of features $\mathcal{F}' = \mathcal{F} \setminus T$ and a new value-function $\nu' : \mathcal{F}' \to \mathbb{R}^+$ such that $\forall S \subseteq \mathcal{F}', \nu'(S) = \nu(S)$

Using this definition, the set of required properties is as follows:

Definition A.2 A valid feature importance function $\phi(\nu)$ in the data-global setting is a function $\phi : 2^{\mathcal{F}} \to \mathbb{R}^+$ that has the following properties:

1. **Marginal Contribution:** The importance of a feature is equal or higher than the increase in the evaluation function when adding it to all the other features, i.e.
   $$\phi(\nu, f) \geq \nu(\mathcal{F}) - \nu(\mathcal{F} \setminus f).$$

2. **Elimination:** Eliminating features from $\mathcal{F}$ can only decrease the importance of each feature. i.e., if $T \subseteq \mathcal{F}$ and $\nu'$ is the value-function which is obtained by eliminating $T$ from $\mathcal{F}$ then
   $$\forall f \in \mathcal{F} \setminus T, \phi(\nu, f) \geq \phi(\nu', f).$$

3. **Minimalism:** If $\phi(\nu)$ is the feature importance function, then for every function $\phi' : 2^{\mathcal{F}} \to \mathbb{R}^+$ for which axioms 1 and 2 hold, and for every $f \in \mathcal{F}$:
   $$\phi(\nu, f) \leq \phi'(\nu, f).$$

A.2 Proofs for Lemmas

When proving the inconsistency between the local and the global settings, we used two lemmas. The first lemma stated that if the consistency holds between the local and the global, then the local function is identical to the global function. The second lemma stated that if the consistency holds, then the global function is linear. The proof for these lemmas appears below:

Proof. [of Lemma 1]

Assume, in contradiction, that $\exists x \in \mathcal{X}$ s.t $\phi_g(\nu_x) \neq \phi_l(\nu_x)$. It holds that
$$\phi_g(\nu_x) = \phi_g(\mathbb{E}[\nu_x]) = \mathbb{E}[\phi_l(\nu_x)]$$

We construct a new sample space $\mathcal{X}_x$ comprised solely of duplicates of $x$, i.e $\forall x \in \mathcal{X}_x, \nu_x \equiv \nu_g$. It implies that $\forall x' \in \mathcal{X}_x,$
$$\phi_g(\nu_x') = \phi_l(\nu_x')$$

in contradiction to our assumption. \qed

Proof. [of Lemma 2]

Let $\alpha \in [0, 1]$, and let $x_1, x_2 \in \mathcal{X}$. We construct a new sample space $\mathcal{X}_{1,2}$ s.t consisting of $\alpha \cdot |\mathcal{X}_{1,2}|$ duplicates of $x_1$ and $(1 - \alpha) \cdot |\mathcal{X}_{1,2}|$ duplicates of $x_2$. it holds that
$$\alpha \cdot \phi_g(\nu_{x_1}) + (1 - \alpha) \cdot \phi_g(\nu_{x_2}) = \mathbb{E}[\phi_l(\nu_x)]$$
$$\alpha \cdot \phi_l(\nu_{x_1}) + (1 - \alpha) \cdot \phi_l(\nu_{x_2}) = \mathbb{E}[\phi_l(\nu_x)]$$

where (2) is valid by lemma 1, (3) and (5) are valid by the expected value of $\mathcal{X}_{1,2}$, and (4) is valid by the consistency property. \qed
A.3 Counter example for Theorem 1

This counter-example proves that MCI is not a linear function, thus leading to a contradiction between the definitions of the data-global setting and the lemma that proved that the global function is linear. In doing so, we demonstrate a contradiction to the claim of consistency between the local and the global settings.

\[
\alpha \cdot \text{MCI}(\nu_{x_1}) + (1 - \alpha) \cdot \text{MCI}(\nu_{x_2}) \neq \text{MCI}(\alpha \cdot \nu_{x_1} + (1 - \alpha) \cdot \nu_{x_2})
\]  

(6)

Let \( \alpha = \frac{1}{2} \) and let \( x_0, x_1 \in X_{1,2} \) be a dataset of instances composed of two features \( f_0, f_1 \) such that

\[
\nu_{x_0} := \begin{pmatrix} \{\emptyset\} := 0 \\ \{f_0\} := 0 \\ \{f_1\} := 2 \end{pmatrix}, \quad \nu_{x_1} := \begin{pmatrix} \{\emptyset\} := 0 \\ \{f_0\} := 1 \\ \{f_1\} := 1 \end{pmatrix}.
\]

