# Explaining by Removing: A Unified Framework for Model Explanation

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#### Abstract

Researchers have proposed a wide variety of model explanation approaches, but it remains unclear how most methods are related or when one method is preferable to another. We establish a new class of methods, removal-based explanations, that are based on the principle of simulating feature removal to quantify each feature's influence. These methods vary in several respects, so we develop a framework that characterizes each method along three dimensions: 1) how the method removes features, 2) what model behavior the method explains, and 3) how the method summarizes each feature's influence. Our framework unifies 25 existing methods, including several of the most widely used approaches (SHAP, LIME, Meaningful Perturbations, permutation tests). This new class of explanation methods has rich connections that we examine using tools that have been largely overlooked by the explainability literature. To anchor removal-based explanations in cognitive psychology, we show that feature removal is a simple application of subtractive counterfactual reasoning. Ideas from cooperative game theory shed light on the relationships and trade-offs among different methods, and we derive conditions under which all removal-based explanations have information-theoretic interpretations. Through this analysis, we develop a unified framework that helps practitioners better understand model explanation tools, and that offers a strong theoretical foundation upon which future explainability research can build. Model explanation, interpretability, information theory, cooperative game theory, psychology

# COVERT, LUNDBERG & LEE

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## 1. Introduction

The proliferation of black-box models has made machine learning (ML) explainability an increasingly important subject, and researchers have now proposed a variety of model explanation approaches (Zeiler and Fergus, 2014; Ribeiro et al., 2016; Lundberg and Lee, 2017). Despite progress in the field, the relationships and trade-offs among these methods have not been rigorously investigated, and researchers have not always formalized their fundamental ideas about how to interpret models (Lipton, 2018). This makes the interpretability literature difficult to navigate and raises questions about whether existing methods relate to human processes for explaining complex decisions (Miller et al., 2017; Miller, 2019).

Here, we present a comprehensive framework that unifies a substantial portion of the model explanation literature. Our framework is based on the observation that many methods can be understood as *simulating feature removal* to quantify each feature's influence on a model. The intuition behind these methods is similar (depicted in Figure 1), but each one takes a slightly different approach to the removal operation: some replace features with neutral values (Zeiler and Fergus, 2014; Petsiuk et al., 2018), others marginalize over a distribution of values (Strobl et al., 2008; Lundberg and Lee, 2017), and still others train separate models for each subset of features (Lipovetsky and Conklin, 2001; Štrumbelj et al., 2009). These methods also vary in other respects, as we describe below.

We refer to this class of approaches as removal-based explanations and identify 25<sup>1</sup> existing methods that rely on the feature removal principle, including several of the most widely used methods (SHAP, LIME, Meaningful Perturbations, permutation tests). We then develop a framework that shows how each method arises from various combinations of three choices: 1) how the method removes features from the model, 2) what model behavior the method analyzes, and 3) how the method summarizes each feature's influence on the model. By characterizing each method in terms of three precise mathematical choices, we are able to systematize their shared elements and reveal that they rely on the same fundamental approach—feature removal.

The model explanation field has grown significantly in the past decade, and we take a broader view of the literature than existing unification theories. Our framework's flexibility lets us establish links between disparate classes of methods (e.g., computer vision-focused methods, global methods, game-theoretic methods, feature selection methods) and show that the literature is more interconnected than previously recognized. However, while exposing these relationships make the literature more coherent, it also raises questions about the degree of novelty in recent work and the unique advantages of each approach.

To address such questions, we thoroughly analyze our framework's theoretical foundation by examining its connections with related fields. In particular, we find that cognitive psychology, cooperative game theory and information theory are intimately connected to removal-based explanations and help shed light on the trade-offs between different approaches. The extent of these links is perhaps surprising because few methods explicitly reference these related fields.

Our approach yields many new results (listed below) and provides a strong theoretical foundation for understanding existing methods and guiding future work. Our contributions include:

<sup>1.</sup> This total count does not include minor variations on the approaches we identified.

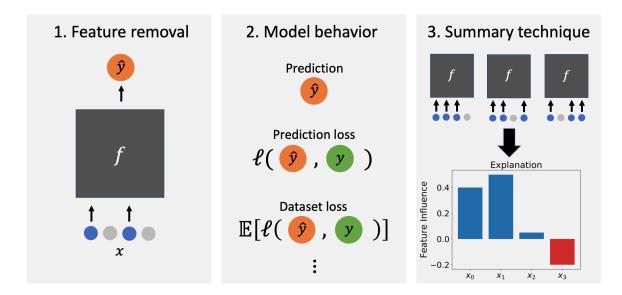


Figure 1: A unified framework for *removal-based explanations*. Each method is determined by three choices: how it removes features, what model behavior it analyzes, and how it summarizes feature influence.

- 1. We present a **unified framework** that characterizes 25 existing explanation methods and establishes a new class of **removal-based explanations**. The framework integrates classes of methods that were previously considered disjoint, including local and global approaches as well as feature attribution and feature selection methods. In our experiments, we develop and compare 60+ new explanation approaches by mixing and matching the choices that methods make in each dimension of our framework.
- 2. We develop **new mathematical tools** to represent different approaches for removing features from ML models. Then, by incorporating an underlying data distribution, we argue that marginalizing out features using their conditional distribution is the only approach that is consistent with standard probability axioms. Finally, we prove that several alternative choices approximate this approach, and that this approach gives all removal-based explanations an **information-theoretic interpretation**.
- 3. We demonstrate that **every removal-based explanation has a precedent in cooperative game theory**, and we leverage decades of game theory research to highlight advantages of the Shapley value over alternative summarization strategies. Building on these findings, we also show that several feature attribution techniques are special cases of LIME (Ribeiro et al., 2016) and several feature selection techniques are generalized by the Masking Model approach (Dabkowski and Gal, 2017).
- 4. We consult social science research to understand the intuition behind feature removal as an approach to model explanation. We find that feature removal is a simple application of subtractive counterfactual reasoning, or, equivalently, of Mill's method of difference from the philosophy of scientific induction (Mill, 1884).

We begin with background on the model explanation problem and a review of prior work (Section 2) and then introduce our framework (Section 3). We then present our framework in detail, describing how methods remove features (Section 4), formalizing the model behaviors analyzed by each method (Section 5), and examining each method's approach to summarizing feature influence (Section 6). We next explore connections to related fields. First, we show how each method has roots in cooperative game theory (Section 7). Next, we prove that under certain conditions, removal-based explanations analyze the information communicated by each feature (Section 8). Then, we refer to the psychology literature to establish a cognitive basis for removal-based explanations (Section 9). Our experiments provide empirical comparisons between existing methods and new combinations of existing approaches (Section 10) before we recap and conclude our discussion (Section 11).

## 2. Background

Here, we introduce the model explanation problem and briefly review existing approaches and related unification theories.

#### 2.1 Preliminaries

Consider a supervised ML model f that is used to predict a response variable  $Y \in \mathcal{Y}$  using the input  $X = (X_1, X_2, \dots, X_d)$ , where each  $X_i$  represents an individual feature, such as a patient's age. We use uppercase symbols (e.g., X) to denote random variables and lowercase ones (e.g., x) to denote their values. We also use  $\mathcal{X}$  to denote the domain of the full feature vector X and  $\mathcal{X}_i$  to denote the domain of each feature  $X_i$ . Finally,  $x_S \equiv \{x_i : i \in S\}$  denotes a subset of features for  $S \subseteq D \equiv \{1, 2, \dots d\}$ , and  $\bar{S} \equiv D \setminus S$  represents a set's complement.

ML interpretability broadly aims to provide insight into how models make predictions. This is particularly important when f is a complex model, such as a neural network or a decision forest. The most active area of research in the field is *local interpretability*, which explains individual predictions, such as an individual patient diagnosis (e.g., Ribeiro et al., 2016; Lundberg and Lee, 2017; Sundararajan et al., 2017); in contrast, *global interpretability* explains the model's behavior across the entire dataset (e.g., Breiman, 2001; Owen, 2014; Covert et al., 2020). Both problems are usually addressed using *feature attribution*, where a score is assigned to explain each feature's influence. However, recent work has also proposed the strategy of *local feature selection* (Chen et al., 2018a), and other papers have introduced methods to isolate sets of relevant features (Zhou et al., 2014; Fong and Vedaldi, 2017; Dabkowski and Gal, 2017).

Whether the aim is local or global interpretability, explaining the inner workings of complex models is fundamentally difficult, so it is no surprise that researchers keep devising new approaches. Commonly cited categories of approaches include perturbation-based methods (e.g., Zeiler and Fergus, 2014; Lundberg and Lee, 2017), gradient-based methods (e.g., Simonyan et al., 2013; Sundararajan et al., 2017), and inherently interpretable models (e.g., Zhou et al., 2016; Rudin, 2019). However, these categories refer to loose collections of approaches that seldom share a precise mechanism.

Besides the inherently interpretable models, virtually all of these approaches generate explanations by considering some class of perturbation to the input and using the outcomes to explain each feature's influence. Certain methods consider infinitesimal perturbations by

calculating gradients (Simonyan et al., 2013; Sundararajan et al., 2017; Smilkov et al., 2017; Erion et al., 2019; Xu et al., 2020), but there are many possible perturbations (Zeiler and Fergus, 2014; Ribeiro et al., 2016; Fong and Vedaldi, 2017; Lundberg and Lee, 2017). Our work is based on the observation that numerous perturbation strategies can be understood as simulating feature removal.

#### 2.2 Related work

Prior work has made solid progress in exposing connections among disparate explanation methods. Lundberg and Lee (2017) proposed the unifying framework of additive feature attribution methods and showed that LIME, DeepLIFT, LRP and QII are all related to SHAP (Bach et al., 2015; Ribeiro et al., 2016; Shrikumar et al., 2016; Datta et al., 2016). Similarly, Ancona et al. (2017) showed that Grad \* Input, DeepLIFT, LRP and Integrated Gradients are all understandable as modified gradient backpropagations. Most recently, Covert et al. (2020) showed that several global explanation methods can be viewed as additive importance measures, including permutation tests, Shapley Net Effects, and SAGE (Breiman, 2001; Lipovetsky and Conklin, 2001).

Relative to prior work, the unification we propose is considerably broader but nonetheless precise. By focusing on the common mechanism of removing features from a model, we encompass far more methods, including both local and global ones. We also provide a considerably richer theoretical analysis by exploring underlying connections with cooperative game theory, information theory and cognitive psychology.

As we describe below, our framework characterizes methods along three dimensions. The choice of how to remove features has been considered by many works (Lundberg and Lee, 2017; Chang et al., 2018; Janzing et al., 2019; Sundararajan and Najmi, 2019; Merrick and Taly, 2019; Aas et al., 2019; Hooker and Mentch, 2019; Agarwal and Nguyen, 2019; Frye et al., 2020). The choice of what model behavior to analyze has been considered explicitly by only a few works (Lundberg et al., 2020; Covert et al., 2020), as has the choice of how to summarize each feature's influence based on a cooperative game (Štrumbelj et al., 2009; Datta et al., 2016; Lundberg and Lee, 2017; Frye et al., 2019; Covert et al., 2020). To our knowledge, ours is the first work to consider all three dimensions simultaneously and unite them under a single framework.

Besides the methods that we focus on, there are also methods that do not rely on the feature removal principle. We direct readers to survey articles for a broader overview of the literature (Adadi and Berrada, 2018; Guidotti et al., 2018).

#### 3. Removal-Based Explanations

We now introduce our framework and briefly describe the methods it unifies.

#### 3.1 A unified framework

We develop a unified model explanation framework by connecting methods that define each feature's influence through the impact of removing it from a model. This perspective encompasses a substantial portion of the explainability literature: we find that 25 exist-

Метнор	Removal	Behavior	Summary
IME (2009)	Separate models	Prediction	Shapley value
IME (2010)	Marginalize (uniform)	Prediction	Shapley value
QII	Marginalize (marginals product)	Prediction	Shapley value
SHAP	Marginalize (conditional/marginal)	Prediction	Shapley value
KernelSHAP	Marginalize (marginal)	Prediction	Shapley value
TreeSHAP	Tree distribution	Prediction	Shapley value
LossSHAP	Marginalize (conditional)	Prediction loss	Shapley value
SAGE	Marginalize (conditional)	Dataset loss (label)	Shapley value
Shapley Net Effects	Separate models	Dataset loss (label)	Shapley value
Shapley Effects	Marginalize (conditional)	Dataset loss (output)	Shapley value
Permutation Test	Marginalize (marginal)	Dataset loss (label)	Remove individual
Conditional Perm. Test	Marginalize (conditional)	Dataset loss (label)	Remove individual
Feature Ablation (LOCO)	Separate models	Dataset loss (label)	Remove individual
Univariate Predictors	Separate models	Dataset loss (label)	Include individual
L2X	Missingness during training	Prediction mean loss	High-value subset
INVASE	Missingness during training	Prediction mean loss	High-value subset
LIME (Images)	Default values	Prediction	Linear model
LIME (Tabular)	Marginalize (replacement dist.)	Prediction	Linear model
PredDiff	Marginalize (conditional)	Prediction	Remove individual

Prediction

Prediction loss

Prediction

Prediction

Prediction

Prediction

Prediction

Prediction

Remove individual

Remove individual

Mean when included

Partitioned subsets

High-value subset Low-value subset

High-value subset

High-value subset

Occlusion

CXPlain

FIDO-CA

RISE

MM

MIR

MP

Table 1: Choices made by existing removal-based explanations.

ing methods rely on this mechanism, including many of the most widely used approaches (Breiman, 2001; Ribeiro et al., 2016; Fong and Vedaldi, 2017; Lundberg and Lee, 2017).

Zeros

Zeros

 ${
m Zeros}$ 

Default values

Extend pixel values

Blurring

Blurring

Generative model

These methods all remove groups of features from the model, but, beyond that, they take a diverse set of approaches. For example, LIME fits a linear model to an interpretable representation of the input (Ribeiro et al., 2016), L2X selects the most informative features for a single example (Chen et al., 2018a), and Shapley Effects examines how much of the model's variance is explained by each feature (Owen, 2014). Perhaps surprisingly, their differences are easy to systematize because each method removes discrete sets of features.

As our main contribution, we introduce a framework that shows how these methods can be specified using only three choices.

**Definition 1 Removal-based explanations** are model explanations that quantify the impact of removing sets of features from the model. These methods are determined by three choices:

- 1. (Feature removal) How the method removes features from the model (e.g., by setting them to default values or by marginalizing over a distribution of values)
- 2. (Model behavior) What model behavior the method analyzes (e.g., the probability of the true class or the model loss)
- 3. (Summary technique) How the method summarizes each feature's impact on the model (e.g., by removing a feature individually or by calculating the Shapley values)

#### Summary technique Feature attribution Feature selection Include Mean when High value Low value Partitioned Remove Linear Shapley value individual individual included model subset subset subsets Occlusion RISE ММ Zeros **CXPlain** HMF Default values (images) MIR **Extend pixels** Blurring MP Generative FIDO-CA Feature removal model LIME (tabular) distribution) Marginalize IME (2010) (uniform) Marginalize (marginals QII product) Marginalize Permutation SHAP KernelSHAP test PredDiff **SHAP SAGE** Marginalize Conditional LossSHAP (conditional) Shapley Effects perm. test Tree TreeSHAP distribution Missingness L2X INVASE during training IME (2009) Univariate Feature Separate Shapley Net Effects Model behavior ■ Prediction loss ■ Prediction ■ Mean prediction loss

Figure 2: Visual depiction of the space of removal-based explanations.

