The Explanation Game: Explaining Machine Learning Models with Cooperative Game Theory

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Abstract

Recently, a number of techniques have been proposed to explain a machine learning (ML) model’s prediction by attributing it to the corresponding input features. Popular among these are techniques that apply the Shapley value method from cooperative game theory. While existing papers focus on the axiomatic motivation of Shapley values, and efficient techniques for computing them, they do not justify the game formulations used. For instance, we find that the SHAP algorithm’s formulation (Lundberg and Lee 2017) may give substantial attributions to features that play no role in a model. In this work, we study the game formulations underpinning several existing methods. Using a series of simple models, we illustrate how their subtle differences can yield large differences in attribution for the same prediction. We then present a general game formulation that unifies existing methods. After discussing the primitive of single-reference games, we decompose the Shapley values of the general game formulation into Shapley values of single-reference games. This is instructive in several ways. First, it enables confidence intervals on estimated attributions, which are not offered by previous works. Second, it enables different contrastive explanations of a prediction through comparisons with different groups of reference inputs. We tie this idea to classic work on Norm Theory (Kahneman and Miller 1986) in cognitive psychology, and propose a general framework for generating explanations for ML models, called formulate, approximate, and explain (FAE). We apply this framework to explaining black-box models trained on two UCI datasets and a Lending Club dataset.

1 Introduction

Complex machine learning (ML) models are rapidly spreading to high-stakes tasks such as credit scoring, underwriting, medical diagnosis, and crime prediction. Consequently, it is becoming increasingly important to interpret and explain individual model predictions to decision-makers, end-users, and regulators. A common form of model explanations are based on feature attributions, wherein a score (attribution) is ascribed to each feature in proportion to the feature’s contribution to the prediction. Over the last few years there has been a surge in feature attribution methods, with methods based on Shapley values from cooperative game theory being prominent among them.

Shapley values (Shapley 1953) provide a mathematically fair and unique method to attribute the payoff of a cooperative game to the players of the game. Due to its strong axiomatic guarantees, the Shapley values method is emerging as the de facto approach to feature attribution, and some researchers even speculate that it may be the only method compliant with legal regulation such as GDPR’s “right to an explanation” (Aas, Jullum, and Løland 2019).

We begin by studying several Shapley-value-based explanation algorithms: TreeSHAP (Lundberg, Erion, and Lee 2018), KernelSHAP (Lundberg and Lee 2017), QII (Datta, Sen, and Zick 2016), and IME (Strumbelj and Kononenko 2010). Paradoxically, while all of these techniques lay claim to the axiomatic uniqueness of Shapley values, we discover that they yield significantly different attributions even when evaluated exactly (without approximation). Although these techniques offer the axiomatic motivations of Shapley values and efficient algorithms for computing them, they do not clearly justify the various explanation game formulations (which we term explanation games) that they rely upon. We find that as a result, these techniques can yield counter-intuitive attributions even on simple toy models. For instance, in Section 3 we show a simple model for which the popular SHAP method gives substantial attribution to a feature that is mathematically irrelevant to the model function. We show mathematically that this is a shortcoming of the explanation game formulated by SHAP.

We next pursue a fundamental understanding of how to formulate explanation games whose Shapley values admit meaningful and relevant explanations. To this end, we first unify KernelSHAP, QII, and IME with a general game formulation parameterized by a single probability distribution. We decompose the Shapley values of this general game formulation into the Shapley values of single-reference games that model a feature’s absence by replacing its value with the corresponding value from a specific counterfactual reference input. This decomposition is instructive in several ways.

First, it allows us to efficiently compute confidence intervals and other supplementary information about attributions, a notable advancement over existing methods (which lack confidence intervals even though they approximate metrics of random variables using finite samples). Second, it offers conceptual clarity. We interpret the (decomposed) feature attributions using the lens of Norm Theory, a clas-
sic work in cognitive psychology. Leveraging insights from Norm Theory, we develop a general formulate, approximate, and explain (FAE) framework to create Shapley-value-based feature attributions that are not only axiomatically justified, but also relevant and meaningful to the humans who consume them. Notably, the FAE framework allows us to contrastively explain a model prediction relative to a chosen group of reference inputs. To illustrate these ideas, we present case studies explaining the predictions of models trained on two UCI datasets (Bike Sharing and Adult Income) and a Lending Club dataset. We find that in these real-world situations, explanations generated using our FAE framework uncover important patterns that previous attribution methods cannot identify.

In summary, we make the following key contributions:

- We highlight several shortcomings of existing Shapley-value-based feature attribution methods (Sections 3), and analyze the root cause of these issues (Section 4.1).
- We present a novel game formulation that unifies and illuminates existing methods, and leverage it to provide confidence bounds and other supplemental information for existing methods (Section 4.2).
- We combine our formulation with principles from Norm Theory (Kahneman and Miller 1986) to establish the formulate, approximate, and explain (FAE) framework (Section 5), and demonstrate noticeable improvements over the prior art through case studies (Section 6).

## 2 Preliminaries

### 2.1 Additive Feature Attributions

Additive feature attributions (Lundberg and Lee 2017) are attributions that sum to the difference between the explained model output \( f(x) \) and a reference output value \( \phi_0 \). In practice, \( \phi_0 \) is typically an average model output or model output for a domain-specific “baseline” input (e.g. an empty string for text sentiment classification).

**Definition 1 (Additive Feature Attributions)** Suppose \( f : \mathcal{X} \rightarrow \mathbb{R} \) is a model mapping an \( M \)-dimensional feature space \( \mathcal{X} \) to a real-valued prediction. Additive feature attributions for \( f(x) \) at input \( x = (x_1, \ldots, x_M) \in \mathcal{X} \) comprise of a reference (or baseline) attribution \( \phi_0 \) and feature attributions \( \phi_1, \phi_2, \ldots, \phi_M \) corresponding to the \( M \) features such that \( f(x) = \phi_0 + \sum_{i=1}^{M} \phi_i \).

There currently exist a number of competing methodologies for computing these attributions (see (Ancona et al. 2018)). Given the difficulty of empirically evaluating attributions, several methods offer an axiomatic justification, often through the Shapley values method.