On one hand,

\[
\frac{1}{2} \cdot \text{MCI}\left( \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix} \right) + \frac{1}{2} \cdot \text{MCI}\left( \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \right) = \frac{1}{2} \cdot \left( \begin{pmatrix} 1 \\ 2 \end{pmatrix} \right) + \frac{1}{2} \cdot \left( \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right) = \left( \begin{pmatrix} 1 \\ 1.5 \end{pmatrix} \right)
\]

On the other hand,

\[
\text{MCI}\left( \frac{1}{2} \cdot \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix} + \frac{1}{2} \cdot \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \right) = \text{MCI}\left( \begin{pmatrix} 0 \\ 1 \\ 1.5 \end{pmatrix} \right) = \left( \begin{pmatrix} 0.5 \\ 1 \end{pmatrix} \right)
\]

Hence, we found a counter example consistent with (6), which contradicts the linearity of MCI.

A.4 Proofs for Lemmas [3][4] and [5]

In proving that there exists a maximal and unique partitioning of \( \mathcal{F} \) into separable sets, we used three lemmas: The first lemma stated that if a set is a separable set, then so is its complement. The second lemma stated that if two sets are separable, so is their union. The third lemma stated that for two separable sets, their intersection is also a separable set. The proofs for the lemmas appear below:

Proof. [of Lemma 3]

The proof follows immediately from the definition. \( \square \)

Proof. [of Lemma 4]

For a set \( T, S_1, S_2 \subseteq \mathcal{F} \) it holds that

\[
\nu(T) = \nu(T \cap S_1) + \nu(T \setminus S_1) = \nu(T \cap S_1) + \nu((T \setminus S_1) \cap S_2) + \nu((T \setminus S_1) \cup S_2)
\]

\[
\nu(T \cap (S_1 \cup S_2)) = \nu(T \cap (S_1 \cup S_2) \cap S_1) + \nu(T \cap (S_1 \cup S_2) \setminus S_1) = \nu(T \cap S_1) + \nu(T \setminus S_1) \cap S_2)
\]

Therefore,

\[
\nu(T) = \nu(T \cap S_1) + \nu((T \setminus S_1) \cap S_2) + \nu((T \setminus S_1) \setminus S_2) = \nu(T \cap (S_1 \cup S_2)) + \nu(T \setminus (S_1 \cup S_2))
\]

\( \square \)

Proof. [of Lemma 5]

From Lemmas 3-4 we have that \((\mathcal{F} \setminus S_1) \cup (\mathcal{F} \setminus S_2)\) is a separable set.

By the fact that \((\mathcal{F} \setminus S_1) \cup (\mathcal{F} \setminus S_2) = \mathcal{F} \setminus (S_1 \cap S_2)\) we get that \(\mathcal{F} \setminus (S_1 \cap S_2)\) is a separable set.

Using Lemma 1 again, we get that \(S_1 \cap S_2\) is a separable set, as required. \( \square \)
A.5 Toy example of separable sets

Here, we illustrate the effects of assigning importance scores to separable sets in the data-global setting. We construct an example in which different feature importance methods disagree on the importance of features. Then, we partition the feature space into separable sets. Consequently, the different feature importance methods merge when applied to these separable sets.

We take the value-function to be the coefficient of determination of a linear regression model without an intercept, i.e.
\[
∀S \subseteq F, ν(S) = 1 - \sum_i(y_i^S - y_i)^2 / \sum_i y_i^2,
\]
where \(y_i^S\) is the prediction for instance \(y_i\) restricted to the feature subset \(S\). This is a common metric of assessing a model’s fit to a continuous target variable.

Assume the world consists of three features, determining the target variable:
\[y = f_1 + f_3 + U.\]
Also, assume that we observe only \(f_1, f_2, f_3\), while \(U\) is a source of unexplained variance. We consider the following dataset:

|   | \(f_1\) | \(f_2\) | \(f_3\) | \(U\) |
|---|---|---|---|---|
| \(x_1\) | 1 | 1 | -1 | \(\sqrt{\frac{1}{6}}\) |
| \(x_2\) | 1 | 1 | 0 | \(\sqrt{\frac{2}{3}}\) |
| \(x_3\) | 1 | 1 | 1 | \(\sqrt{\frac{1}{6}}\) |

Note that these features were selected to be orthogonal, besides \(f_1\) and \(f_2\) which are duplicates.