This precise yet flexible framework represents each choice as a specific type of mathematical function, as we show later. The framework unifies disparate explanation methods, and, by unraveling each method's choices, offers a step towards a better understanding of the literature by allowing explicit reasoning about the trade-offs among different approaches.

## 3.2 Overview of existing approaches

We now outline some of our findings, which we present in more detail in the next several sections. In particular, we preview how existing methods fit into our framework and highlight groups of methods that appear similar in light of our feature removal perspective.

Table 2: Common combinations of choices in existing methods. Check marks  $(\checkmark)$  indicate choices that are identical between methods.

Removal	Behavior	Summary	Methods	
	✓	✓	IME, QII, SHAP, KernelSHAP, TreeSHAP	
✓		✓	SHAP, LossSHAP, SAGE, Shapley Effects	
✓	✓		Occlusion, LIME (images), MM, RISE	
	✓	✓	Feature ablation (LOCO), permutation tests, conditional permutation tests	
✓	✓		Univariate predictors, feature ablation (LOCO), Shapley Net Effects	
	✓	✓	SAGE, Shapley Net Effects	
<b>√</b>	✓		SAGE, conditional permutation tests	
✓		✓	Shapley Net Effects, IME (2009)	
✓		✓	Occlusion, CXPlain	
	✓	✓	Occlusion, PredDiff	
✓		✓	Conditional permutation tests, PredDiff	
✓	✓		SHAP, PredDiff	
✓	✓		MP, EP	
	✓	✓	EP, FIDO-CA	
✓	✓	✓	L2X, INVASE	

Table 1 lists the methods unified by our framework (with acronyms introduced in the next section). These methods represent diverse parts of the interpretability literature, including global interpretability methods (Breiman, 2001; Owen, 2014), computer vision-focused methods (Zeiler and Fergus, 2014; Zhou et al., 2014; Fong and Vedaldi, 2017; Petsiuk et al., 2018), game-theoretic methods (Štrumbelj and Kononenko, 2010; Lundberg and Lee, 2017; Covert et al., 2020) and feature selection methods (Chen et al., 2018a; Yoon et al., 2018; Fong et al., 2019). They are all unified by their reliance on feature removal.

Disentangling the details of each method shows that many approaches share one or more of the same choices. For example, most methods choose to explain individual predictions (model behavior), and the most popular summary technique is the Shapley value (Shapley, 1953). These common choices raise important questions about how different these methods truly are and how their choices are justified; we explore these questions in the remainder of the paper.

To highlight similarities among the methods, we visually depict the space of removalbased explanations in Figure 2. Visualizing our framework reveals several regions of the space of methods that are crowded (e.g., methods that marginalize out removed features with their conditional distribution and that calculate Shapley values), while certain methods are relatively unique and spatially isolated (e.g., RISE; LIME for tabular data; L2X and INVASE). Empty positions in the grid reveal opportunities to develop new methods; we explore these possibilities in our experiments by partially filling out the space of removal-based explanations (Section 10).

Finally, Table 2 shows groups of methods that differ in only one dimension of the framework. These methods are neighbors in the space of explanation methods (Figure 2), and it is remarkable how many instances of neighboring methods exist in the literature. Certain methods even have neighbors along every dimension of the framework (e.g., SHAP, SAGE, Occlusion, PredDiff, conditional permutation tests), reflecting how intimately connected the literature has become. The explainability literature is evolving and maturing, and our perspective provides a new approach for reasoning about the subtle relationships and trade-offs among existing approaches.

## 4. Feature Removal

Here, we define the mathematical tools necessary to remove features from ML models and then examine how existing explanation methods remove features.

#### 4.1 Functions on subsets of features

Most ML models make predictions given a specific set of features  $X = (X_1, \ldots, X_d)$ . Mathematically, these models are functions are of the form  $f : \mathcal{X} \mapsto \mathcal{Y}$ , and we use  $\mathcal{F}$  to denote the set of all such possible mappings. The principle behind removal-based explanations is to remove certain features to understand their impact on a model, but since most models require all the features to make predictions, removing a feature is more complicated than simply not giving the model access to it.

To remove features from a model, or to make predictions given a subset of features, we require a different mathematical object than  $f \in \mathcal{F}$ . Instead of functions with domain  $\mathcal{X}$ , we consider functions with domain  $\mathcal{X} \times \mathcal{P}(D)$ , where  $\mathcal{P}(D)$  denotes the power set of  $D \equiv \{1, \ldots, d\}$ . To ensure invariance to the held out features, these functions must depend only on features specified by the subset  $S \in \mathcal{P}(D)$ , so we formalize *subset functions* as follows.

**Definition 2** A subset function is a mapping of the form

$$F: \mathcal{X} \times \mathcal{P}(D) \mapsto \mathcal{Y}$$

that is invariant to the dimensions that are not in the specified subset. That is, we have F(x,S) = F(x',S) for all (x,x',S) such that  $x_S = x'_S$ . We define  $F(x_S) \equiv F(x,S)$  for convenience because the held out values  $x_{\bar{S}}$  are not used by F.

A subset function's invariance property is crucial to ensure that only the specified feature values determine the function's output, while guaranteeing that the other feature values do not matter. Another way of viewing subset functions is that they simulate the presence of missing data. While we use  $\mathcal{F}$  to represent standard prediction functions, we use  $\mathfrak{F}$  to denote the set of all possible subset functions.

We introduce subset functions here because they help conceptualize how different methods remove features from ML models. Removal-based explanations typically begin with an existing model  $f \in \mathcal{F}$ , and in order to quantify each feature's influence, they must establish a convention for removing it from the model. A natural approach is to define a subset function  $F \in \mathfrak{F}$  based on the original model f. To formalize this idea, we define a model extension as follows.

**Definition 3** An extension of a model  $f \in \mathcal{F}$  is a subset function  $F \in \mathfrak{F}$  that agrees with f in the presence of all features. That is, the model f and its extension F must satisfy

$$F(x) = f(x) \quad \forall x \in \mathcal{X}.$$

As we show next, extending an existing model is the first step towards specifying a removal-based explanation method.

## 4.2 Removing features from machine learning models

Existing methods have devised numerous ways to evaluate models while withholding groups of features. Although certain methods use different terminology to describe their approaches (e.g., deleting information, ignoring features, using neutral values, etc.), the goal of these methods is to measure a feature's influence through the impact of removing it from the model. Most proposed techniques can be understood as extensions  $F \in \mathfrak{F}$  of an existing model  $f \in \mathcal{F}$  (Definition 3).

We now examine each method's approach (see Appendix A for more details):

• (Zeros) Occlusion (Zeiler and Fergus, 2014), RISE (Petsiuk et al., 2018) and causal explanations (CXPlain, Schwab and Karlen, 2019) remove features simply by setting them to zero:

$$F(x_S) = f(x_S, 0). \tag{1}$$

• (Default values) LIME for image data (Ribeiro et al., 2016) and the Masking Model method (MM, Dabkowski and Gal, 2017) remove features by setting them to user-defined default values (e.g., gray pixels for images). Given default values  $r \in \mathcal{X}$ , these methods calculate

$$F(x_S) = f(x_S, r_{\bar{S}}). \tag{2}$$

This is a generalization of the previous approach, and in some cases features may be given different default values (e.g., their mean).

• (Missingness during training) Learning to Explain (L2X, Chen et al., 2018a) and Instance-wise Variable Selection (INVASE, Yoon et al., 2018) use a model that has missingness introduced at training time. Removed features are replaced with zeros so that the model makes the following approximation:

$$F(x_S) = f(x_S, 0) \approx p(Y|X_S = x_S). \tag{3}$$

This approach differs from Occlusion and RISE because the model is trained to recognize zeros as missing values rather than zero-valued features. A model trained with a loss function other than cross entropy loss would approximate a different quantity (e.g., the conditional expectation  $\mathbb{E}[Y|X_S=x_S]$  for MSE loss).

- (Extend pixel values) Minimal image representation (MIR, Zhou et al., 2014) removes features in images by extending the values of neighboring pixels. This effect is achieved through a gradient-space manipulation.
- (Blurring) Meaningful Perturbations (MP, Fong and Vedaldi, 2017) and Extremal Perturbations (EP, Fong et al., 2019) remove features from images by blurring them with a Gaussian kernel. This approach is *not* an extension of f because the blurred image retains dependence on the removed features. Blurring fails to remove large, low frequency objects (e.g., mountains), but it provides an approximate way to remove information from images.
- (Generative model) FIDO-CA (Chang et al., 2018) removes feature by replacing them with a sample from a conditional generative model (e.g. Yu et al., 2018). The held out features are drawn from a generative model represented by  $p_G(X_{\bar{S}}|X_S)$ , or  $\tilde{x}_{\bar{S}} \sim p_G(X_{\bar{S}}|X_S)$  and predictions are made as follows:

$$F(x_S) = f(x_S, \tilde{x}_{\bar{S}}). \tag{4}$$

• (Marginalize with conditional) SHAP (Lundberg and Lee, 2017), LossSHAP (Lundberg et al., 2020) and SAGE (Covert et al., 2020) present a strategy for removing features by marginalizing them out using their conditional distribution  $p(X_{\bar{S}} \mid X_S = x_S)$ :

$$F(x_S) = \mathbb{E}[f(X) \mid X_S = x_S]. \tag{5}$$

This approach is computationally challenging in practice, but recent work tries to achieve close approximations (Aas et al., 2019; Frye et al., 2020). Shapley Effects (Owen, 2014) implicitly uses this convention to analyze function sensitivity, while conditional permutation tests (Strobl et al., 2008) and Prediction Difference Analysis (PredDiff, Zintgraf et al., 2017) do so to remove individual features.

• (Marginalize with marginal) KernelSHAP (a practical implementation of SHAP) removes features by marginalizing them out using their joint marginal distribution  $p(X_{\bar{S}})$ :

$$F(x_S) = \mathbb{E}[f(x_S, X_{\bar{S}})]. \tag{6}$$

This is the default behavior in SHAP's implementation,<sup>2</sup> and recent work discusses the benefits of this approach (Janzing et al., 2019). Permutation tests (Breiman, 2001) use this approach to remove individual features from a model.

<sup>2.</sup> https://github.com/slundberg/shap

• (Marginalize with product of marginals) Quantitative Input Influence (QII, Datta et al., 2016) removes held out features by marginalizing them out using the product of the marginal distributions  $p(X_i)$ :

$$F(x_S) = \mathbb{E}_{\prod_{i \in D} p(X_i)} [f(x_S, X_{\bar{S}})]. \tag{7}$$

• (Marginalize with uniform) The updated version of the Interactions Method for Explanation (IME, Štrumbelj and Kononenko, 2010) removes features by marginalizing them out with a uniform distribution over the feature space. If we let  $u_i(X_i)$  denote a uniform distribution over  $\mathcal{X}_i$  (with extremal values defining the boundaries for continuous features), then features are removed as follows:

$$F(x_S) = \mathbb{E}_{\prod_{i \in D} u_i(X_i)} [f(x_S, X_{\bar{S}})]. \tag{8}$$

• (Marginalize with replacement distributions) LIME for tabular data replaces features with independent draws from replacement distributions (our term), each of which depends on the original feature values. When a feature  $X_i$  with value  $x_i$  is removed, discrete features are drawn from the distribution  $p(X_i | X_i \neq x_i)$ ; when quantization is used for continuous features (LIME's default behavior<sup>3</sup>), continuous features are simulated by first generating a different quantile and then simulating from a truncated normal distribution within that bin. If we denote each feature's replacement distribution given the original value  $x_i$  as  $q_{x_i}(X_i)$ , then LIME for tabular data removes features as follows:

$$F(x,S) = \mathbb{E}_{\prod_{i \in D} q_{x_i}(X_i)} [f(x_S, X_{\bar{S}})]. \tag{9}$$

Although this function F agrees with f given all features, it is *not* an extension because it does not satisfy the invariance property for subset functions.

- (Tree distribution) Dependent TreeSHAP (Lundberg et al., 2020) removes features using the distribution induced by the model, which roughly approximates the conditional distribution. When splits for removed features are encountered in the model's trees, TreeSHAP averages predictions from the multiple paths in proportion to how often the dataset follows each path.
- (Separate models) Shapley Net Effects (Lipovetsky and Conklin, 2001) and the original version of IME (Štrumbelj et al., 2009) are not based on a single model f but rather on separate models trained for each subset,  $\{f_S : S \subseteq D\}$ . The prediction for a subset of features is given by that subset's model:

$$F(x_S) = f_S(x_S). (10)$$

Although this approach is technically an extension of the model  $f_D$  trained with all features, its predictions given subsets of features are not based on  $f_D$ . Similarly,

<sup>3.</sup> https://github.com/marcotcr/lime

feature ablation, also known as leave-one-covariate-out (LOCO, Lei et al., 2018), trains models to remove individual features, and the univariate predictors approach (used mainly for feature selection) uses models trained with individual features (Guyon and Elisseeff, 2003).

Most of these approaches are extensions of an existing model f, so our formalisms provide useful tools for understanding how removal-based explanations remove features from models. However, consider two exceptions: the blurring technique (MP and EP) and LIME's approach with tabular data. Both provide functions of the form  $F: \mathcal{X} \times \mathcal{P}(D) \mapsto \mathcal{Y}$  that agree with f given all features, but that still exhibit dependence on removed features. Based on our mathematical characterization of subset functions and their invariance to held out features, we argue that these two approaches do not fully remove features from the model.

We conclude that the first dimension of our framework amounts to choosing an extension  $F \in \mathfrak{F}$  of the model  $f \in \mathcal{F}$ . We defer consideration of the trade-offs among these approaches until Section 8, where we show that one approach to removing features yields to connections with information theory (marginalizing out removed features with the conditional distribution, Eq. 5).

## 5. Explaining Different Model Behaviors

Removal-based explanations all aim to demonstrate how a model works, but they can do so by analyzing a variety of model behaviors. We now consider the various choices of target quantities to observe as different features are withheld from the model.

The feature removal principle is flexible enough to explain virtually any function. For example, methods can explain a model's prediction, a model's loss function, a hidden layer in a neural network, or any node in a computation graph. In fact, removal-based explanations need not be restricted to the ML context: any function that accommodates missing inputs can be explained via feature removal by examining either its output or some function of its output as groups of inputs are removed. This perspective shows the broad potential applications for removal-based explanations.

However, since our focus is the ML context, we proceed by examining how existing methods work. Each method's target quantity can be understood as a function of the model output, which is represented by a subset function  $F(x_S)$ . Many methods explain the model output or a simple function of the output, such as the log-odds ratio. Other methods take into account a measure of the model's loss, for either an individual input or the entire dataset. Ultimately, as we show below, each method generates explanations based on a set function of the form

$$u: \mathcal{P}(D) \mapsto \mathbb{R},$$

which represents a value associated with each subset of features  $S \subseteq D$ . This set function represents the model behavior that a method is designed to explain.