### 2.2 Shapley Values

The Shapley values method is a classic technique from game theory that fairly attributes the total payoff from a cooperative game to the game’s players (Shapley 1953). Recently, this method has found numerous applications in explaining ML models (e.g. (Cohen, Ruppin, and Dror 2005; Lundberg and Lee 2017; Ghorbani and Zou 2019)).

| \( x_{male} \) | \( x_{lift} \) | \( \Pr\{X = x\} \) | \( f_{male}(x) \) | \( f_{both}(x) \) |
|---|---|---|---|---|
| 0 | 0 | 0.1 | 0.0 | 0.0 |
| 0 | 1 | 0.0 | 0.0 | 0.0 |
| 1 | 0 | 0.4 | 1.0 | 0.0 |
| 1 | 1 | 0.5 | 1.0 | 1.0 |

Table 1: Probability mass function and model outputs for the mover hiring system example.

Formally, a cooperative game between a set of players \( \mathcal{M} = \{1, \ldots, M\} \) is characterized by a set function \( v : 2^\mathcal{M} \rightarrow \mathbb{R} \) such that \( v(S) \) is the payoff for any subset of players \( S \subseteq \mathcal{M} \), and \( v(\emptyset) = 0 \). Shapley values are built by examining the marginal contribution of a player to an existing subset \( S \), i.e., \( v(S \cup \{i\}) - v(S) \). The Shapley value of a player \( i \), denoted \( \phi_i(v) \), is a certain weighted aggregation of its marginal contribution to all possible subsets of players:

\[
\phi_i(v) = \frac{1}{M} \sum_{S \subseteq \mathcal{M} \setminus \{i\}} \left( \frac{M - 1}{|S|} \right)^{-1} (v(S \cup \{i\}) - v(S)) \tag{1}
\]

The Shapley value method is the unique method satisfying four desirable axioms: Dummy, Symmetry, Efficiency, and Linearity. We informally describe the axioms in the Supplemental Material, and refer the reader to (Young 1985) for formal definitions and proofs. The rest of this paper deals with the application of Shapley values to model explanation, focusing on game formulation rather than the Shapley value method itself.

## 3 A Motivating Example

To probe existing Shapley-value-based model explanation methods, we evaluate them on two toy models for which it is easy to intuit correct attributions. We leverage a modified version of the example provided in (Datta, Sen, and Zick 2016): a system that recommends whether a moving company should hire a mover applicant. Models consider an input vector of the binary features “is male” and “is good lifter” (notated \( x = (x_{male}, x_{lift}) \)), and output a recommendation score between 0 (“no hire”) and 1 (“hire”). We define \( f_{male}(x) := f_{male}(x_{male}) \) (only hire males), and \( f_{both}(x) := f_{male}(x) \wedge f_{lift}(x_{lift}) \) (only hire males who are good lifters). Table 1 specifies a probability distribution over the input space, along with the predictions from the two models.

Consider the input \( x = (1, 1) \) (i.e. a male who is a good lifter), for which both models output a recommendation score of 1. Table 2 lists these predictions’ attributions from several existing methods. Focusing on the relative attribution between \( x_{male} \) and \( x_{lift} \) (ignoring for now the magnitude of the attributions and the reference term \( \phi_0 \)), we make the following surprising observations. First, even though \( x_{lift} \) is irrelevant to \( f_{male} \), the popular SHAP algorithm results in equal attribution to both features, contradicting our intuition around the Dummy axiom of Shapley values. Additionally, these SHAP attributions are misleading from a fairness perspective: \( f_{male} \) relies solely on \( x_{male} \), yet the attributions

\[\text{As defined by Equation 9 in (Lundberg and Lee 2017).}\]
downplay this gender bias by claiming the model uses both features equally. Second, although \( f_{\text{both}} \) treats its features symmetrically and \( x \) has identical values in both its features, many of the methods considered do not provide symmetrical attributions. This again is intuitively at odds with the Shapley value axioms, as Symmetry appears to be violated. These unintuitive behaviors surfaced by the above observations demand an in-depth study of these methods’ internal design choices. We carry out this study in the next section.

\section{Explanation Games}

In order to explain a model prediction with the Shapley values method, it is necessary to formulate a cooperative game with players that correspond to the features and a payoff that corresponds to the prediction. In this section, we analyze the methods examined in Section 3 and show that their surprising attributions are an artifact of their game formulations. We then discuss a unified game formulation and its decomposition to single-reference games, enabling conceptual clarity about the meanings of existing methods’ attributions.

**Notation.** Let \( D_{\text{inp}} \) be the input distribution, which characterizes the process that generates model inputs. We denote the input of an explained prediction as \( x = (x_1, \ldots, x_M) \) and use \( r \) to denote another “reference” input. We use boldface to indicate when a variable or function is vector-valued, and we use capital letters for random variable inputs (although \( S \) continues to represent the set of contributing players/features). Thus, \( x_i \) is a scalar input, \( x \) is an input vector, and \( X \) is a random input vector. We use \( x_S = \{x_i, i \in S\} \) to represent a sub-vector of features indexed by \( S \). Lastly, we introduce the composite input \( z(x, r, S) \), which agrees with the input \( x \) on all features in \( S \) and with \( r \) on all features not in \( S \). Note that \( z(x, r, \emptyset) = r \), and \( z(x, r, M) = x \).

\[ z(x, r, S) = (z_1, z_2, \ldots, z_M), \text{ where } z_i = \begin{cases} x_i & \text{if } i \in S \\ r_i & \text{if } i \notin S \end{cases} \]  

\subsection{Existing Game Formulations}

The explanation game payoff function \( \nu_x \) must be defined for every feature subset \( S \) such that \( \nu_x(S) \) captures the contribution of \( x_S \) to the model’s prediction. This allows us to compute each feature’s possible marginal contributions to the prediction and derive its Shapley value (see Section 2). By the definition of additive feature attributions (Definition 1) and the Shapley values’ Efficiency axiom, we must define \( \nu_x(M) = f(x) - \phi_0 \) (i.e., the payoff of the full coalition must be the difference between the explained model prediction and a baseline prediction). Although this definition is fixed, it leaves us the challenge of coming up with the payoff when some features do not contribute (that is, when they are absent). We find that all existing approaches handle this feature-absent payoff by randomly sampling absent features according to a particular counterfactual reference distribution and then computing the expected value of the prediction. The resulting game formulations differ from one another only in the counterfactual distribution they use.