For the observed feature space, the value-function is as follow:
\[
ν(S) = \begin{cases} 
0, & S = \emptyset \\
\frac{1}{2}, & S = \{f_1\} \\
\frac{1}{2}, & S = \{f_2\} \\
\frac{1}{3}, & S = \{f_3\} \\
\frac{5}{6}, & S = \{f_1, f_3\} \\
\frac{5}{6}, & S = \{f_2, f_3\} \\
\frac{5}{6}, & S = \{f_1, f_2, f_3\} 
\end{cases}
\]

Therefore, we can easily see that the common methods for calculating feature importance produce different results:
- Ablation assigns each of the duplicates features \(f_1, f_2\) with zero importance.
- For Shapley, each duplicate feature has a non-zero importance, but as we introduce more duplicates, their importance decreases.
- The bivariate feature importance and MCI assign \(\frac{1}{2}\) importance to each of the duplicate features, and do not change this value upon introduction of additional duplicates.

On the other hand, we can see that \(\{f_1, f_2\}\) and \(f_3\) are separable sets w.r.t \(ν\). By partitioning the feature space into \(G := \{\{f_1, f_2\}, f_3\}\), all the feature importance functions mentioned above yield
\[
φ(ν, g) = \begin{cases} 
\frac{1}{2}, & g = \{f_1, f_2\} \\
\frac{1}{3}, & g = f_3
\end{cases}
\]

A.6 Additional properties

In this work we presented a framework that consist of a small set of properties for the various settings of feature importance. For the sake of completeness, we present here additional properties that were not required for our results, but might be useful for future work:

Definition A.3 (Empty-Set Value) \(ν(\emptyset) = 0\)
The Empty-Set Value property is a technical property that aims to prevent edge cases.

**Definition A.4 (Monotonicity)** The Monotonicity property holds if:

- \( \forall S_1, S_2 \subseteq \mathcal{F} \text{ s.t } S_2 \subseteq S_1, \text{ it holds that } \nu_g(S_2) \leq \nu_g(S_1) \)

The Monotonicity property states that the value in the global setting of each subset is less than or equal to the value of each set in which it is contained.

Notice that the Monotonicity property is defined only for the global setting. There are cases where the value of a local instance might not be monotonic. Also, we observe that Empty-set Value and Monotonicity imply non-negativity for the value-function in the global setting.

**Definition A.5 (Symmetry)** The symmetry property holds if \( \forall f_1, f_2 \in \mathcal{F} \):

- If \( \forall S \subseteq \mathcal{F} \setminus z \text{ it holds that } \nu(S \cup \{f_1\}) = \nu(S \cup \{f_2\}) \) then 
  \[ \phi(\nu, f_1) = \phi(\nu, f_2) \]

where \( z \) can be defined as \( \emptyset \) or \( \{f_1, f_2\} \).

The Symmetry property states that if two features are identical in their contribution to each subset with respect to the value, their importance should be identical. Using \( z \) one can define two different definitions of symmetry, both of which are accepted in the literature.

**Corollary 1 (Triviality)** The Triviality property implies that \( \forall f \in \mathcal{F} \):

- If \( \forall S \subseteq \mathcal{F}, \nu(S \cup f) = \nu(S) \) then \( \phi(\nu, f) = 0 \)

This corollary to the Triviality property aims to emphasize an important trait of this property.

**Definition A.6 (Separable Importance)** The separable importance property consists of two parts:

1. If \( S \) is a separable set w.r.t \( \nu \), then \( \forall f \in \mathcal{F}, \phi(\nu, f) = \phi^S(\nu, f) + \phi^{\mathcal{F} \setminus S}(\nu, f) \)

2. If \( \forall f \in \mathcal{F}, \phi(\nu, f) = \phi^S(\nu, f) + \phi^{\mathcal{F} \setminus S}(\nu, f) \) then \( S \) is a separable set w.r.t \( \nu \).

where \( \phi^S \) denotes the feature importance function restricted to the subset \( S \).

The first item of the Separable Importance property claims that if a set is separable, the importance function can also be separated with respect to this set. The second item of the Separable Importance property states that if the importance function can be separated with respect to a set, this set is a separable set.