We now examine the specific choices made by existing methods (see Appendix A for further details). The various model behaviors that methods analyze, and their corresponding set functions, include:

• (Prediction) Occlusion, RISE, PredDiff, MP, EP, MM, FIDO-CA, MIR, LIME, SHAP (including KernelSHAP and TreeSHAP), IME and QII all analyze a model's prediction for an individual input  $x \in \mathcal{X}$ :

$$v_x(S) = F(x_S). (11)$$

These methods examine how holding out different features makes an individual prediction either higher or lower. For multi-class classification models, methods often use a single output that corresponds to the class of interest. They can also apply a simple function to the model's output (for example, using the log-odds ratio rather than classification probability).

• (Prediction loss) LossSHAP and CXPlain take into account the true label y for an input x and calculate the prediction loss using a loss function  $\ell$ :

$$v_{xy}(S) = -\ell(F(x_S), y). \tag{12}$$

By incorporating label information, these methods quantify whether certain features make the prediction more or less correct. The minus sign is necessary to give the set function a higher value when more informative features are included.

• (Prediction mean loss) L2X and INVASE consider the expected loss for a given input x according to the label's conditional distribution p(Y|X=x):

$$w_x(S) = -\mathbb{E}_{p(Y|X=x)} \Big[ \ell \big( F(x_S), Y \big) \Big]. \tag{13}$$

By averaging the loss across the label's distribution, these methods highlight features that correctly predict what *could* have occurred, on average.

• (Dataset loss w.r.t. label) Shapley Net Effects, SAGE, feature ablation (LOCO), permutation tests and univariate predictors consider the expected loss across the entire dataset:

$$v(S) = -\mathbb{E}_{XY} \Big[ \ell \big( F(X_S), Y \big) \Big]. \tag{14}$$

These methods quantify how much the model's performance degrades when different features are removed. This set function can also be viewed as the predictive power derived from sets of features (Covert et al., 2020). Recent work has proposed a SHAP value aggregation scheme that is a special case of this approach (Frye et al., 2020).

• (Dataset loss w.r.t. output) Shapley Effects considers the expected loss with respect to the full model output:

$$w(S) = -\mathbb{E}_X \Big[ \ell \big( F(X_S), F(X) \big) \Big]. \tag{15}$$

Though related to the previous approach (Covert et al., 2020), Shapley Effects focuses on each feature's influence on the model output rather than on the model performance.

Each set function serves a distinct purpose in exposing a model's dependence on different features. The first three approaches listed above analyze the model's behavior for individual predictions (local explanations); the last two take into account the model's behavior across the entire dataset (global explanations). Although their aims differ, these set functions are all in fact related. Each builds upon the previous ones by accounting for either the loss or data distribution, and their relationships can be summarized as follows:

$$v_{xy}(S) = \ell(v_x(S), y) \tag{16}$$

$$w_x(S) = \mathbb{E}_{p(Y|X=x)} \left[ v_{xY}(S) \right] \tag{17}$$

$$v(S) = \mathbb{E}_{XY}[v_{XY}(S)] = \mathbb{E}_X[w_X(S)]$$
(18)

$$w(S) = \mathbb{E}_X \left[ \ell \left( v_X(S), v_X(D) \right) \right] \tag{19}$$

These relationships show that explanations based on one set function are in some cases related to explanations based on another. For example, Covert et al. (2020) showed that SAGE explanations are the expectation of explanations provided by LossSHAP—a relationship reflected in Eq. 18.

Understanding these connections is possible only because our framework disentangles each method's choices rather than viewing each method as a monolithic algorithm. We conclude by reiterating that removal-based explanations can explain virtually any function, and that choosing what to explain amounts to selecting a set function  $u: \mathcal{P}(D) \to \mathbb{R}$  to represent the model's dependence on different sets of features.

#### 6. Summarizing Feature Influence

The third choice for removal-based explanations is how to summarize each feature's influence on the model. We examine the various summarization techniques and then discuss their computational complexity and approximation approaches.

#### 6.1 Explaining set functions

The set functions we used to represent a model's dependence on different features (Section 5) are complicated mathematical objects that are difficult to communicate fully due to the exponential number of feature subsets and underlying feature interactions. Removal-based explanations confront this challenge by providing users with a concise summary of each feature's influence.

We distinguish between two main types of summarization approaches: feature attributions and feature selections. Many methods provide explanations in the form of feature attributions, which are numerical scores  $a_i \in \mathbb{R}$  given to each feature  $i = 1, \ldots, d$ . If we use  $\mathcal{U}$  to denote the set of all functions  $u : \mathcal{P}(D) \mapsto \mathbb{R}$ , then we can represent feature attributions as mappings of the form  $E : \mathcal{U} \mapsto \mathbb{R}^d$ , which we refer to as explanation mappings. Other methods take the alternative approach of summarizing set functions with a set  $S^* \subseteq D$  of the most influential features. We represent these feature selection summaries as explanation mappings of the form  $E : \mathcal{U} \mapsto \mathcal{P}(D)$ . Both approaches provide users with simple summaries of a feature's contribution to the set function.

We now consider the specific choices made by each method (see Appendix A for further details). For simplicity, we let u denote the set function each method analyzes. Surveying the various removal-based explanation methods, the techniques for summarizing each feature's influence include:

• (Remove individual) Occlusion, PredDiff, CXPlain, permutation tests and feature ablation (LOCO) calculate the impact of removing a single feature from the set of all features, resulting in the following attribution values:

$$a_i = u(D) - u(D \setminus \{i\}). \tag{20}$$

Occlusion, PredDiff and CXPlain can also be applied with groups of features in image contexts.

• (Include individual) The univariate predictors approach calculates the impact of including individual features, resulting in the following attribution values:

$$a_i = u(\{i\}) - u(\{\}).$$
 (21)

This is essentially the reverse of the previous approach: while that approach removes individual features from the complete set, this one adds individual features to the empty set.

 (Linear model) LIME fits a regularized weighted linear model to a dataset of perturbed examples. In the limit of an infinitely large dataset, this process approximates the following attribution values:

$$a_1, \dots, a_d = \underset{b_0, \dots, b_d}{\operatorname{arg \, min}} \sum_{S \subseteq D} \pi(S) \Big( b_0 + \sum_{i \in S} b_i - u(S) \Big)^2 + \Omega(b_1, \dots, b_d).$$
 (22)

In this problem,  $\pi$  represents a weighting kernel and  $\Omega$  is a regularization function that is often set to the  $\ell_1$  penalty to encourage sparse attributions (Tibshirani, 1996). Since this summary is based on an additive model, the learned coefficients  $(a_1, \ldots, a_d)$  represent values associated with including each feature.

• (Mean when included) RISE determines feature attributions by sampling many subsets  $S \subseteq D$  and then calculating the mean value when a feature is included. Denoting the distribution of subsets as p(S) and the conditional distribution as  $p(S \mid i \in S)$ , the attribution values are defined as

$$a_i = \mathbb{E}_{p(S|i \in S)}[u(S)]. \tag{23}$$

In practice, RISE samples the subsets  $S \subseteq D$  by removing each feature i independently with probability p, using p = 0.5 in their experiments (Petsiuk et al., 2018).

- (Shapley value) Shapley Net Effects, IME, Shapley Effects, QII, SHAP (including KernelSHAP, TreeSHAP and LossSHAP) and SAGE all calculate feature attribution values using the Shapley value, which we denote as  $a_i = \phi_i(u)$ . Described in more detail in Section 7, Shapley values are the only attributions that satisfy numerous desirable properties (Shapley, 1953).
- (Low-value subset) MP selects a small set of features  $S^*$  that can be removed to give the set function a low value. It does so by solving the following optimization problem:

$$S^* = \underset{S}{\operatorname{arg\,min}} \ u(D \setminus S) + \lambda |S|. \tag{24}$$

In practice, MP uses additional regularizers and solves a relaxed version of this problem (see Section 6.2).

• (High-value subset) MIR solves an optimization problem to select a small set of features  $S^*$  that alone can give the set function a high value. For a user-defined minimum value t, the problem is given by:

$$S^* = \underset{S}{\operatorname{arg\,min}} |S| \quad \text{s.t. } u(S) \ge t. \tag{25}$$

L2X and EP solve a similar problem but switch the terms in the constraint and optimization objective. For a user-defined subset size k, the optimization problem is given by:

$$S^* = \underset{S}{\operatorname{arg\,max}} \ u(S) \quad \text{s.t.} \ |S| = k. \tag{26}$$

Finally, INVASE and FIDO-CA solve a regularized version of the problem with a parameter  $\lambda > 0$  controlling the trade-off between the subset value and subset size:

$$S^* = \underset{S}{\operatorname{arg\,max}} \ u(S) - \lambda |S|. \tag{27}$$

• (Partitioned subsets) MM solves an optimization problem to partition the features into  $S^*$  and  $D \setminus S^*$  while maximizing the difference in the set function's values. This approach is based on the idea that removing features to find a low-value subset (as in MP) and retaining features to get a high-value subset (as in MIR, L2X, EP, INVASE and FIDO-CA) are both reasonable approaches for identifying influential features. The problem is given by:

$$S^* = \underset{S}{\operatorname{arg \, max}} \ u(S) - \lambda u(D \setminus S) - \gamma |S|. \tag{28}$$

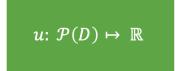
In practice, MM incorporates regularizers and monotonic link functions to enable a more flexible trade-off between u(S) and  $u(D \setminus S)$  (see Appendix A).

#### 1. Feature removal

## 2. Model behavior

# 3. Summary technique

$$F \colon \mathcal{X} \times \mathcal{P}(D) \mapsto \mathcal{Y}$$



 $E: U \mapsto \mathbb{R}^d$  or  $E: U \mapsto \mathcal{P}(D)$ 

Figure 3: Removal-based explanations are specified by three precise mathematical choices: a subset function  $F \in \mathfrak{F}$ , a set function  $u \in \mathcal{U}$ , and an explanation mapping E (for feature attribution or selection).

As this discussion shows, every removal-based explanation generates summaries of each feature's influence on the underlying set function. In general, a model's dependencies are too complex to communicate fully, so explanations must provide users with a concise summary instead. As noted, most methods we discuss generate feature attributions, but several others generate explanations by selecting the most important features. These feature selection explanations are essentially coarse attributions that assign binary importance rather than a real number.

Interestingly, if the high-value subset optimization problems solved by MIR, L2X, EP, INVASE and FIDO-CA were applied to the set function that represents the dataset loss (Eq. 18), they would resemble conventional global feature selection problems (Guyon and Elisseeff, 2003). The problem in Eq. 26 determines the set of k features with maximum predictive power, the problem in Eq. 25 determines the smallest possible set of features that achieve the performance represented by t, and the problem in Eq. 27 uses a parameter  $\lambda$  to control the trade-off. Though not generally viewed as a model explanation approach, global feature selection serves an identical purpose of identifying highly predictive features.

We conclude by reiterating that the third dimension of our framework amounts to a choice of explanation mapping, which takes the form  $E: \mathcal{U} \mapsto \mathbb{R}^d$  for feature attribution or  $E: \mathcal{U} \mapsto \mathcal{P}(D)$  for feature selection. Our discussion so far has shown that removal-based explanations can be specified using three precise mathematical choices, as depicted in Figure 3. These methods, which are often presented in ways that make their connections difficult to discern, are constructed in a remarkably similar fashion. The remainder of this work addresses the relationships and trade-offs among these different choices, beginning by examining the computational complexity of each summarization approach.

## 6.2 Complexity and approximations

Showing how certain explanation methods fit into our framework requires distinguishing between their substance and the approximations that make them practical. Our presentation of these methods deviates from the original papers, which often focus on details of a method's implementation. We now bridge the gap by describing these methods' significant computational complexity and the approximations they use out of necessity.

The challenge with most summarization techniques described above is that they require calculating the underlying set function's value u(S) for many subsets of features. In fact, without making any simplifying assumptions about the model or data distribution, several techniques must examine all  $2^d$  subsets of features. This includes the Shapley value, RISE's summary technique and LIME's linear model. Finding exact solutions to several of the optimization problems (MP, MIR, MM, INVASE, FIDO-CA) also requires examining all subsets of features, and solving the constrained optimization problem (EP, L2X) for k features requires examining  $\binom{d}{k}$  subsets, or  $2^d d^{-\frac{1}{2}}$  subsets in the worst case.<sup>4</sup>

The only approaches with lower computational complexity are those that remove individ-

The only approaches with lower computational complexity are those that remove individual features (Occlusion, PredDiff, CXPlain, permutation tests, feature ablation) or include individual features (univariate predictors). These require only one subset per feature, or d total feature subsets.

Many summarization techniques have superpolynomial complexity in d, making them intractable for large numbers of features. However, these methods work in practice due to fast approximation approaches, and in some cases methods have even been devised to generate explanations in real-time. Strategies that yield fast approximations include:

- Attribution values that are the expectation of a random variable can be estimated
  using Monte Carlo approximations. IME (Štrumbelj and Kononenko, 2010), Shapley
  Effects (Song et al., 2016) and SAGE (Covert et al., 2020) use sampling strategies
  to approximate Shapley values, and RISE also estimates its attributions via sampling
  (Petsiuk et al., 2018).
- KernelSHAP and LIME are both based on linear regression models fitted to datasets containing an exponential number of datapoints. In practice, these techniques fit models to smaller sampled datasets, which means optimizing an approximate version of their objective function.
- TreeSHAP calculates Shapley values in polynomial time using a dynamic programming algorithm that exploits the structure of tree-based models. Similarly, L-Shapley and C-Shapley exploit the properties of models for structured data to provide fast Shapley value approximations (Chen et al., 2018b).
- Several of the feature selection methods (MP, L2X, EP, MM, FIDO-CA) solve continuous relaxations of their discrete optimization problems. While these optimization problems could be solved by representing the set of features  $S \subseteq D$  as a mask  $m \in \{0,1\}^d$ , these methods instead use a mask variable of the form  $m \in [0,1]^d$ . When these methods incorporate a penalty on the subset size |S|, they often use the convex relaxation  $||m||_1$ .
- One feature selection method (MIR) uses a greedy optimization algorithm. MIR determines a set of influential features  $S \subseteq D$  by iteratively removing groups of features that do not reduce the predicted probability for the correct class.
- One feature attribution method (CXPlain) and three feature selection methods (L2X, INVASE, MM) generate real-time explanations by learning separate explainer models.

<sup>4.</sup> This can be seen by applying Stirling's approximation to  $\binom{d}{d/2}$  as d becomes large.

CXPlain learns an explainer model using a dataset consisting of manually calculated explanations, which removes the need to iterate over each feature after training. L2X learns a model that outputs a set of features (represented by a k-hot vector) and IN-VASE learns a similar selector model that can output an arbitrary number of features; similarly, MM learns a model that outputs masks of the form  $m \in [0,1]^d$  for images. These techniques can be viewed as amortized optimization approaches (Shu, 2017) because they learn models that output approximate solutions in a single forward pass (similar to amortized inference, see Kingma and Welling, 2013).

In conclusion, many methods provide efficient explanations despite using summarization techniques that are inherently intractable. Each approximation significantly speeds up computation relative to a brute-force calculation, but we predict that more approaches could be made to run in real-time by learning explainer models, as in the MM, L2X, INVASE and CXPlain approaches (Dabkowski and Gal, 2017; Chen et al., 2018a; Yoon et al., 2018; Schwab and Karlen, 2019).