**Conditional Distribution.** The game formulation of SHAP \cite{lundberg2017consistent}, TreeSHAP \cite{lundberg2017unified}, and \{Aas, Jullum, and Løland 2019\} simulates feature absence by sampling absent features from the input distribution conditional on knowing the values of the present (or contributing) features:

\[ \nu_x^{\text{Cond}}(S) = \mathbb{E}_{R \sim D_{\text{inp}}} [f(z(x, R, S)) | R_S = x_S] - \mathbb{E}_{R \sim D_{\text{inp}}} [f(R)] \]  

Unfortunately, this formulation does not properly simulate the absence of a feature. This flaw explains why the irrelevant feature \( x_{\text{lift}} \) receives a nonzero attribution in the \( f_{\text{male}} \) example from Section 3. Specifically, since the event \( x_{\text{male}} = 1 \) is correlated\footnote{Here correlation refers to any statistical dependence, not just a nonzero Pearson correlation coefficient.} with \( x_{\text{lift}} = 1 \), once \( x_{\text{lift}} = 1 \) is given, the expected prediction becomes 1. This causes the \( x_{\text{lift}} \) feature to have a non-zero marginal contribution (relative to when both features are absent), and therefore a nonzero Shapley value. More generally, whenever a feature is correlated with a model’s prediction on inputs drawn from \( D_{\text{inp}} \), this game formulation results in non-zero attribution to the feature regardless of whether the feature causally impacts the prediction.

**Input Distribution.** Another option for simulating feature absence, which is used by KernelSHAP, is to sample absent features from the corresponding marginal distribution in \( D_{\text{inp}} \):

\[ \nu_x^{\text{marg}}(S) = \mathbb{E}_{R \sim D_{\text{inp}}} [f(z(x, R, S))] - \mathbb{E}_{R \sim D_{\text{inp}}} [f(R)] \]  

Since this formulation breaks correlation with the contributing features, it ensures irrelevant features receive no attribution (e.g., no attribution to \( x_{\text{lift}} \) when explaining \( f_{\text{male}}(1, 1) = 1 \)). We formally describe this property via the Insentivity axiom in Section 4.2.

Unfortunately, this formulation is still subject to artifacts of the input distribution, as evident from the asymmetrical

| Payoff formulation         | \( \phi_0 \) (baseline) | \( f_{\text{male}} \) | \( \phi_2 \) (lifting) | \( \phi_0 \) (baseline) | \( f_{\text{both}} \) | \( \phi_1 \) (male) | \( \phi_2 \) (lifting) |
|----------------------------|-------------------------|----------------------|----------------------|-------------------------|-------------------------|----------------------|----------------------|
| SHAP (Conditional Distribution) | 0.9                     | 0.05                 | 0.05                 | 0.50                    | 0.028                    | 0.472                 |                      |
| KernelSHAP (Input Distribution) | 0.9                     | 0.10                 | 0.00                 | 0.50                    | 0.050                    | 0.450                 |                      |
| QII (Joint Marginal Distribution) | 0.9                     | 0.10                 | 0.00                 | 0.45                    | 0.075                    | 0.475                 |                      |
| IME (Uniform Distribution)   | 0.5                     | 0.50                 | 0.00                 | 0.25                    | 0.375                    | 0.375                 |                      |

\textbf{Table 2: Attributions for the input } x_{\text{male}} = 1, x_{\text{lift}} = 1.
attributions when explaining the prediction \( f_{\text{both}}(1, 1) = 1 \) (see Table 2). The features receive different attributions because they have different marginal distributions in \( D^{\text{inp}} \), not because they impact the model differently.

**Joint-Marginal Distribution.** QII (Datta, Sen, and Zick 2016) simulates feature absence by sampling absent features one at a time from their own univariate marginal distributions. In addition to breaking correlation with the contributing features, this breaks correlation between absent features as well. Formally, the QII formulation uses a distribution we term the “joint-marginal” distribution \( (D^{J,M}) \), where:

\[
\Pr_{X \sim D^{J,M}} [X = (x_1, \ldots, x_M)] = \prod_{i=1}^{M} \Pr_{X_i \sim D^{\text{inp}}} [X_i = x_i]
\]

The joint-marginal formulation \( v_x^{J,M} \) is similar to \( v_x^{\text{inp}} \), except that the reference distribution is \( D^{J,M} \) instead of \( D^{\text{inp}} \):

\[
v_x^{J,M}(S) = \mathbb{E}_{R \sim D^{J,M}} [f(z(x, R, S))] - \mathbb{E}_{R \sim D^{\text{inp}}} [f(R)]
\]

Unfortunately, like \( v_x^{\text{inp}} \), this game formulation is also tied to the input distribution and under-attributes features that take on common values in the background data. This is evident from the attributions for the \( f_{\text{both}} \) model shown in Table 2.

**Uniform Distribution.** The last formulation we study simulates feature absence by drawing values from a uniform distribution \( \mathcal{U} \). Completely ignoring the input distribution, this payoff \( v_x^{\text{uni}} \) considers all possible feature values (edge-cases and common cases) with equal weighting.

\[
v_x^{\text{uni}}(S) = \mathbb{E}_{R \sim \mathcal{U}} [f(z(x, R, S))] - \mathbb{E}_{R \sim \mathcal{U}} [f(R)]
\]

In Table 2, we see that this formulation yields intuitively correct attributions for \( f_{\text{male}} \) and \( f_{\text{both}} \). However, the uniform distribution can sample so heavily from irrelevant outlier regions of \( \mathcal{X} \) that relevant patterns of model behavior become masked (we study the importance of relevant references both theoretically in Section 5.1 and empirically in Section 6).