## 7. Game-Theoretic Explanations

The set functions analyzed by removal-based explanations (Section 5) can be viewed as cooperative games—mathematical objects studied by cooperative game theory. Few explanation methods explicitly consider game-theoretic connections, but we show that every method described thus far has a precedent in the cooperative game theory literature.

#### 7.1 Cooperative game theory background

Cooperative games are functions of the form  $u: \mathcal{P}(D) \to \mathbb{R}$  (i.e., set functions) that describe the value achieved when sets of players  $S \subseteq D$  participate in a game. Intuitively, a game might represent the profit made when a particular group of employees chooses to work together. Cooperative game theory research focuses on understanding the properties of different payoffs that can be offered to incentivize participation in the game and predicting which groups of players will ultimately agree to participate.

For this discussion, we use u to denote a cooperative game. To introduce terminology from cooperative game theory, the features  $i=1,2,\ldots d$  are referred to as players, sets of players  $S\subseteq D$  are referred to as coalitions, and the output u(S) is referred to as the value of S. Player i's marginal contribution to the coalition  $S\in D\setminus\{i\}$  is defined as the difference in value  $u(S\cup\{i\})-u(S)$ . Allocations are vectors  $z\in\mathbb{R}^d$  that represent payoffs proposed to each player in return for participating in the game.

Several fundamental concepts in cooperative game theory are related to the properties of allocations: the *core* of a game, a game's *nucleolus*, and its *bargaining sets* are all based on whether players view certain allocations as favorable (Narahari, 2014). Perhaps surprisingly, every summarization technique used by removal-based explanations (Section 6) can be understood in terms of allocations to players in the underlying game.

## 7.2 Allocation strategies

Several summarization techniques used by removal-based explanations relate to *solution* concepts, which in the cooperative game theory context are allocation strategies designed

to be fair to the players. If we let  $\mathcal{U}$  represent the set of all cooperative games with d players, then solution concepts are represented by mappings of the form  $E: \mathcal{U} \to \mathbb{R}^d$ , similar to explanation mappings that represent feature attributions.

We first discuss the Shapley value, which assumes that the grand coalition (the coalition containing all players) is participating and distributes the total value in proportion to each player's contributions (Shapley, 1953). The Shapley value can be derived axiomatically, and we list several of its properties below; we provide more axioms than are necessary to derive the Shapley value uniquely in order to highlights its many desirable properties. The Shapley values  $\phi_i(u) \in \mathbb{R}$  for a game u are the unique allocations that satisfy the following:

• (Efficiency) The allocations  $\phi_1(u), \ldots, \phi_d(u)$  add up to the difference in value between the grand coalition and the empty coalition:

$$\sum_{i \in D} \phi_i(u) = u(D) - u(\{\}).$$

• (Symmetry) Two players i, j that make equal marginal contributions to all coalitions receive the same allocation:

$$u(S \cup \{i\}) = u(S \cup \{j\}) \ \forall \ S \implies \phi_i(u) = \phi_j(v).$$

• (Dummy) A player i that makes zero marginal contribution receives zero allocation:

$$u(S \cup \{i\}) = u(S) \ \forall \ S \implies \phi_i(u) = 0.$$

• (Additivity) If we consider two games u, u' and their respective allocations  $\phi_i(u)$  and  $\phi_i(u')$ , then the cooperative game defined as their sum u + u' has allocations defined as the sum of each game's allocations:

$$\phi_i(u+u') = \phi_i(u) + \phi_i(u') \ \forall \ i.$$

• (Marginalism) For two games u, u' where all players have identical marginal contributions, the players receive equal allocations:

$$u(S \cup \{i\}) - u(S) = u'(S \cup \{i\}) - u'(S) \ \forall \ (i, S) \implies \phi_i(u) = \phi_i(u') \ \forall \ i.$$

The Shapley values are the unique allocations that satisfy these properties (Shapley, 1953), and the expression for each Shapley value  $\phi_i(u)$  is:

$$\phi_i(u) = \frac{1}{d} \sum_{S \subseteq D \setminus \{i\}} {d-1 \choose |S|}^{-1} \Big( u(S \cup \{i\}) - u(S) \Big). \tag{29}$$

The Shapley value has found widespread use because of its axiomatic derivation, both within game theory and in other disciplines (Aumann, 1994; Shorrocks, 1999; Petrosjan and Zaccour, 2003; Tarashev et al., 2016). In the context of model explanation, Shapley values

define each feature's contribution while accounting for complex feature interactions, such as correlations, redundancy, and complementary behavior (Lipovetsky and Conklin, 2001; Štrumbelj et al., 2009; Owen, 2014; Datta et al., 2016; Lundberg and Lee, 2017; Lundberg et al., 2020; Covert et al., 2020).

Like the Shapley value, the Banzhaf value attempts to define fair allocations for each player in a cooperative game. It generalizes the Banzhaf power index, which is a technique for measuring the impact of players in the context of voting games (Banzhaf, 1964). Links between Shapley and Banzhaf values are described by Dubey and Shapley (1979), who show that the Shapley value can be understood as an enumeration over all *permutations* of players, while the Banzhaf value can be understood as an enumeration over all *subsets* of players. The expression for each Banzhaf value  $\psi_i(u)$  is:

$$\psi_i(u) = \frac{1}{2^{d-1}} \sum_{S \subseteq D \setminus \{i\}} \left( u(S \cup \{i\}) - u(S) \right). \tag{30}$$

The Banzhaf value has multiple interpretations, but the most useful for our purpose is that it represents the difference between the mean value of coalitions that do and do not include the ith player when coalitions are chosen uniformly at random. With this perspective, we observe that the RISE summarization technique is closely related to the Banzhaf value: RISE calculates the mean value of coalitions that include i, but, unlike the Banzhaf value, it disregards the value of coalitions that do not include i. While the RISE technique (Petsiuk et al., 2018) was not motivated by the Banzhaf value, it is unsurprising that such a natural idea has been explored in cooperative game theory.

Both Shapley and Banzhaf values are mathematically appealing because they can be understood as the weighted average of a player's marginal contributions (Eq. 29-30). This is a stronger version of the marginalism property introduced by Young's axiomatization of the Shapley value (Young, 1985), and solution concepts of this form are known as *probabilistic values* (Weber, 1988). Probabilistic values have their own axiomatic characterization—they have been shown to be the unique values that satisfy a specific subset of the Shapley value's properties (Monderer et al., 2002).

The notion of probabilistic values reveals links with two other solution concepts. The techniques of removing individual players (Occlusion, PredDiff, CXPlain, permutation tests, feature ablation) and including individual players (univariate predictors) can also be understood as probabilistic values, although they are trivial averages that put all their weight on a single marginal contribution (Eqs. 20-21). Unlike the Shapley and Banzhaf values, these methods do not consider complex interactions when quantifying a player's contribution.

The methods discussed thus far (Shapley value, Banzhaf value, removing individual players, including individual players) all satisfy the symmetry, dummy, additivity, and marginalism axioms. What makes the Shapley value unique among these methods is its efficiency axiom, which lets us view it as a distribution of the grand coalition's value among the players (Dubey and Shapley, 1979).

#### 7.3 Modeling cooperative games

Unlike the methods discussed so far, LIME provides a flexible approach for summarizing each player's influence. LIME fits a regularized weighted least squares model to the coop-

erative game (Eq. 22), leaving the user the option of specifying a weighting kernel  $\pi$  and a regularization term  $\Omega$ .

Although fitting a linear model to a cooperative game seems distinct from the allocation strategies already discussed, these ideas are in fact intimately connected. Fitting models to cooperative games, including both linear and nonlinear models, has been studied by numerous works in cooperative game theory (Charnes et al., 1988; Hammer and Holzman, 1992; Grabisch et al., 2000; Ding et al., 2008, 2010; Marichal and Mathonet, 2011), and specific choices for the weighting kernel yield recognizable LIME attribution values.

If we use LIME with no regularization ( $\Omega = 0$ ), then several choices of weighting kernels and their corresponding solutions to LIME's optimization problem include:

- When we use the weighting kernel  $\pi_{\text{Rem}}(S) = \mathbb{1}(|S| \geq d-1)$ , where  $\mathbb{1}(\cdot)$  is an indicator function, LIME attribution values are the marginal contributions from removing individual players from the grand coalition, or the values  $a_i = u(D) u(D \setminus \{i\})$ . This special case is identical to Occlusion, PredDiff, CXPlain, permutation tests, and feature ablation.
- When we use the weighting kernel  $\pi_{\text{Inc}}(S) = \mathbb{1}(|S| \leq 1)$ , LIME attribution values are the marginal contributions from adding individual players to the empty coalition, or the values  $a_i = u(\{i\}) u(\{\})$ . This special case is identical to the univariate predictors approach.
- Results from Hammer and Holzman (1992) imply that when we use the weighting kernel  $\pi_B(S) = 1$ , LIME attribution values are the Banzhaf values  $a_i = \psi_i(u)$ .
- Results from Charnes et al. (1988) and Lundberg and Lee (2017) show that LIME attribution values are equal to the Shapley values  $a_i = \phi_i(u)$  when we use the weighting kernel  $\pi_{\text{Sh}}$ , defined as:

$$\pi_{\rm Sh}(S) = \frac{d-1}{\binom{d}{|S|}|S|(d-|S|)}.$$
 (31)

Although the Shapley value connection has been noted in the model explanation context, the other results we present are new observations about LIME (with proofs provided in Appendix B). These results show that the weighted least squares problem solved by LIME provides sufficient flexibility to express both the Shapley and Banzhaf values, as well as simpler quantities such as the marginal contributions from removing or including individual players. The LIME approach captures every feature attribution technique discussed so far, with the caveat that RISE uses a modified version of the Banzhaf value. And, like the other attribution strategies, LIME attributions satisfy different sets of Shapley axioms under certain conditions (Appendix C).

We have thus demonstrated that the LIME approach for summarizing feature influence not only has precedent in cooperative game theory, but is intimately connected to the other allocation strategies. This suggests that the feature attributions generated by removal-based explanations should be viewed as additive decompositions of the underlying cooperative game u.

## 7.4 Identifying coalitions using excess

To better understand removal-based explanations that perform feature selection, we look to a more basic concept in cooperative game theory: the notion of *excess*. Excess is defined for a given allocation  $z \in \mathbb{R}^d$  and for a given coalition  $S \subseteq D$  as the difference between the coalition's value and its total allocation (Narahari, 2014). More formally, it is defined as follows.

**Definition 4** Given a cooperative game  $u : \mathcal{P}(D) \to \mathbb{R}$ , a coalition  $S \subseteq D$ , and an allocation  $z = (z_1, z_2, \dots, z_d) \in \mathbb{R}^d$ , the excess of S at z is defined as

$$e(S, z) = u(S) - \sum_{i \in S} z_i.$$

The excess e(S, z) represents the coalition S's degree of unhappiness under the allocation z, because an allocation is unfavorable to a coalition if its value u(S) exceeds its cumulative allocation  $\sum_{i \in S} z_i$ . For cooperative game theory concepts including the core, the nucleolus and bargaining sets, a basic assumption is that coalitions with higher excess (greater unhappiness) are more likely to break off and refuse participation in the game (Narahari, 2014). We have no analogue for features refusing participation in ML, but the notion of excess is useful for understanding several removal-based explanation methods.

The feature selection explanations in our framework can be understood in terms of excess. Below, we show that these summarization techniques are equivalent to proposing equal allocations to all players and then determining a high-valued coalition by considering each coalition's excess. Given equal allocations, players with high contributions will be less satisfied than players with low contributions, so solving this problem implicitly identifies a set of high- and low-valued players. We observe this by reformulating each method's optimization problem as follows.

• (Minimize excess) MP isolates a low-value coalition by finding the coalition with the lowest excess, or the highest satisfaction, given the equal allocation  $z = 1\lambda$ :

$$S^* = \underset{S}{\operatorname{arg\,min}} \ e(\bar{S}, \mathbf{1}\lambda). \tag{32}$$

The result  $S^*$  is a coalition whose complement  $D \setminus S^*$  is most satisfied with the equal allocation.

• (Maximize excess) MIR isolates the smallest possible coalition that achieves a sufficient level of excess given allocations equal to zero. For a level of excess t, the optimization problem is given by:

$$S^* = \underset{S}{\operatorname{arg\,min}} |S| \quad \text{s.t. } e(S, \mathbf{0}) \ge t.$$
 (33)

L2X and EP solve a similar problem but switch the objective and constraint. The optimization problem represents the coalition of size k with the highest excess given allocations of zero to each player:

$$S^* = \underset{S}{\arg\max} \ e(S, \mathbf{0}) \quad \text{s.t.} \ |S| = k.$$
 (34)

Finally, FIDO-CA and INVASE find the coalition with the highest excess given equal allocations  $z = \mathbf{1}\lambda$ :

$$S^* = \underset{S}{\operatorname{arg\,max}} \ e(S, \mathbf{1}\lambda). \tag{35}$$

• (Maximize difference in excess) MM combines the previous approaches. Rather than focusing on a coalition with low or high excess, MM partitions players into two coalitions while maximizing the difference in excess given allocations  $z = \mathbf{1} \frac{\gamma}{1+\lambda}$ :

$$S^* = \underset{S}{\operatorname{arg \, max}} \ e\left(S, \mathbf{1} \frac{\gamma}{1+\lambda}\right) - \lambda e\left(\bar{S}, \mathbf{1} \frac{\gamma}{1+\lambda}\right). \tag{36}$$

The result  $S^*$  is a coalition of dissatisfied players whose complement  $D \setminus S^*$  is comparably more satisfied.

All of the approaches listed above are different formulations of the same multi-objective optimization problem. The intuition behind these methods is that there is a small set of high-valued players S and a comparably larger set of low-valued players  $D \setminus S$ . Most methods focus on just one of these coalitions (MP focuses on  $D \setminus S$ , while MIR, L2X, EP, INVASE and FIDO-CA focus on S), but the optimization problem solved by MM considers both coalitions.

MM can therefore be understood as a generalization of the other methods. The MP and INVASE/FIDO-CA problems (Eqs. 32, 35) are clearly special cases of the MM problem. The other problems (Eq. 33, 34) cannot necessarily be cast as special cases of the MM problem (Eq. 36), but the MM problem resembles the Lagrangians of these constrained problems. More precisely, a special case of the MM problem shares the same optimal set as the dual to these constrained problems (Boyd et al., 2004).

By reformulating the optimization problems solved by each method, we show that each feature selection summarization can be described as minimizing or maximizing excess given equal allocations for all players. In cooperative game theory, examining each coalition's level of excess (or dissatisfaction) helps determine whether allocations will incentivize participation, but the same tool is used by removal-based explanations to find the most influential features for a model.

These feature selection approaches can be viewed as mappings of the form  $E: \mathcal{U} \mapsto \mathcal{P}(D)$  because they identify coalitions  $S^* \subseteq D$ . The Shapley axioms apply only to mappings of the form  $E: \mathcal{U} \mapsto \mathbb{R}^d$ , but these feature selection approaches satisfy certain analogous properties (Appendix C).