### 4.2 A Unified Formulation

We observe that the existing game formulations \( v_x^{\text{inp}}, v_x^{J,M}, \) and \( v_x^{\text{uni}} \) can be unified as a single game formulation \( v_x^{\mathcal{U}} \) that is parametric on the reference distribution \( \mathcal{D} \):

\[
v_x^{\mathcal{U}}(S) = \mathbb{E}_{R \sim \mathcal{D}} [f(z(x, R, S))] - \mathbb{E}_{R \sim \mathcal{D}} [f(R)]
\]

For instance, the formulation for KernelSHAP is recovered when \( \mathcal{D} = D^{\text{inp}} \), and QII is recovered when \( \mathcal{D} = D^{J,M} \). In the rest of this section, we discuss several properties of this general formulation that help us better understand its attributions. Notably, the formulation \( v_x^{\text{cond}} \) cannot be expressed in this framework; we discuss the reason for this later.

\footnote{It is somewhat unclear whether IME proposes \( \mathcal{U} \) or \( D^{\text{inp}} \), as (Strumbelj and Kononenko 2010) assumes \( D^{\text{inp}} = \mathcal{U} \), while (Strumbelj and Kononenko 2014) calls for values to be sampled from \( \mathcal{X} \) “at random.”}

### A Decomposition in Terms of Single-Reference Games

We now introduce single-reference games, a conceptual building block that helps us interpret the Shapley values of the \( v_x^{r,D} \) game. A single-reference game \( v_x^{r,D} \) simulates feature absence by replacing the feature value with a counterfactual value from a specific reference input \( r \):

\[
v_x^{r,D}(S) = f(z(x, r, S)) - f(r)
\]

The attributions from a single-reference game explain the difference between the prediction for the input and the prediction for the reference (i.e. \( \sum_i \phi_i(v_x^{r,D}) = v_x^{r,D}(M) = f(z(x) - f(r)) \)). Computing attributions relative to a single reference point (also referred to as a “baseline”) is common to several others methods (Sundararajan, Taly, and Yan 2017) [Shrikumar, Greenside, and Kundaje 2017] [Dhurandhar et al. 2018] [Ancona, Oztireli, and Gross 2019]. However, while those works seek a neutral “informationless” reference (e.g. an all-black image for image models), we find it beneficial to consider arbitrary references and interpret the resulting attributions relative to the reference. We develop this idea further in our FAE framework (see Section 5).

We now state Lemma 1 which shows how the Shapley values of \( v_x^{\mathcal{U}} \) can be expressed as the expected Shapley values of a (randomized) single-reference game \( v_x^{r,D} \) where \( \mathcal{D} = \mathcal{R} \). The proof (given in full in the Supplemental Material) follows from the Shapley values’ Linearity axiom and the linearity of expectation.

**Lemma 1** \( \phi(v_x^{\mathcal{U}}) = \mathbb{E}_{R \sim \mathcal{D}} [\phi(v_x^{r,D})] \)

Despite its mathematical simplicity, Lemma 1 brings conceptual clarity and practical improvements (confidence intervals and supplementary metrics) to existing methods. For instance, through this lemma we can contrast the attributions from existing games \( (v_x^{\text{inp}}, v_x^{J,M}, \text{and } v_x^{\text{uni}}) \) as different weighted aggregations of attributions from a space of single-reference games. While \( v_x^{\text{uni}} \) weighs attributions relative to all reference points equally, \( v_x^{r,D} \) weights them using the input distribution \( D^{\text{inp}} \).

### Insensitivity Axiom

**Insensitivity Axiom.** We show that attributions from the game \( v_x^{\mathcal{U}} \) satisfy the Insensitivity axiom from (Sundararajan, Taly, and Yan 2017), which states that a feature that is mathematically irrelevant to the model must receive zero attribution. Formally, a feature \( i \) is irrelevant to a model \( f \) if for any input, changing the feature does not change the model output. That is, \( \forall x, r \in \mathcal{X} : x_{M\setminus{i}} = r_{M\setminus{i}} \implies f(x) = f(r) \).

**Lemma 2** If a feature \( i \) is irrelevant to a model \( f \) then \( \phi_i(v_x^{\mathcal{U}}) = 0 \) for all distributions \( \mathcal{D} \).

The proof (given in the Supplemental Material) is based on showing that the axiom is obeyed by all single-reference games, and therefore by Lemma 1 is also obeyed by \( v_x^{\mathcal{U}} \) games. Notably, the \( v_x^{\text{cond}} \) formulation does not obey the Insensitivity axiom (a counter-example being the \( f_{\text{male}} \) attributions from Section 3). Accordingly, our general formulation (Equation 5) cannot express this formulation. In the rest
of the paper, we focus on game formulations that satisfy the Insensitivity axiom.

Confidence Intervals On Attributions. Existing game formulations involve computing an expected value in every invocation of the payoff function. In practice, this expectation is approximated via sampling, which introduces uncertainty. However, none of the existing methods except (Štrumbelj and Kononenko 2010) discuss confidence intervals for the attributions they provide. The decomposition in Lemma 1 shows that the attributions themselves can be expressed as an expectation over (deterministic) attributions from a distribution of single-reference games. Consequently, one can approximate the expectation by computing the mean attribution from a sample of single-reference games, and estimate confidence intervals (CIs) by estimating the standard error of the mean (SEM). In terms of the sample standard deviation (SSD), 95% CIs on the mean attribution ($\phi$) from a sample of size $N$ are given by

$$\phi \pm \frac{1.96 \times \text{SSD} (\{\phi (v_{n,x})\})}{\sqrt{N}}$$

The original formulations of these games do not lend themselves these CI estimates. While one could use bootstrap to obtain CIs, the SEM approach is more efficient as it requires no additional Shapley value computations.

5 A Framework For Model Explanations

In Section 4, we noted that existing Shapley value feature attribution methods can yield misleading and unintuitive attributions. In Section 4.1, we traced these issues to the game formulations that these methods use. We are now left with the question: How do we formulate better explanation games that yield meaningful explanations? To understand how explanations acquire meaning, we turn to Norm Theory (Kahneman and Miller 1986), a classic work from cognitive psychology. Norm Theory describes the psychological norms which shape the emotional responses, social judgments, and explanations of humans. Using insights from Norm Theory and the unified game formulation from Section 4.2, we create a conceptual framework for feature attributions called formulate, approximate, and explain (FAE).