Table 3: Each method's summarization technique can each be understood in terms of concepts from cooperative game theory.

SUMMARIZATION	Methods	Related To
Shapley value	Shapley Net Effects, IME, QII, SHAP (TreeSHAP, KernelSHAP, LossSHAP), Shapley Effects, SAGE	Shapley value, probabilistic values, modeling cooperative games
Mean value when included	Mean value when included RISE mod	
Remove/include individual players	Occlusion, PredDiff, CXPlain, permutation tests, univariate predictors, feature ablation (LOCO)	Probabilistic values, modeling cooperative games
Linear model	Linear model LIME	
High/low value coalitions	MP, EP, MIR, MM, L2X, INVASE, FIDO-CA	Maximum/minimum excess

## 7.5 Summary

Our discussion establishes that every removal-based explanation has a precedent in cooperative game theory. Table 3 displays our findings regarding each method's game-theoretic interpretation. Among the various techniques, we argue that the Shapley value provides the preferred explanation because it satisfies many desirable properties and provides a granular view of each player's contributions. Unlike the other methods, it divides the grand coalition's value (due to the efficiency property) while capturing the nuances of each player's contributions.

In contrast, the other methods have clear shortcomings. Measuring a single marginal contribution, either by removing or including individual players, provides an inadequate summary because it ignores player interactions. The Banzhaf value provides a more nuanced view of each player's contributions, but it cannot be regarded as a division of the grand coalition's value because it fails to satisfy the efficiency axiom (Dubey and Shapley, 1979). Finally, feature selection explanations provide only a coarse summary of each player's value contribution, and their results depend on user-specified hyperparameters.

## 8. Information-Theoretic Explanations

We now examine how removal-based explanations are connected to information theory. We begin by describing how features can be removed using knowledge of the underlying data distribution, and we then prove that many feature removal approaches approximate

marginalizing out features with their conditional distribution. Finally, we show that this approach gives every removal-based explanation an information-theoretic interpretation.

## 8.1 Removing features consistently

The first choice for removal-based explanations is how to evaluate a model while withholding certain features. Recall that this is done using a subset function  $F \in \mathfrak{F}$ , which is typically an extension of an existing model  $f \in \mathcal{F}$  (Definition 3). There are many ways to remove features from a model (Section 4.2), so we consider whether there is an approach that is consistent with the underlying data distribution. We begin by introducing a specific perspective on how to interpret a subset function's predictions  $F(x_S)$ .

Supervised ML models approximate the response variable's conditional distribution given the input. This is clear for classification models that estimate the conditional probability  $f(x) \approx p(Y|X=x)$ , but it is also true for regression models that estimate the conditional expectation  $f(x) \approx \mathbb{E}[Y|X=x]$ . (These approximations are implicit in conventional loss functions such as cross entropy and MSE.) We propose that a subset function  $F \in \mathfrak{F}$  can be viewed equivalently as a conditional probability/expectation estimate given subsets of features.

To illustrate this idea in the classification case, we denote the model's estimate as  $q(Y|X=x) \equiv f(x)$ . Although it is not necessarily equal to the true conditional distribution p(Y|X=x), the estimate q(Y|X=x) represents a valid probability distribution for all  $x \in \mathcal{X}$ . Similarly, we denote the subset function's estimate as  $q(Y|X_S=x_S) \equiv F(x_S)$ . A subset function F implies a set of conditional distributions  $\{q(Y|X_S): S \subseteq D\}$ , and this interpretation is important because we must consider whether these distributions are probabilistically valid. In particular, we must verify that standard probability laws (nonnegativity, unitarity, countable additivity, Bayes rule) are satisfied.

As we show below, this is not guaranteed. The laws of probability impose a relationship between q(Y|X=x) and  $q(Y|X_S=x_S)$  for any  $x\in\mathcal{X}$  and  $S\subset D$ : they are linked by the underlying distribution on  $\mathcal{X}$ , or, more specifically, by the conditional distribution  $X_{\bar{S}}|X_S=x_S$ . In fact, any data distribution q(X) implies a unique definition for  $q(Y|X_S)$  based on q(Y|X) due to Bayes rule and the countable additivity property. The flexibility of subset functions regarding how to remove features is therefore problematic, because certain removal approaches (e.g., replacing features with default values) will not yield a valid set of conditional distributions.

Constraining the feature removal approach to be probabilistically valid ensures that the model extension F is faithful both to the original model f and to an underlying data distribution. Building on this perspective, we define a notion of *consistency* between a subset function and a data distribution as follows.

**Definition 5** A subset function  $F \in \mathfrak{F}$  that estimates a random variable Y's conditional distribution is **consistent** with a data distribution q(X) if its estimates satisfy the following properties:

1. (Countable additivity) The probability of the union of a countable number of disjoint events is the sum of their probabilities. Given events  $A_1, A_2, \ldots$  such that  $A_i \cap A_j = \emptyset$  for  $i \neq j$ , we have

$$P\Big(\bigcup_{i=1}^{\infty} A_i\Big) = \sum_{i=1}^{\infty} P(A_i).$$

2. (Bayes rule) The conditional probability P(A|B) for events A and B is defined as

$$P(A|B) = \frac{P(A,B)}{P(B)}.$$

This definition of consistency describes a class of subset functions that obey fundamental probability axioms (Kolmogorov, 1950; Laplace, 1986). Restricting a subset function to be consistent does not necessarily make its predictions correct, but it makes them compatible with a particular data distribution q(X). Allowing for a distribution q(X) that differs from the true distribution p(X) reveals that certain approaches implicitly assume an incorrect data distribution.

Based on this definition, the next two results show that there is a unique extension  $F \in \mathfrak{F}$  of a model  $f \in \mathcal{F}$  that is consistent with a given data distribution q(X). (Proofs are provided in Appendix D.) The first result relates to extensions of classification models that estimate conditional probabilities.

**Proposition 6** For a classification model  $f \in \mathcal{F}$  that estimates a discrete Y's conditional probability, there is a unique extension  $F \in \mathfrak{F}$  that is consistent with q(X). It is given by

$$F(x_S) = \mathbb{E}_{q(X_{\bar{S}}|X_S = x_S)} [f(x_S, X_{\bar{S}})],$$

where  $q(X_{\bar{S}} \mid X_S = x_S)$  is the conditional distribution induced by q(X).

The next result arrives at a similar conclusion, but it is specific to extensions of regression models that estimate the response variable's conditional expectation.

**Proposition 7** For a regression model  $f \in \mathcal{F}$  that estimates Y's conditional expectation, there is a unique extension  $F \in \mathfrak{F}$  that is consistent with q(X). It is given by

$$F(x_S) = \mathbb{E}_{q(X_{\bar{S}}|X_S = x_S)} [f(x_S, X_{\bar{S}})],$$

where  $q(X_{\bar{S}} \mid X_S = x_S)$  is the conditional distribution induced by q(X).

These results differ in their focus on classification and regression models, but the conclusion in both cases is the same: the only extension of a model f that is consistent with q(X) is one that averages the full model output f(X) over the distribution of values  $X_{\bar{S}}$  given by  $q(X_{\bar{S}}|X_{\bar{S}})$ .

When defining a model extension in the explanation setting, the natural choice is to make it consistent with the true data distribution p(X). This yields precisely the approach presented by SHAP (the conditional version), SAGE, and several other methods, which is to marginalize out the removed features using their conditional distribution  $p(X_{\bar{S}}|X_S=x_S)$  (Strobl et al., 2008; Zintgraf et al., 2017; Lundberg and Lee, 2017; Aas et al., 2019; Covert et al., 2020; Frye et al., 2020).

Besides this approach, only a few other approaches are consistent with any distribution. The QII approach (Eq. 7) is consistent with a distribution that is the product of marginals,  $q(X) = \prod_{i=1}^d p(X_i)$ . The latest IME approach (Eq. 8) is consistent with a distribution that is the product of uniform distributions,  $q(X) = \prod_{i=1}^d u_i(X_i)$ . And any approach that sets features to default values  $r \in \mathcal{X}$  (Eqs. 1-2) is consistent with a distribution that puts all of its mass on those values—which we refer to as a *constant distribution*. These approaches all achieve consistency because they are based on a simplifying assumption of feature independence.

## 8.2 Approximations of the conditional distribution

While few removal-based explanations explicitly suggest marginalizing out features using their conditional distribution, several methods can be viewed as approximations of this approach. These represent practical alternatives to the exact conditional distribution, which is unavailable in practice and often difficult to estimate.

The core challenge in using the conditional distribution is modeling it accurately. Methods that use the marginal distribution sample rows from the dataset (Breiman, 2001; Lundberg and Lee, 2017), and it is possible to filter for rows that agree with the features to be conditioned on (Sundararajan and Najmi, 2019); however, this technique does not work well for high-dimensional or continuous-valued data. A relaxed version of this approach is to use cohorts of rows with similar values (Mase et al., 2019).

While properly representing the conditional distribution for every subset of features is challenging, there are several approaches that provide either rough or high-quality approximations. These approaches include:

- Assume feature independence. If we assume that the features  $X_1, \ldots, X_d$  are independent, then the conditional distribution  $p(X_{\bar{S}}|X_S)$  is equivalent to the joint marginal distribution  $p(X_{\bar{S}})$ , and it is even equivalent to the product of marginals  $\prod_{i \in \bar{S}} p(X_i)$ . The removal approaches used by KernelSHAP and QII can therefore be understood as rough approximations to the conditional distribution that assume feature independence (Datta et al., 2016; Lundberg and Lee, 2017).
- Assume model linearity. As Lundberg and Lee (2017) pointed out, replacing features with their mean can be interpreted as an additional assumption of model linearity:

$$\mathbb{E}\big[f(X)\mid X_S=x_S\big] = \mathbb{E}_{p(X_{\bar{S}}\mid X_S=x_S)}\big[f(x_S,X_{\bar{S}})\big] \qquad \text{(Conditional distribution)}$$
 
$$\approx \mathbb{E}_{p(X_{\bar{S}})}\big[f(x_S,X_{\bar{S}})\big] \qquad \text{(Assume feature independence)}$$
 
$$\approx f\big(x_S,\mathbb{E}[X_{\bar{S}}]\big). \qquad \text{(Assume model linearity)}$$

While this pair of assumptions rarely holds in practice, particularly for the complex models that are the focus of explainability research, it provides some justification for methods that replace features with default values (LIME, Occlusion, MM, CXPlain, RISE).

• Generative model. FIDO-CA proposes removing features by drawing samples from a conditional generative model (Chang et al., 2018). If the generative model  $p_G$  (e.g., a conditional GAN) is trained to optimality, then it produces samples from the true conditional distribution. We can then write

$$p_G(X_{\bar{S}}|X_S) \stackrel{d}{=} p(X_{\bar{S}}|X_S), \tag{37}$$

where  $\stackrel{d}{=}$  denotes equality in distribution. Given a sample  $\tilde{x}_{\bar{S}} \sim p_G(X_{\bar{S}}|X_S=x_S)$ , the prediction  $f(x_S, \tilde{x}_{\bar{S}})$  can be understood as a single-sample Monte Carlo approximation of the expectation  $\mathbb{E}[f(X)|X_S=x_S]$ . Agarwal and Nguyen (2019) substituted the generative model approach into several existing methods (Occlusion, MP, LIME) and improved their performance across numerous metrics. Frye et al. (2020) demonstrated a similar approach using a variational autoencoder-like model (Ivanov et al., 2018), and future work could leverage other conditional generative models (Douglas et al., 2017; Belghazi et al., 2019).

• Supervised surrogate. Frye et al. (2020) proposed removing features using a supervised surrogate model. The surrogate is given access to subsets of features and is trained to predict the original model's predictions, with missing features represented by zeros (or values that do not appear in the dataset). This circumvents the task of modeling an exponential number of conditional distributions, and it is equivalent to parameterizing a subset function  $F \in \mathfrak{F}$  and training it with the following objective:

$$\min_{F} \mathbb{E}_{X} \Big[ \mathbb{E}_{S} \big[ \ell(F(X_{S}), f(X)) \big] \Big]. \tag{38}$$

In Appendix E, we prove that for certain loss functions  $\ell$ , the subset function F that optimizes this objective is equivalent to marginalizing out features using their conditional distribution. While Frye et al. (2020) focused on MSE loss, we show that a cross entropy loss can be used for classification models.

• Missingness during training. Rather than training a surrogate with missing features, we may learn the original model with missingness during training. This is equivalent to parameterizing a subset function  $F \in \mathfrak{F}$  and optimizing the following objective, which resembles standard empirical risk minimization:

$$\min_{F} \mathbb{E}_{XY} \Big[ \mathbb{E}_{S} \big[ \ell(F(X_S), Y) \big] \Big]. \tag{39}$$

In Appendix E, we prove that if the model optimizes this objective for MSE or cross entropy loss, then it is equivalent to marginalizing out features from  $f(x) \equiv F(x)$  using the conditional distribution. An important aspect of this objective is that S must be independently distributed from the data (X,Y). L2X (Chen et al., 2018a) and INVASE (Yoon et al., 2018) use a similar approach, but because the subsets depend on the data X, the resulting subset function F is not necessarily equivalent to the conditional distribution approach.

• Separate models. Finally, Shapley Net Effects (Lipovetsky and Conklin, 2001) and the original IME (Štrumbelj et al., 2009) propose training separate models for every subset of features. If each model  $\{f_S: S\subseteq D\}$  is optimal, then this approach is equivalent to marginalizing out features with their conditional distribution. This is due to a relationship that arises between models that optimize the population risk for different sets of features. For example, with cross entropy loss, the optimal model (the Bayes classifier) for  $X_S$  is given by  $f_S(x_S) = p(Y|X_S = x_S)$ , which is equivalent to  $\mathbb{E}[f_D(X)|X_S = x_S]$  because the optimal model given access to all the features is  $f_D(x) = p(Y|X = x)$ . Appendix E presents this argument in more detail.

This discussion shows that although few methods suggest removing features with the conditional distribution, numerous methods approximate this approach. Training separate models should provide the best approximation because each model is given a relatively simple task, but this is also the least scalable approach for high-dimensional datasets. The generative model amortizes knowledge of an exponential number of conditional distributions into a single model, which is scalable and effective for image data (Yu et al., 2018); the supervised surrogate and missingness during training approaches also require up to one additional model, and these are trained with far simpler optimization objectives (Eq. 38, 39) than conditional generative models.

We conclude that, under certain assumptions (feature independence, model optimality), several removal strategies are consistent with the data distribution p(X). Our definition of consistency provides a new lens for comparing different removal strategies, and Table 4 summarizes our findings.

## 8.3 Connections with information theory

Conventional wisdom suggests that explanation methods quantify the information contained in each feature. However, we find that precise information-theoretic connections can be identified only when removed features are marginalized out with their conditional distribution. Our analysis expands on prior work by showing that every removal-based explanation has a probabilistic or information-theoretic interpretation when features are removed appropriately (Owen, 2014; Chen et al., 2018a; Covert et al., 2020).

To aide our presentation, we assume that the model f is optimal, i.e., the Bayes classifier f(x) = p(Y|X = x) for classification tasks or the conditional expectation  $f(x) = \mathbb{E}[Y|X = x]$  for regression tasks. This assumption is optimistic in practice, but because models are typically trained to approximate one of these functions, model explanations are approximately based on the information-theoretic quantities derived here.

By assuming model optimality and marginalizing out removed features with their conditional distribution, we can guarantee that the prediction given any subset of features is optimal for those features. Specifically, we have the Bayes classifier  $F(x_S) = p(Y|X_S = x_S)$  in the classification case and the conditional expectation  $F(x_S) = \mathbb{E}[Y|X_S = x_S]$  in the regression case. Using these subset functions, we can derive probabilistic and information-theoretic interpretations for each explanation method.

These connections focus on the set functions analyzed by each removal-based explanation (Section 5). We present results for classification models that use cross entropy loss here,

Table 4: Consistency properties of feature removal strategies.

Removal	Methods	Consistency	
Marginalize (conditional)	Cond. permutation tests, PredDiff, SHAP, LossSHAP, SAGE, Shapley Effects	Consistent with $p(X)$	
Generative model	FIDO-CA		
Supervised surrogate	Frye et al. (2020)	Consistent with $p(X)$	
Missingness during training	L2X, INVASE		
Separate models	Feature ablation (LOCO), univariate predictors, Shapley Net Effects, IME (2009)	(assuming model optimality)	
Marginalize (marginal)	Permutation tests, KernelSHAP	Consistent with $p(X)$	
Marginalize (marginals product)	QII	(assuming independence)	
Marginalize (marginals product)	QII	Consistent with $q(X)$	
Marginalize (uniform)	IME (2010)	with feature independence	
Zeros	Occlusion, PredDiff RISE, CXPlain	Consistent with constant distributions $q(X)$	
Default values	LIME (images), MM		
Tree distribution	TreeSHAP	Not consistent with	
Extend pixel values	MIR	any $q(X)$	
Blurring	MP, EP	N 4 1:1 E 6 2	
Marginalize (replacement dist.)	LIME (tabular)	Not valid $F \in \mathfrak{F}$	

and we show analogous results for regression models in Appendix F. Under the assumptions described above, the set functions analyzed by each method can be interpreted as follows:

• The set function  $v_x(S) = F(x_S)$  represents the response variable's conditional probability for the chosen class y:

$$v_x(S) = p(y \mid X_S = x_S).$$
 (40)

This lets us examine each feature's true association with the response variable.

• The set function  $v_{xy}(S) = -\ell(F(x_S), y)$  represents the log probability of the correct class y, which is equivalent to the *pointwise mutual information* (up to a constant value):

$$v_{xy}(S) = I(y; x_S) + c. \tag{41}$$

This quantifies how much information  $x_S$  contains about the outcome y or, intuitively, how much less surprising y is given knowledge of  $x_S$  (Fano, 1961).

• The set function  $w_x(S) = -\mathbb{E}_{p(Y|X=x)}[\ell(F(x_S),Y)]$  represents the negative Kullback-Leibler divergence of the conditional probability distribution with the partial conditional probability distribution (up to a constant value):

$$w_x(S) = c - D_{KL} (p(Y \mid X = x) \mid | p(Y \mid X_S = x_S)).$$
 (42)

This is an information-theoretic measure of the deviation between the response variable's true distribution and its distribution conditioned on a subset of features (Cover and Thomas, 2012).

• The set function  $v(S) = -\mathbb{E}_{XY}[\ell(F(X_S), Y)]$  represents the mutual information with the response variable (up to a constant value):

$$v(S) = I(Y; X_S) + c. \tag{43}$$

This quantifies the amount of information, or the amount of predictive power, that the features  $X_S$  communicate about the response variable Y (Cover and Thomas, 2012).

• The set function  $w(S) = -\mathbb{E}_{XY}[\ell(F(X_S), f(X))]$  represents how much information  $X_S$  communicates about the model output f(X). Specifically, if we define Z to be a categorical random variable  $Z \sim \text{Cat}(f(X))$ , then we have:

$$w(S) = I(Z; X_S) + c. (44)$$

This result does not require model optimality, but under the assumption that f is the Bayes classifier, this quantity is equivalent to the mutual information with the response variable (up to a constant value):

$$w(S) = I(Y; X_S) + c. (45)$$

As noted, two assumptions are required to derive these results. The first is that features are marginalized out using the conditional distribution; although many methods use different removal approaches, they can be modified to use this approach or an approximation (Section 8.2). The second is that models are optimal; this assumption rarely holds in practice, but since conventional loss functions train models to approximate either the Bayes

Table 5: Each method's underlying set function has an information-theoretic interpretation when features are removed appropriately.

Model Behavior	SET FUNCTION	Methods	Related To
Prediction	$v_x$	Occlusion, MIR, MM, IME, QII, LIME, MP, EP, FIDO-CA, RISE, SHAP, KernelSHAP, TreeSHAP	Conditional probability, conditional expectation
Prediction loss	$v_{xy}$	LossSHAP, CXPlain	Pointwise mutual information
Prediction mean loss	$w_x$	L2X, INVASE	KL divergence with conditional distribution
Dataset loss (label)	v	Permutation tests, univariate predictors, feature ablation (LOCO), Shapley Net Effects, SAGE	Mutual information (with label)
Dataset loss (output)	w	Shapley Effects	Mutual information (with output)

classifier or the conditional expectation, we can view these information-theoretic quantities as the values that each set function approximates.

We conclude that when features are removed appropriately, explanation methods quantify the information communicated by each feature (see summary in Table 5). No single set function provides the "right" approach to model explanation; rather, these information-theoretic quantities span a range of perspectives that could be useful for understanding a complex ML model.

Removal-based explanations that are consistent with the observed data distribution can provide well-grounded insight into intrinsic statistical relationships in the data, and this is useful for finding hidden model influences (e.g., detecting bias from sensitive attributes) or when using ML as a tool to discover real-world relationships. However, this approach has the potentially surprising property that features may appear important even if they are not used by the model in a functional sense (Merrick and Taly, 2019; Chen et al., 2020). When users are more interested in the model's mechanism for calculating predictions, other removal approaches may be preferable, such as interventional approaches motivated by a causal analysis of the model (Janzing et al., 2019).

## 9. A Cognitive Perspective on Removal-Based Explanations

Model explanation tools are not typically designed based on research from the social sciences (Miller et al., 2017), but removal-based explanations have clear parallels with cognitive theories about how people understand causality. We first discuss our framework's foundation

in counterfactual reasoning and then describe the trade-off between simple explanations and those that convey richer information about models.

### 9.1 Subtractive counterfactual reasoning

Explaining a model's predictions is fundamentally a causality question: what makes the model behave this way? Each input feature is a candidate cause, multiple features may be causal, and explanations should quantify each feature's degree of influence on the model. We emphasize the distinction between this model-focused causality and causality between the input and response (e.g., whether a feature causes the outcome) because real-world causality is difficult to discern from observational data (Pearl, 2009).

In philosophy and psychology, counterfactual reasoning is a dominant tool for understanding causality. A counterfactual example changes certain facts of a situation (e.g., the route a person drove to get home) to potentially achieve a different outcome (e.g., getting home safely), and counterfactuals shed light on whether each aspect of a situation caused the actual outcome (e.g., a fatal car crash). In an influential philosophical account of causality, John Stuart Mill presented five methods of induction that use counterfactual reasoning to explain cause-effect relationships (Mill, 1884; Mackie, 1974). In the psychology literature, counterfactual thinking is the basis of multiple theories about how people explain the causes of events (Kahneman and Tversky, 1982; Hilton, 1990).

Removal-based explanations perform a specific type of counterfactual reasoning. In psychology, the process of removing an event to understand its influence on an outcome is called a *subtractive counterfactual* (Epstude and Roese, 2008), and this is precisely how removal-based explanations work. In philosophy, the same principle is called the *method of difference*, and it is one of Mill's five methods for inferring cause-effect relationships (Mill, 1884). This type of logic is also found in cognitive theories about how people understand and discuss causality (Kahneman and Tversky, 1982; Jaspars et al., 1983; Hilton, 1990).

The principle of removing something to examine its influence is pervasive in social sciences, not only as a philosophical approach but as part of descriptive psychological theories; this accounts for the remarkable prevalence of the feature removal principle in model explanation. Perhaps surprisingly, the reliance on subtractive counterfactual reasoning (or equivalently, the method of difference) has been overlooked thus far, even by work that examined the psychological basis for SHAP (Merrick and Taly, 2019; Kumar et al., 2020).

Some prior work describes the use of counterfactual reasoning in model explanation. One influential approach suggests showing users counterfactuals that adjust a small number of features to change the model output (Wachter et al., 2017). This approach undoubtedly provides information about how a model works, but many such counterfactuals may be required to represent each feature's influence. Removal-based explanations can provide more insight by concisely summarizing the results of many subtractive counterfactuals (e.g., via the Shapley value).

#### 9.2 Norm theory and the downhill rule

Subtractive counterfactuals are an intuitive way to quantify each feature's influence, but their implementation is not straightforward. Removal-based explanations aim to remove the information that a feature communicates, or subtract the fact that it was observed,

but it is not obvious how to do this: given an input  $x \in \mathcal{X}$ , it is not clear how to retain  $x_S$  while removing  $x_{\bar{S}}$ . We consult two psychological theories to contextualize the different approaches methods take.

Many removal-based explanations remove features by averaging the model output over a distribution of possible values for those features, which has a clear correspondence with the cognitive model described by Norm theory (Kahneman and Miller, 1986). According to this theory, people assess normality by gathering summary statistics from a set of recalled and simulated representations of a phenomenon (e.g., loan application outcomes for individuals with a set of characteristics). In these representations, certain features are fixed (or *immutable*) while others are allowed to vary (*mutable*); in our case these correspond to the retained and removed features, respectively.

Taking inspiration from Norm theory, we may equate a model's behavior when certain features are blocked from exerting influence (i.e., the removed features) with a "normal" outcome for the remaining features. With this perspective, we can see that Norm theory provides a cognitive justification for averaging the model output over a distribution of values for the removed features. Merrick and Taly (2019) make a similar observation to justify how SHAP removes features.

The choice of distribution when averaging outcomes is important, but Norm theory does not prescribe a specific distribution. Rather, Norm theory is a descriptive cognitive model that recognizes that individuals may have different perspectives of normality based on their experiences (Kahneman and Miller, 1986). Future model explanation research may consider how to cater explanations to users, as suggested by Miller (2019), but we also require systematic methods that do not solicit user input. We therefore consider whether any approach used by existing methods is justifiable from a cognitive perspective.

For guidance on the choice of distribution, we look to research on human tendencies when assigning blame. In their study of mental undoing, Kahneman and Tversky (1982) examined people's biases when proposing counterfactuals that change an undesirable event's outcome. Their clearest finding was the *downhill rule*, which states that people are more likely to propose changes that remove a surprising aspect of a story or otherwise increase the story's internal coherence. In other words, people are more likely to assign blame to an aspect of a situation if it has a more likely alternative that would change the outcome.

One feature removal strategy is reminiscent of the downhill rule because it considers alternative values in proportion to their plausibility. When marginalizing out removed features using their conditional distribution, alternative values and their corresponding outcomes are averaged in proportion to the coherence of the full feature set, which is represented by the data distribution  $p(X_{\bar{S}}|X_S) \propto p(X)$ . This is consistent with the downhill rule because if certain high likelihood values change the outcome, then their influence on the model will be apparent when integrating f(X) over the distribution  $p(X|X_S = x_S)$ .

In summary, Norm theory provides a cognitive analogue for removing features by averaging over a distribution of alternative values, and the downhill rule suggests that the plausibility of alternative values should be taken into account. These theories provide cognitive justification for certain approaches to removing features, but our review of relevant psychology research is far from comprehensive. However, interestingly, our findings lend support to the same approach that yields connections with information theory (Section 8), which is marginalizing out features according to their conditional distribution.

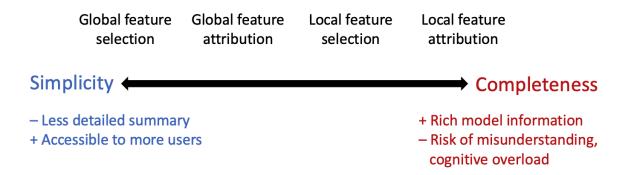


Figure 4: Each model explanation strategy represents a trade-off between an explanation's simplicity and its completeness.

## 9.3 Simplicity versus completeness

Building on our discussion of the human psychology aspect of removal-based explanations, we now discuss a trade-off between the amount of information conveyed by an explanation and the user's likelihood of drawing the correct conclusions. We describe this trade-off and then show that our framework provides the flexibility to balance these competing objectives.

Consider two explanation strategies with different levels of complexity. A counterfactual example that perturbs several features to change the model output is easy to understand, but it does not convey detailed information about a model's dependence on each feature (Wachter et al., 2017). By contrast, SHAP's feature attributions provide a complex summary of each feature's influence by quantifying the impact of removing different groups of features. Perhaps due to their greater complexity, a recent user study showed that users were less likely to understand SHAP visualizations, experiencing a higher cognitive load than users who viewed simpler explanations (Kaur et al., 2020). Similarly, a different study found that longer explanations required more time and effort to understand, and in some cases they impeded a user's ability to draw appropriate conclusions (Lage et al., 2019).

We view this as a trade-off between simplicity and completeness because explanations are typically more complex when they provide a more complete picture of a model. Providing a more complete picture seems preferable for helping users build a mental picture of how a model works, but complicated explanations risk overloading users, potentially providing them with a false or limited sense of model comprehension.

Recognizing this trade-off and its implications motivates us to consider simplicity as a design principle, and fortunately our framework has the flexibility to balance these goals. To reduce cognitive burden, one might focus on global rather than local explanations, e.g., by providing visualizations that aggregate results of many local explanations (Lundberg et al., 2020). Alternatively, one might provide global explanations that represent a model's behavior across the entire dataset by using methods such as Shapley Effects or SAGE (Owen, 2014; Covert et al., 2020).

Certain explanation formats convey richer information than others (Figure 4). Feature attributions provide a granular view of a model by considering every feature as a cause

and quantifying each feature's influence. However, psychology research shows that people report higher satisfaction with explanations that cite fewer causes (Thagard, 1989; Read and Marcus-Newhall, 1993; Lombrozo, 2007; Miller, 2019). Users may therefore derive more insight from explanations that highlight fewer causes, such as the sparse feature attributions provided by LIME (Ribeiro et al., 2016).

Feature selection explanations go even further in the direction of simplicity. These explanations directly penalize the number of selected features (Section 6.1), guaranteeing that fewer features are labeled as important, and they omit information about the granularity of each feature's influence. For a non-technical user, it may be preferable to communicate that a model's prediction was dominated by a small number of features; it may take a more sophisticated user to recognize each feature's role as a coefficient in an additive decomposition of the model's behavior (Section 7.3).

Put simply, an explanation that paints an incomplete picture of a model may prove to be more useful if the user can understand it properly. Designers of explanation methods should be wary of overestimating people's abilities to store complex mental models (Norman, 1983), and the ML community can be mindful of this by tailoring explanations to the user's degree of sophistication.