5.1 Norm Theory and Explanations

Explanations Are Contrastive. Every explanation seeks to answer a certain “why” question (for example, model explanations seek to answer the question “Why did the model make this prediction for this input?”). Kahneman and Miller posit that the interpretation of a “why” question implicitly refers to one or more counterfactual norms, stating “A why question indicates that a particular event is surprising and requests the explanation of an effect, denoted as a contrast between an observation and a more normal alternative.” Thus, our first insight from Norm Theory is that explanations are always contrastive, that is, they explain an event relative to one or more norms. In a single-reference game, the reference serves as the norm against which attributions explain the model prediction contrastively. For the $v_{\text{uni}}$ games, we see from Lemma 1 that norms are drawn from a distribution $\mathcal{D}$, and the resulting attributions (explanations) are averaged.

Different Norms May Lead to Different Explanations Norms vary across individuals, and consequently explanations vary as well. Therefore, explanations must always be interpreted relative to the chosen norm. In this sense, the choice of norm(s) or reference(s) is an important knob for obtaining different explanations. The following example Kahneman and Miller take from (Hart and Honoré 1985) illustrates this well: “A woman married to a man who suffers from an ulcerated condition of the stomach might identify eating parsnips as the cause of his indigestion. The doctor might identify the ulcerated condition as the cause and the meal as a mere occasion.” Here, both explanations are valid but differ since they are relative to different norms.

Norms Must Be Relevant. A second norm-theoretic principle we focus on is that norms (references) must be relevant to the question at hand. As (Hitchcock and Knobe 2009) note: “Our capacity for counterfactual reasoning seems to show a strong resistance to any consideration of irrelevant counterfactuals.” Without getting into the philosophical details of what “relevance” means for references, we motivate it using concrete examples. Consider the task of explaining why a bank’s model rejected a loan applicant. If low debt is a prerequisite for high credit score, then an example with high debt and high credit score is impossible, and therefore an irrelevant reference. We also recognize that other rejected applicants may be irrelevant references for the question of explaining a rejection. In fact, irrelevant references are the reason why the $v_{\text{uni}}$ game is problematic: sampling references from the uniform distribution can lead to contrasts against references that are impossible or otherwise irrelevant to the question at hand.

5.2 Formulate, Approximate, and Explain

We now introduce the formulate, approximate, and explain (FAE) framework to translate these ideas from Norm Theory into actionable steps for Shapley value model explanations.

Formulate. Since explanations are contrastive against relevant norms, we must first formulate a contrastive explanation question that specifies a relevant reference relative to which we shall obtain explanations. From Norm Theory, we know that different references may lead to different explanations. Consequently, one may wish to formulate multiple contrastive explanation questions. For each question, the goal is to pin down the input to be explained (x), and the reference distribution ($\mathcal{D}_{\text{ref}}$).

Approximate. Next we bring to bear the axiomatic power of Shapley values. In this step, we approximate the distribution of Shapley values from single-reference games whose

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\[\text{Explanations Are Contrastive. Every explanation seeks to answer a certain “why” question (for example, model explanations seek to answer the question “Why did the model make this prediction for this input?”). Kahneman and Miller posit that the interpretation of a “why” question implicitly refers to one or more counterfactual norms, stating “A why question indicates that a particular event is surprising and requests the explanation of an effect, denoted as a contrast between an observation and a more normal alternative.” Thus, our first insight from Norm Theory is that explanations are always contrastive, that is, they explain an event relative to one or more norms. In a single-reference game, the reference serves as the norm against which attributions explain the model prediction contrastively. For the $v_{\text{uni}}$ games, we see from Lemma 1 that norms are drawn from a distribution $\mathcal{D}$, and the resulting attributions (explanations) are averaged.}

\[\text{Different Norms May Lead to Different Explanations}

\[\text{Norms vary across individuals, and consequently explanations vary as well. Therefore, explanations must always be interpreted relative to the chosen norm. In this sense, the choice of norm(s) or reference(s) is an important knob for obtaining different explanations. The following example Kahneman and Miller take from (Hart and Honoré 1985) illustrates this well: “A woman married to a man who suffers from an ulcerated condition of the stomach might identify eating parsnips as the cause of his indigestion. The doctor might identify the ulcerated condition as the cause and the meal as a mere occasion.” Here, both explanations are valid but differ since they are relative to different norms.}

\[\text{Norms Must Be Relevant. A second norm-theoretic principle we focus on is that norms (references) must be relevant to the question at hand. As (Hitchcock and Knobe 2009) note: “Our capacity for counterfactual reasoning seems to show a strong resistance to any consideration of irrelevant counterfactuals.” Without getting into the philosophical details of what “relevance” means for references, we motivate it using concrete examples. Consider the task of explaining why a bank’s model rejected a loan applicant. If low debt is a prerequisite for high credit score, then an example with high debt and high credit score is impossible, and therefore an irrelevant reference. We also recognize that other rejected applicants may be irrelevant references for the question of explaining a rejection. In fact, irrelevant references are the reason why the $v_{\text{uni}}$ game is problematic: sampling references from the uniform distribution can lead to contrasts against references that are impossible or otherwise irrelevant to the question at hand.}

\[\text{5.2 Formulate, Approximate, and Explain}

\[\text{We now introduce the formulate, approximate, and explain (FAE) framework to translate these ideas from Norm Theory into actionable steps for Shapley value model explanations.}

\[\text{Formulate. Since explanations are contrastive against relevant norms, we must first formulate a contrastive explanation question that specifies a relevant reference relative to which we shall obtain explanations. From Norm Theory, we know that different references may lead to different explanations. Consequently, one may wish to formulate multiple contrastive explanation questions. For each question, the goal is to pin down the input to be explained (x), and the reference distribution ($\mathcal{D}_{\text{ref}}$).}

\[\text{Approximate. Next we bring to bear the axiomatic power of Shapley values. In this step, we approximate the distribution of Shapley values from single-reference games whose}
references are drawn from $D_{ref}$. Formally, we approximate the attribution distribution $\hat{\Phi}_{x,R} = \Phi(v_x,R)$, where $R \sim D_{ref}$. This involves two steps: (1) sampling a set of references $\{r_i\}_{i=1}^N$ from $D_{ref}$, and (2) estimating the Shapley values of each corresponding single-reference game.

For models with few features, it is possible to exactly compute the Shapley values of these games via Equation 1. For models with many features, however, the Shapley values must be approximated. Recently there has been much progress towards the efficient estimation of Shapley values. The details of these techniques are beyond the scope of this work, but we refer the reader to [Maleki et al. 2013; Chen et al. 2018; Aas, Jullum, and Løland 2019; Hunt et al. 2019; Ancona, Oztireli, and Gross 2019].

**Explain.** In the final step, we use our sampled Shapley value vectors to summarize $\hat{\Phi}_{x,R}$, and we present this summary in the context of the formulation. The summarization should also quantify uncertainty arising from the Approximate step. A simple summarization consists of the sample mean (approximating $\mathbb{E}[\hat{\Phi}_{x,R}]$), which is equivalent to the attributions from the games $v_x^{inp}$, $v_x^{J.M.}$, and $v_x^{unif}$. As discussed in Section 4.2, we can also report confidence intervals computed from the sample standard error of the mean.

A caveat with using the mean is that it may hide important information. For instance, a feature’s attributions may have opposite signs relative to different references. Averaging these will cause them to cancel each other out, yielding a small mean that incorrectly suggests the feature is unimportant. Thus, we recommend visualizing the sampled distribution of attributions and noting other patterns not captured by the mean. Additionally, in Section 6 we present examples of alternate summarizations based on clustering.

6 Case Studies

In this section we apply the formulate, approximate and explain framework (FAE) to LightGBM [Ke et al. 2017] Gradient Boosted Decision Trees (GBDT) models trained on real data: the UCI Bike Sharing and Adult Income datasets, and a Lending Club dataset. For parsimony, we analyze models that use only five features. For the Bike Sharing model, we explain a randomly selected prediction of 210 rentals for a certain hour. For the Adult Income model, we explain a counter-intuitively low prediction for an individual with high *education-num*. For the Lending Club model, we explain a counter-intuitive rejection (assuming a threshold that accepts 15% of loan applications) for a high-income borrower.

6.1 Shortcomings of Existing Methods

Recall from Section 3.2 that the attributions from existing methods amount to computing the mean attribution for the

| Game Formulation | Avg. Prediction ($\phi_0$) | hr | temp | work | hum | season |
|------------------|--------------------------|----|------|------|-----|--------|
| $v_x^{inp}$      | 151                      | 3  | 47   | 1    | 7   | 2      |
| $v_x^{J.M.}$     | 141                      | 6  | 50   | 1    | 9   | 3      |
| $v_x^{unif}$     | 128                      | 3  | 60   | 3    | 12  | 3      |

Table 3: Bike Sharing comparison of mean attributions. 95% CIs ranged from ±0.4 (*hum* in $D_{inp}$ and $D^{J.M.}$) to ±2.5 (*hr* in $D_{inp}$ and $D^{J.M.}$).

![Figure 1: Distribution of attributions from the $v_x^{inp}$ formulation with $R \sim D_{inp}$ for the Bike Sharing example.](image)

single-reference game $v_x^{inp}$, where the reference $R$ is sampled from a certain distribution.

**Misleading Means.** In Section 5 we discussed that the mean attribution can be a misleading summarization. Here we illustrate this using the attributions from the KernelSHAP game $v_x^{inp}$ for the Bike Sharing example (see Table 6). The mean attribution to the feature *hr* is tiny, suggesting that the feature has little impact. However, the distribution of single-reference game attributions (Figure 1) reveals a large spread centered close to zero. In fact, we find that absolute value *hr* receives the largest attribution in over 60% of the single-reference games. Consequently, only examining the mean of the distribution may be misleading.

| Game Formulation | Size | Avg. Prediction ($\phi_0$) | rel | cap | edu | mar | age |
|------------------|------|--------------------------|-----|-----|-----|-----|-----|
| $v_x^{inp}$      | 0.24 | -0.04                    | -0.03 | -0.01 | -0.10 | -0.00 |
| $v_x^{J.M.}$     | 0.19 | -0.02                    | -0.03 | -0.01 | -0.08 | 0.01 |
| $v_x^{unif}$     | 0.82 | 0.01                     | -0.79 | 0.02 | -0.03 | 0.04 |

Table 4: Adult Income comparison of mean attributions. 95% CIs ranged from ±0.0004 (Cluster 2, *relationship*) to ±0.0115 (Cluster 5, *marital-status* and *age*).

**Unquantified Uncertainty.** Lack of uncertainty quantification in existing techniques can result in misleading attributions. For instance, taking the mean attribution of 100 randomly-sampled Bike Sharing single-reference games}\[9] raises a warning if over 100 references are used.

\[9] The official implementation of KernelSHAP [Lundberg and Lee 2017] raises a warning if over 100 references are used.
Our first contribution is an in-depth study of various Shapley-value-based model explanation methods. We find cases where existing methods yield counter-intuitive attributions, and we trace these misleading attributions to the cooperative games these methods formulate. We propose a generalizing formulation that unifies attribution methods, offers conceptual clarity for interpreting each method’s attributions, and admits straightforward confidence intervals for attributions.

Our second contribution is a framework for model explanations, called formulate, approximate, and explain (FAE), which is built on principles from Norm Theory (Kahneman and Miller 1986). We advise practitioners to formulate contrastive explanation questions that specify the references relative to which a prediction should be explained, for example “Why did this rejected loan application receive a score of 0.28 compared to the applications that were accepted?” By approximating the Shapley values of games formulated relative to the chosen references and explaining the distribution of approximated Shapley values, we provide a meaningful and relevant answer to the explanation question at hand.

We conclude that axiomatic guarantees do not inherently guarantee relevant explanations, and that game formulations may need to be constructed carefully. In summarizing attribution distributions, we caution practitioners to avoid coarse-grained summaries that hide information, and to appropriately quantify any uncertainty resulting from approximation.
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Supplemental Material: The Explanation Game

8 Shapley Value Axioms

We briefly summarize the four Shapley value axioms.