## 10. Experiments

We have thus far analyzed removal-based explanations from a theoretical standpoint, so we now conduct experiments to provide a complementary empirical perspective. Our experiments aim to accomplish three goals:

- 1. Implement and compare many new explanation methods by partially filling out the space of removal-based explanations (recall Figure 2).
- 2. Demonstrate the advantages of removing features by marginalizing them out using their conditional distribution.
- 3. Validate the existence of relationships between certain explanation methods, as predicted by our previous analysis. Explanations may be similar if they use (i) summary techniques that are probabilistic values of the same cooperative game (Section 7), or (ii) feature removal strategies that are approximately equivalent (Section 8).

To cover a wide range of possible methods, we consider many combinations of removal strategies (Section 4), model behaviors (Section 5) and summary techniques (Section 6). Code for our experiments is available online,<sup>5</sup> and we implemented 80 total methods (68 of which are new) that span our framework as follows:

• For feature removal, we considered replacing features with default values and marginalizing out features using either uniform distributions, the product of marginals, or the joint marginal. To approximate marginalizing out features using their conditional distribution, we trained supervised surrogate models to match the original model's predictions when features are held out (Frye et al., 2020). Finally, for one dataset we also trained separate models with all feature subsets.

<sup>5.</sup> https://github.com/iancovert/removal-explanations

- Our experiments analyze three *model behaviors* using three different datasets. We explained individual classification probabilities using the census income dataset (Lichman et al., 2013), the model's loss on individual predictions using MNIST images (LeCun et al., 2010), and the dataset loss for a breast cancer subtype classification task (Berger et al., 2018).
- For summary techniques, we considered removing or including individual features, the mean when included strategy, and Banzhaf and Shapley values. We used sampling-based approximations for methods that involve an exponential number of feature subsets, and we detected convergence based on the width of confidence intervals (similar to the technique described in Covert et al., 2020).

Implementing and comparing all combinations of these choices helps us better understand the similarities between methods and identify the most promising approaches. For more details about the models, datasets and hyperparameters, see Appendix G.

# 10.1 Census income

The census income dataset provides basic demographic information and the task is to predict whether a person's annual income exceeds \$50k. We trained a LightGBM model (Ke et al., 2017) and then generated explanations using the combinations of removal and summary strategies described above, including training separate models for all feature subsets (because there are only 12 features). When using the default values removal strategy, we used the mean for continuous features and the mode for discrete ones.

These combinations of choices result in 30 distinct explanation methods, several of which are equivalent to existing approaches (SHAP, QII, IME 2009, IME 2010, Occlusion, RISE, PredDiff), but most of which are new. Figure 5 shows a grid of explanations generated for a single person whose income did not exceed \$50k. We offer two remarks about these explanations:

- 1. Explanations are sometimes similar despite using different removal strategies (see the bottom four rows of Figure 5). This is likely because these removal strategies (product, marginal, surrogate, separate models) all approximate the conditional distribution. The first two rows (default values, uniform) deviate from the others because they use poor approximations of the conditional distribution.
- 2. Explanations are sometimes similar despite using different feature removal strategies (see the columns for include individual, Banzhaf and Shapley values). This may be because these summaries are probabilistic values of the same cooperative game. The remove individual strategy deviates from the others, possibly due to saturation effects when most features are included, and the mean when included strategy is not a probabilistic value (in the game-theoretic sense).

To check if these observations hold in general, we generated explanations using the same methods for 256 instances and measured the similarity between methods. To allow for a flexible comparison across removal and summary strategies, we calculated the mean correlation between explanations generated by each pair of methods. The results are shown in Figure 6, with methods grouped by removal strategy (top) or summary technique (bottom).



Figure 5: Grid of prediction explanations for a single example in the census income dataset. Each bar chart represents attribution values for a different explanation method. The vertical axis represents feature removal strategies, and the horizontal axis represents summary techniques.

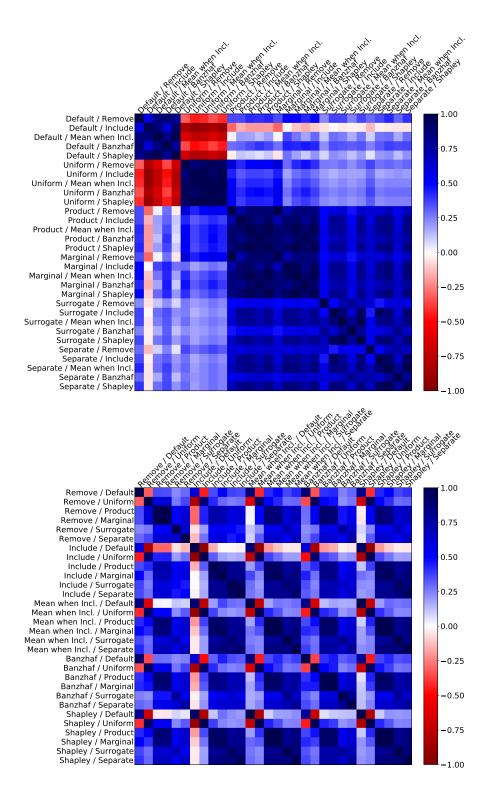


Figure 6: Mean correlation between different explanation methods on the census income dataset. Methods are grouped by their feature removal strategy (top) or summary technique (bottom).

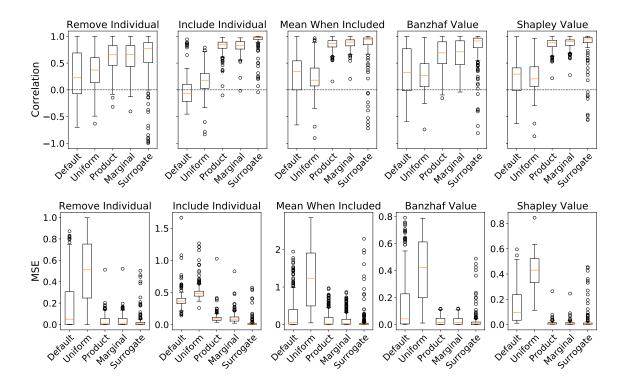


Figure 7: Boxplots quantifying the similarity of census income explanations to comparable explanations generated using separate models (a proxy for using the true conditional distribution). The similarity metrics are correlation (top, higher is better) and MSE (bottom, lower is better).

Figure 6 (top) shows that, for the census dataset, four removal strategies produce similar explanations regardless of the summary technique (default values, uniform, product, marginal). It also shows that the product of marginals and joint marginal strategies are nearly identical, suggesting that feature dependencies are not strong in this dataset. By closely examining Figure 6 (bottom), we also see that explanations generated with the Shapley value are most similar to those that include individual features or use the mean when included summary, while they are less similar to those that use the Banzhaf value.

Since many methods approximate removing features with the conditional distribution (Section 8.3), it would be useful to compare each explanation to one generated using the true conditional distribution. This is not possible in practice, so we consider the explanations generated using separate models to be our ground truth because this is our most reliable proxy. To measure each method's faithfulness to the underlying data distribution, we grouped explanations by their summary technique (e.g., include individual, Shapley value) and quantified their similarity to explanations generated using separate models (Figure 7).

For the two similarity metrics we considered (MSE and correlation), the closest approximation to using separate models is the surrogate approach, which is designed to mimic marginalizing out features with the conditional distribution. The product and marginal approaches are sometimes competitive, while the default and uniform approaches often

produce very different explanations. We remark that the surrogate has several large outliers; this suggests that although it is closer to using separate models most of the time, the surrogate is prone to occasionally making large errors.

These results suggest that to produce explanations that are faithful to the underlying data distribution, the surrogate approach provides a reliable proxy for training separate models, which itself is a proxy for marginalizing out features using the conditional distribution. However, because the surrogate approach requires training a single additional model, it provides a more scalable approach for high-dimensional datasets. Fortunately, the surrogate produces relatively fast explanations because it does not require sampling, unlike several other approaches (uniform, product, marginal).

#### **10.2 MNIST**

For the MNIST digit recognition dataset, we trained a 14 layer CNN and then generated explanations for the model's loss (rather than classification probabilities). We used zeros as default values, and, as in the previous experiment, we trained a surrogate model to approximate the conditional distribution.

The combinations of removal and summary strategies result in 25 explanation methods, only two of which correspond to existing approaches (LossSHAP, and CXPlain without the amortized explainer model). Using these methods, we generated a grid of explanations for a single example in the dataset (Figure 8). Unlike in the previous experiment, we now observe significant differences between explanations generated by each method. We make the following qualitative observations about these explanations:

- 1. The empty region at the top of the digit should be highlighted because it clearly distinguishes fours from nines. This is successfully indicated by most methods, particularly those that remove individual features or use Shapley or Banzhaf values.
- 2. Two removal strategies (uniform, product) frequently produce low quality explanations. The default value explanations are clean, but zero pixels always receive zero attribution because removing them does not impact the model; this is not ideal, because zero pixels can be highly informative.
- 3. The mean when included technique is difficult to visualize because its attributions are not marginal contributions (in the game-theoretic sense) where positive (negative) values improve (hurt) the model's loss.
- 4. When using the surrogate approach, the Shapley value explanation is most similar to the one that includes individual features. Removing individual features has a negligible impact on the model, leading to noise artifacts even when unimportant features are removed (Figure 8 bottom left). This suggests that removing individual features, which is far more common than including individual features (see Table 1), is sometimes incompatible with close approximations to the conditional distribution.

Overall, the explanation produced by the surrogate and Shapley value combination is the most visually appealing (Figure 8 bottom right); this method roughly corresponds to LossSHAP (Lundberg et al., 2020), although it uses the surrogate as an approximation of

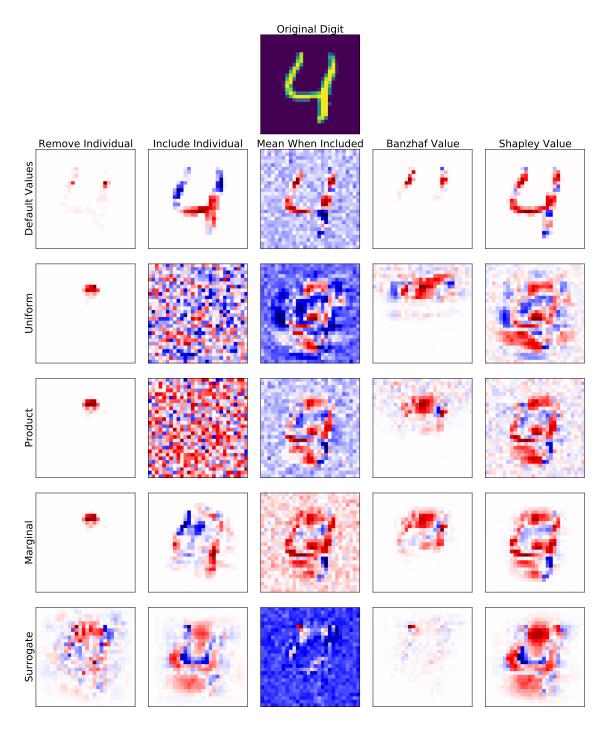


Figure 8: Grid of prediction loss explanations for a single MNIST example. The vertical axis represents feature removal strategies and the horizontal axis represents summary techniques. Red pixels improve the loss, and blue ones hurt it (except for mean when included).

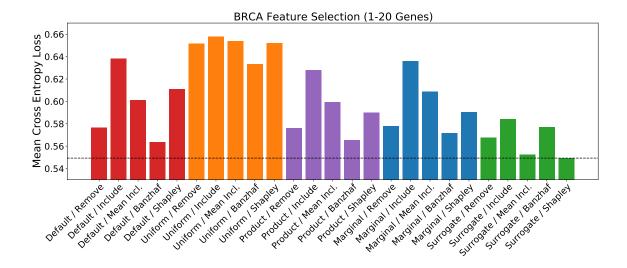


Figure 9: Feature selection results when using the top genes identified by each global explanation method (based on the dataset loss). Each bar represents the average loss for models trained using 1-20 top genes (lower is better).

the conditional distribution. For the digit displayed in Figure 8, the explanation highlights two regions at the top and bottom that distinguish the four from an eight or a nine; it has minimal noise artifacts; and it suggests that the curvature on the left side of the four may hurt the model's loss, which is highlighted by only a few other explanations. Appendix G shows more LossSHAP explanations on MNIST digits.

#### 10.3 Breast cancer subtype classification

In our final experiment, we analyzed gene microarray data from The Cancer Genome Atlas (TCGA)<sup>6</sup> for breast cancer (BRCA) patients whose tumors were classified into different molecular subtypes (Berger et al., 2018). Due to the small dataset size (only 510 patients), we prevented overfitting by analyzing a random subset of 100 genes (details in Appendix G) and training a regularized logistic regression model. Rather than explaining individual predictions, we explained the dataset loss (Section 5) to determine which genes contain the most information about BRCA subtypes.

We used the same combinations of removal and summary strategies as in the previous experiments, including using the mean expression as default values and training a surrogate model to approximate the conditional distribution. Figure 10 shows a grid of explanations generated by each method. Three of these explanations correspond to existing approaches (permutation tests, conditional permutation tests, SAGE), but many are new methods. We observe that most explanations identify the same gene as being most important (ESR1), but, besides this, the explanations are difficult to compare qualitatively. In Appendix G, we measure the similarity between each of these explanations, finding that there are often

<sup>6.</sup> https://www.cancer.gov/tcga

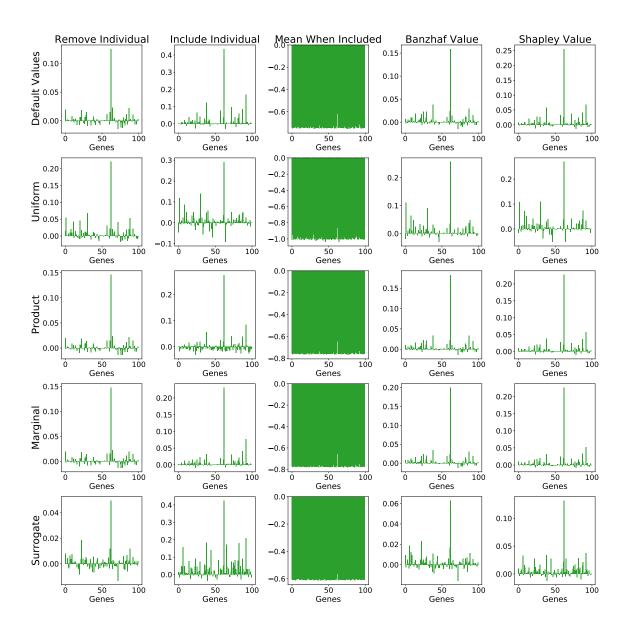


Figure 10: Grid of dataset loss explanations for BRCA subtype classification. Each bar chart represents gene attribution values for a different explanation method. The vertical axis represents feature removal strategies and the horizontal axis represents summary techniques. Positive values improve the dataset loss and negative values hurt it (except for mean when included).

similarities across removal strategies (product, marginal, surrogate) and sometimes across summary techniques (remove individual, Banzhaf, mean when included).

For a quantitative assessment of these global explanations, we evaluated each method by training new models with the most important genes. Focusing specifically on the top n genes for a particular value of n (e.g., n=10) may be misleading because different methods perform best for different values of n. Therefore, we trained separate models with the top  $n=1,2,\ldots,20$  genes and averaged their performance (Figure 9). This approach is similar to the insertion evaluation metric proposed by Petsiuk et al. (2018), and the results summarize each method's utility for performing global feature selection.