- The Dummy axiom requires that if player $i$ has no possible contribution (i.e. $v(S \cup \{i\}) = v(S)$ for all $S \subseteq M$), then that player receives zero attribution.
- The Symmetry axiom requires that two players that always have the same contribution receive equal attribution. Formally, if $v(S \cup \{i\}) = v(S \cup \{j\})$ for all $S$ not containing $i$ or $j$ then $\phi_i(v) = \phi_j(v)$.
- The Efficiency axiom requires that the attributions to all players sum to the total payoff of all players. Formally, $\sum_i \phi_i(v) = v(M)$.
- The Linearity axiom states that for any payoff function $v$ that is a linear combination of two other payoff functions $u$ and $w$ (i.e. $v(S) = \alpha u(S) + \beta w(S)$), the Shapley values of $v$ equal the corresponding linear combination of the Shapley values of $u$ and $w$ (i.e. $\phi_i(v) = \alpha \phi_i(u) + \beta \phi_i(w)$).

9 Proofs

In what follows, we prove the lemmas from the main paper. The proofs refer to equations and definition from the main paper.

9.1 Proof of Lemma 1

From the definitions of $v_{x,D}$ (Equation 7) and $v_{x,r}$ (Equation 8), it follows that $v_{x,D}(S) = \mathbb{E}_{R \sim D}[v_{x,R}(S)]$. Thus, the game $v_{x,D}$ is a linear combination of games $\{v_{x,r} | r \in X\}$ (with weights defined by the distribution $D$). From the Linearity axiom of Shapley values, it follows that the Shapley values of the game $v_{x,D}$ must be corresponding Shapley values of the games $v_{x,r}$ and therefore, $\phi(v_{x,D}) = \mathbb{E}_{R \sim D}[\phi(v_{x,R})]$.

9.2 Proof of Lemma 2

From Lemma 1, we have $\phi_i(v_{x,D}) = \mathbb{E}_{R \sim D}[\phi_i(v_{x,R})]$. Thus, to prove this lemma, it suffices to show that for any irrelevant feature $i$, the Shapley value from the game $v_{x,r}$ is zero for all references $r \in X$. That is,

$$\forall r \in X \phi_i(v_{x,r}) = 0$$

(10)

From the definition of Shapley values (Equation 1), we have:

$$\phi_i(v_{x,r}) = \frac{1}{M} \sum_{S \subseteq M \setminus \{i\}} \left( \frac{M - 1}{|S|} \right)^{-1} (v_{x,r}(S \cup \{i\}) - v_{x,r}(S))$$

(11)

Thus, to prove Equation (10) it suffices to show the marginal contribution $(v_{x,r}(S \cup \{i\}) - v_{x,r}(S))$ of an irrelevant feature $i$ to any subset of features $S \subseteq M \setminus \{i\}$ is always zero. From the definition of the game $v_{x,r}$, we have:

$$v_{x,r}(S \cup \{i\}) - v_{x,r}(S) = f(z(x, r, S \cup \{i\})) - f(z(x, r, S))$$

(12)

From the definition of composite inputs $z$ (Equation 2), it follows that the inputs $z(x, r, S \cup \{i\})$ and $z(x, r, S)$ agree on all features except $i$. Thus, if feature $i$ is irrelevant, $f(z(x, r, S \cup \{i\})) = f(z(x, r, S))$, and consequently by Equation (11) $v_{x,r}(S \cup \{i\}) - v_{x,r}(S) = 0$. Thus feature $i$ has zero marginal contribution to all subsets $S \subseteq M \setminus \{i\}$ in the game $v_{x,r}$. Combining this with the definition of Shapley values (Equation 1) proves Equation (10).

10 Reproducibility

For brevity, we omitted from the main paper many of the mundane choices in the design of our toy examples and case studies. To further transparency and reproducibility, we include them here.

10.1 Fitting models

For both case studies, we used the LightGBM package configured with default parameters to fit a Gradient Boosted Decision Trees (GBDT) model.

For the Bike Sharing dataset, we fit on all examples from 2011 while holding out the 2012 examples for testing. We omitted the atemp feature, as it is highly correlated to temp ($r = 0.98$), and the instant feature because the tree-based GBDT model cannot capture its time-series trend. For parsimony, we refitted the model to the top five most important features by cumulative gain (hr, temp, workingday, hum, and season). This lowered test-set $r^2$ from 0.64 to 0.63.

For the Adult Income dataset, we used the pre-defined train/test split. Again, we refitted the model to the top five features by cumulative gain feature importance (relationship, capitalgain, education-num, marital-status, and age). This increased test-set misclassification error from 14.73% to 10.97%.
10.2 Selection of points to explain

For the Bike Share case study, we sampled ten points at random from the test set. We selected one whose prediction was close to the middle of the range observed over the entire test set (predictions ranged approximately from 0 to 600). Specifically, we selected instant 11729 (2012-05-08, 9pm). We examined other points from the same sample of ten to suggest a random but meaningful comparative question. We found another point with comparable \textit{workingday}, \textit{hum}, and \textit{season}: instant 11362. This point caught our eye because it differed only in \textit{hr} (2pm rather than 9pm), and \textit{temp} (0.36 rather than 0.64) but had a much lower prediction.

For the Adult Income case study, we wanted to explain why a point was scored as likely to have low income, a task roughly analogous to that of explaining why an application for credit is rejected by a creditworthiness model in a lending setting. We sampled points at random with scores between 0.01 and 0.1, and chose the 9880th point in the test set due to its strikingly high \textit{education-num} (most of the low-scoring points sampled had lower \textit{education-num}).

For the Lending Club data, we chose an open-source subset of the dataset that has been pre-cleaned to a predictive task on 3-year loans. For the five-feature model, we selected the top five features by cumulative gain feature importance from a model fit to the full set of features.

10.3 K-means clustering

We choose $k = 5$ arbitrarily, having observed a general tradeoff of conciseness for precision as $k$ increases. In the extremes, $k = 1$ maintains the overall attribution distribution, while $k = N$ examines each single-reference game separately.

11 Case Study Supplemental Material

Here we present the full results of the case studies, including tables and boxplot visualizations of attribution distributions.

Table 6: Bike Sharing comparison of mean attributions. 95% CIs ranged from ±0.4 (\textit{hum} in $D^{inp}$ and $D^{J.M.}$) to ±2.5 (\textit{hr} in $D^{inp}$ and $D^{J.M.}$).

| Game Formulation | Size | Avg. Prediction ($\phi_0$) | hr | temp | work. | hum | season |
|------------------|------|---------------------------|----|------|-------|-----|--------|
| $v^{inp}$        | 100% | 151                       | 3  | 47   | 1     | 7   | 2      |
| $v^{J.M.}$       | 100% | 141                       | 6  | 50   | 1     | 9   | 3      |
| $v^{unif}$       | 100% | 128                       | 3  | 60   | 3     | 12  | 3      |
| Cluster 1        | 12.9%| 309                       | -86| 14   | -28   | 3   | -1     |
| Cluster 2        | 27.6%| 28                        | 140| 32   | 0     | 9   | 0      |
| Cluster 3        | 10.5%| 375                       | -247| 58   | 16    | 9   | -1     |
| Cluster 4        | 32.5%| 131                       | 31 | 38   | 3     | 4   | 2      |
| Cluster 5        | 16.5%| 128                       | -57| 107  | 13    | 9   | 9      |

Table 7: Adult Income comparison of mean attributions. 95% CIs ranged from ±0.0004 (Cluster 2, \textit{relationship}) to ±0.0115 (Cluster 5, \textit{marital-status} and \textit{age}).

| Game Formulation | Size | Avg. Prediction ($\phi_0$) | rel. | cap. | edu. | mar. | age   |
|------------------|------|---------------------------|------|------|------|------|-------|
| $v^{inp}$        | 100% | 0.24                      | -0.04| -0.03| -0.01| -0.10| -0.00 |
| $v^{J.M.}$       | 100% | 0.19                      | -0.02| -0.03| -0.01| -0.08| 0.01  |
| $v^{unif}$       | 100% | 0.82                      | 0.01 | -0.79| 0.02 | -0.03| 0.04  |
| Cluster 1        | 10.2%| 0.67                      | -0.15| -0.01| -0.15| -0.28| -0.02 |
| Cluster 2        | 55.3%| 0.04                      | 0.01 | 0.00 | 0.00 | -0.01| 0.02  |
| Cluster 3        | 4.4% | 0.99                      | -0.04| -0.70| -0.06| -0.12| -0.01 |
| Cluster 4        | 28.0%| 0.31                      | -0.09| 0.00 | 0.08 | -0.21| -0.03 |
| Cluster 5        | 2.1% | 0.67                      | -0.04| 0.01 | -0.47| -0.14| 0.03  |
Table 8: Lending Club comparison of mean attributions. 95% CIs ranged from ±0.0004 to ±0.0007 for both games.

| Game Formulation | Size | Avg. Prediction (φ₀) | fico. | addr. | inc. | acc. | dti |
|------------------|------|----------------------|-------|-------|------|------|-----|
| v_x, D^inp      | 20%  | 0.05                 | 0.02  | 0.04  | 0.02 | 0.11 | 0.03|
| v_x, D^J.M.     | 100% | 0.14                 | 0.00  | 0.03  | 0.00 | 0.10 | 0.00|
| v_x, D^unif     | 100% | 0.14                 | 0.01  | 0.03  | 0.01 | 0.10 | 0.00|
| v_x, D^unif     | 100% | 0.11                 | 0.05  | 0.07  | -0.01| 0.03 | 0.02|

| Cluster | Size | Avg. Prediction (φ₀) | fico. | addr. | inc. | acc. | dti |
|---------|------|----------------------|-------|-------|------|------|-----|
| Cluster 1 | 28.5% | 0.11                | 0.01  | 0.06  | 0.00 | 0.08 | 0.01|
| Cluster 2 | 24.4% | 0.10                | 0.01  | 0.00  | 0.01 | 0.11 | 0.04|
| Cluster 3 | 15.4% | 0.18                | 0.00  | 0.01  | 0.00 | 0.14 | -0.05|
| Cluster 4 | 17.6% | 0.16                | -0.01 | 0.01  | 0.03 | 0.09 | -0.01|
| Cluster 5 | 14.0% | 0.22                | -0.01 | 0.05  | -0.02| 0.08 | -0.06|

(a) Attributions for $v_x, RR$ when $RR \sim D^{inp}$.
(b) Attributions for $v_x, RR$ when $RR \sim D^{J.M.}$.
(c) Attributions for $v_x, RR$ when $RR \sim U$.

Figure 2: Bike Sharing attributions for decompositions of $v_x$, $v_x^{J.M.}$, and $v_x^{unif}$.

(a) Attributions for $v_x, RR$ when $RR \sim D^{inp}$.
(b) Attributions for $v_x, RR$ when $RR \sim D^{J.M.}$.
(c) Attributions for $v_x, RR$ when $RR \sim U$.

Figure 3: Adult Income attributions for decompositions of $v_x^{inp}$, $v_x^{J.M.}$, and $v_x^{unif}$.

(a) Attributions for $v_x, RR$ when $RR \sim D^{inp}$.
(b) Attributions for $v_x, RR$ when $RR \sim D^{J.M.}$.
(c) Attributions for $v_x, RR$ when $RR \sim U$.

Figure 4: Lending Club attributions for decompositions of $v_x^{inp}$, $v_x^{J.M.}$, and $v_x^{unif}$.
Figure 5: Bike Sharing predictions by cluster and attributions from contrastive games against counterfactual clusters.
Figure 6: Adult Income predictions by cluster and attributions from contrastive games against counterfactual clusters.
(a) Model predictions by cluster

(b) Attributions contrasting against cluster 1

(c) Attributions contrasting against cluster 2

(d) Attributions contrasting against cluster 3

(e) Attributions contrasting against cluster 4

(f) Attributions contrasting against cluster 5

Figure 7: Lending Club predictions by cluster and attributions from contrastive games against counterfactual clusters.