According to Figure 9, the surrogate and Shapley value combination performs best overall; this method roughly corresponds to SAGE (Covert et al., 2020), although it uses the surrogate as an approximation of the conditional distribution. The mean when included summary performs comparably, and results are generally better when using the surrogate rather than any other removal approach. Including individual features performs poorly, possibly because it neglects feature interactions; and removing features with uniform distributions consistently yields poor results.

When we performed a literature review for the most important genes identified by the surrogate and Shapley value combination, we found that many had documented BRCA associations, including ESR1 (Robinson et al., 2013), CCNB2 (Shubbar et al., 2013) and TXNL4B (Nordgard et al., 2008). Other highly ranked genes had known associations with other cancers, including DDC (Koutalellis et al., 2012) and GSS (Kim et al., 2015). We did not evaluate explanation methods based their ability to identify true associations because of the ambiguity in verifying an association from the literature. However, beyond confirming known relationships, we point out that these explanations can also be used to generate new scientific hypotheses.

# 11. Discussion

In this work, we developed a unified framework that characterizes a significant portion of the model explanation literature (25 existing methods). Removal-based explanations have a great degree of flexibility, and we systematized their differences by showing that each method is specified by three precise mathematical choices:

- 1. How the method removes features. Each method specifies a subset function  $F \in \mathfrak{F}$  to make predictions with subsets of features, often based on an existing model  $f \in \mathcal{F}$ .
- 2. What model behavior the method analyzes. Each method implicitly relies on a set function  $u: \mathcal{P}(D) \mapsto \mathbb{R}$  to represent the model's dependence on different groups of features. The set function describes the model's behavior either for an individual prediction or across the entire dataset.
- 3. How the method summarizes each feature's influence. Methods generate explanations that provide a concise summary of each feature's contribution to the set function  $u \in \mathcal{U}$ . Mappings of the form  $E : \mathcal{U} \mapsto \mathbb{R}^d$  generate feature attribution explanations, and mappings of the form  $E : \mathcal{U} \mapsto \mathcal{P}(D)$  generate feature selection explanations.

Our framework reveals that the literature is highly interconnected, and it demonstrates that many popular approaches are constructed in a similar manner and based on combinations of interchangeable choices. This perspective raises questions about the degree of novelty in recent work, but we also believe that each method has the potential to offer unique advantages, either computationally or conceptually.

To shed light on the relationships and trade-offs between different methods, we explored perspectives from three related fields that have been overlooked by most explainability research: cooperative game theory (Section 7), information theory (Section 8) and cognitive psychology (Section 9). We found that removal-based explanations are a simple application of subtractive counterfactual reasoning, or, equivalently, of Mill's method of difference, and we showed that most explanation methods can be framed through existing ideas in cooperative game theory and information theory.

Consulting the game theory literature helped us draw connections between several approaches that can be viewed as *probabilistic values* (in the game-theoretic sense), and which are equivalent to fitting a weighted linear regression model to a cooperative game (Ribeiro et al., 2016). We also found that many feature selection methods can be understood in terms of coalitional *excess*, and that these approaches are generalized by the Masking Model method (Dabkowski and Gal, 2017). These competing summarization techniques can be compared through the axioms they satisfy (e.g., the Shapley axioms) and through their ease of interpretation for users (Section 9).

Because of its axiomatic derivation and its many desirable properties, the Shapley value provides, in our view, the most complete summary of how a model works. However, while several approaches have accelerated Shapley value approximation (Štrumbelj and Kononenko, 2010; Lundberg and Lee, 2017; Lundberg et al., 2020), these techniques remain considerably slower than the fastest removal-based explanations (Dabkowski and Gal, 2017; Chen et al., 2018a; Schwab and Karlen, 2019), particularly in the model-agnostic setting. Shapley value-based explanations may not always be the best choice: they can be difficult for users to interpret due to their complexity, and variations of the Shapley value may be required to reflect causal relationships in the data (Frye et al., 2019).

Building on work that discusses probabilistic and information-theoretic explanations (Owen, 2014; Chen et al., 2018a; Covert et al., 2020), we found that multiple model behaviors can be understood as information-theoretic quantities. These connections require that removed features are marginalized out using their conditional distribution, and although this approach is challenging to implement, we showed that several removal strategies provide high-quality approximations (e.g., generative modeling approaches and models trained with missing features). Our work is among a growing number of papers lending support to this approach (Strobl et al., 2008; Zintgraf et al., 2017; Agarwal and Nguyen, 2019; Aas et al., 2019; Slack et al., 2020; Covert et al., 2020; Frye et al., 2020), but we present a novel perspective on why this choice is justified (Section 8).

We recognize, however, that users will not always want information-theoretic explanations. These explanations have the potentially undesirable property that features may be deemed important even if they are not used by the model in a functional sense; this property is useful in certain applications (e.g., bias detection), but in other cases it may seem misleading to users. Another concern with this approach is spreading credit among correlated features (Merrick and Taly, 2019; Kumar et al., 2020), but recent work argues

for sparsifying attributions using a variant on the Shapley value (Frye et al., 2019); interestingly, this is a solution in the third dimension of our framework (summary technique) for a problem that arises from a choice in the first dimension (removal strategy).

The growing interest in black-box ML models has spurred a remarkable amount of model explanation research, and in the past decade we have seen a number of publications proposing innovative new methods. However, as the field has matured we have also seen a growing number of unifying theories that reveal underlying similarities and implicit relationships (Lundberg and Lee, 2017; Ancona et al., 2017; Covert et al., 2020). Our framework for removal-based explanations is perhaps the broadest unifying theory yet, and it bridges the gap between disparate parts of the explainability literature. We believe that this work represents an important step towards making the field more organized and rigorous.

An improved understanding of the literature presents new opportunities for both explainability practitioners and researchers. For practitioners, our framework enables more explicit reasoning about the trade-offs between available explanation tools. The unique advantages of different methods are difficult to understand when each approach is viewed as a monolithic algorithm, but disentangling their choices makes it simpler to reason about their strengths and weaknesses and potentially develop hybrid methods (as demonstrated in Section 10).

For researchers, our framework offers a new theoretical perspective that can guide and strengthen ongoing research. Using the tools we developed, future work will be better equipped to (i) specify the dimensions along which new methods differ from existing ones, (ii) distinguish the substance of new approaches from their approximations (to avoid presenting methods as monolithic algorithms), (iii) fix shortcomings in existing explanation methods using solutions along different dimensions of the framework, and (iv) rigorously justify new approaches in light of their connections with cooperative game theory, information theory and psychology. As the number of removal-based explanations continues to grow, we hope that our framework will serve as a strong foundation upon which future research can build.

# Appendix A. Method Details

Here, we provide additional details about some of the explanation methods discussed in the main text. In several cases, we presented generalized versions of methods that deviated from their explanations in the original papers.

## A.1 Meaningful Perturbations (MP)

Meaningful Perturbations (Fong and Vedaldi, 2017) considers multiple ways of deleting information from an input image, and the approach it recommends is a blurring operation. Given a mask  $m \in [0,1]^d$ , MP uses a function  $\Phi(x,m)$  to denote the modified input and suggests that the mask may be used to 1) set pixels to a constant value, 2) replace them with Gaussian noise, or 3) blur the image. In the blurring approach, each pixel  $x_i$  is blurred separately using a Gaussian kernel with standard deviation given by  $\sigma \cdot m_i$  (for a user specified  $\sigma > 0$ ).

To prevent adversarial solutions, MP incorporates a total variation norm on the mask, upsamples it from a low-resolution version, and uses a random jitter on the image during optimization. Additionally, MP uses a continuous mask  $m \in [0,1]^d$  in place of a binary mask  $\{0,1\}^d$  and the  $\ell_1$  penalty on the mask in place of the  $\ell_0$  penalty. Although MP's optimization tricks are key to providing visually compelling explanations, our presentation focuses on the most essential part of the optimization objective, which is reducing the classification probability while blurring only a small part of the image (Eq. 24).

## A.2 Extremal Perturbations (EP)

Extremal Perturbations (Fong et al., 2019) is an extension of MP with several modifications. The first is switching the objective from a "removal game" to a "preservation game," which means learning a mask that retains rather than removes the salient information. The second is replacing the penalty on the subset size (or the mask norm) with a constraint. In practice, the constraint is enforced using a penalty, but the authors argue that it should still be viewed as a constraint due to the use of a large regularization parameter.

EP uses the same blurring operation as MP and introduces new tricks to ensure a smooth mask, but our presentation focuses on the most important part of the optimization problem, which is maximizing the classification probability while blurring a fixed portion of the image (Eq. 26).

#### A.3 FIDO-CA

FIDO-CA (Chang et al., 2018) is similar to EP but it replaces the blurring operation with features drawn from a generative model. The generative model  $p_G$  can condition on arbitrary subsets of features, and although its samples are non-deterministic, FIDO-CA achieves strong results using a single sample. The authors consider multiple generative models but recommend a generative adversarial network (GAN) that uses contextual attention (Yu et al., 2018). The optimization objective is based on the same "preservation game" as EP, and the authors use the Concrete reparameterization trick (Maddison et al., 2016) for optimization.

## A.4 Minimal Image Representation (MIR)

In the Minimal Image Representation approach, Zhou et al. (2014) remove information from an image to determine which regions are salient for the desired class. MIR works by creating a segmentation of edges and regions and iteratively removing segments from the image (selecting those that least decrease the classification probability) until the remaining image is incorrectly classified. We view this as a greedy approach for solving the constrained optimization problem

$$\min_{S} |S| \quad \text{s.t. } u(S) \ge t,$$

where u(S) represents the prediction with the specified subset of features and t represents the minimum allowable classification probability. Our presentation of MIR in the main text focuses on this view of the optimization objective rather than the specific greedy algorithm MIR uses (Eq. 25).

## A.5 Masking Model (MM)

The Masking Model approach (Dabkowski and Gal, 2017) observes that removing salient information (while preserving irrelevant information) and removing irrelevant information (while preserving salient information) are both reasonable approaches to understanding image classifiers. The authors refer to these tasks as discovering the smallest destroying region (SDR) and smallest sufficient region (SSR).

The authors adopt notation similar to Fong and Vedaldi (2017), using  $\Phi(x, m)$  to denote the transformation to the input given a mask  $m \in [0, 1]^d$ . For an input  $x \in \mathcal{X}$ , the authors aim to solve the following optimization problem:

$$\min_{m} \lambda_1 \text{TV}(m) + \lambda_2 ||m||_1 - \log f(\Phi(x, m)) + \lambda_3 f(\Phi(x, 1 - m))^{\lambda_4}.$$

The TV (total variation) and  $\ell_1$  penalty terms are both similar to MP and respectively encourage smoothness and sparsity in the mask. Unlike MP, MM learns a global explainer model that outputs approximate solutions to this problem in a single forward pass. In the main text, we provide a simplified presentation of the problem that does not include the logarithm in the third term or the exponent in the fourth term (Eq. 28). We view these as monotonic link functions that provide a more complex trade-off between the objectives but that are not necessary for finding informative solutions.

### A.6 Learning to Explain (L2X)

The first theorem of the L2X paper (Chen et al., 2018a) says that the explanation they seek is the distribution that optimizes the following objective:

$$\epsilon^*(x) = \underset{|S|=k}{\arg\min} \ -\mathbb{E}\big[\log p(Y \mid X_S = x_S) \mid X = x\big].$$

If we replace the conditional probability with a subset function  $F(x_S) = p(Y|X_S = x_S)$  and allow for loss functions other than cross entropy, then we recover the version of this problem that we present in the main text. The L2X paper focuses on classification problems

and an interpretation of their approach in terms of mutual information maximization; for a regression task evaluated with MSE loss, the approach could be interpreted analogously as performing conditional variance minimization. Our presentation of L2X's information-theoretic interpretation does not allude to mutual information because we focus on what L2X represents for individual predictions (Section 8.3).

## A.7 Instance-wise Variable Selection (INVASE)

The INVASE method (Yoon et al., 2018) is very similar to L2X, but it parameterizes the selector model differently. Rather than constraining the explanations to contain exactly k features, INVASE generates a set of features from a factorized Bernoulli distribution conditioned on the input  $x \in \mathcal{X}$ , using a regularization parameter  $\lambda > 0$  to control the trade-off between the number of features and the expected value of the loss function. Instead of optimizing the selector model with reparameterization gradients, INVASE is learned using an actor-critic approach.

### A.8 Prediction Difference Analysis (PredDiff)

Prediction Difference Analysis (Zintgraf et al., 2017) removes individual features (or groups of features) and analyzes the difference in a model's prediction. Removed pixels are imputed by conditioning on their bordering pixels, which approximates sampling from the full conditional distribution. Rather than measuring the prediction difference directly, the authors use attribution scores based on the log-odds ratio:

$$a_i = \log \frac{F(x)}{1 - F(x)} - \log \frac{F(x_{D \setminus \{i\}})}{1 - F(x_{D \setminus \{i\}})}.$$

We view this as another way of analyzing the difference in the model output for an individual prediction.

#### A.9 Causal Explanations (CXPlain)

CXPlain removes single features (or groups of features) for individual inputs and measures the change in the loss function (Schwab and Karlen, 2019). The authors propose calculating the attribution values

$$a_i(x) = \ell(F(x_{D\setminus\{i\}}), y) - \ell(F(x, y))$$

and then computing the normalized values

$$w_i(x) = \frac{a_i(x)}{\sum_{j=1}^d a_j(x)}.$$

The normalization step enables the use of a learning objective based on Kullback-Leibler divergence for the explainer model, which is ultimately used to calculate attribution values in a single forward pass. The authors explain that this approach is based on a "causal objective," but CXPlain is causal in the same sense as every other method described in our work (Section 9).

## A.10 Randomized Input Sampling for Explanation (RISE)

The RISE method (Petsiuk et al., 2018) begins by generating a large number of randomly sampled binary masks. In practice, the masks are sampled by dropping features from a low-resolution mask independently with probability p, upsampling to get an image-sized mask, and then applying a random jitter. Due to the upsampling, the masks have values  $m \in [0,1]^d$  rather than  $m \in \{0,1\}^d$ .

The mask generation process induces a distribution over the masks, which we denote as p(m). The method then uses the randomly generated masks to obtain a Monte Carlo estimate of the following attribution values:

$$a_i = \frac{1}{\mathbb{E}[M_i]} \mathbb{E}_{p(M)} [f(x \odot M) \cdot M_i].$$

If we ignore the upsampling step that creates continuous mask values, we see that these attribution values are the mean prediction when a given pixel is included:

$$a_{i} = \frac{1}{\mathbb{E}[M_{i}]} \mathbb{E}_{p(M)} [f(x \odot M) \cdot M_{i}]$$

$$= \sum_{m \in \{0,1\}^{d}} f(x \odot m) \cdot m_{i} \cdot \frac{p(m)}{\mathbb{E}[M_{i}]}$$

$$= \mathbb{E}_{p(M|M_{i}=1)} [f(x \odot M)].$$

# A.11 Interactions Methods for Explanations (IME)

IME was presented in two separate papers (Štrumbelj et al., 2009; Štrumbelj and Kononenko, 2010). In the original version, the authors recommended training a separate model for each subset of features. In the second version, the authors proposed the more efficient approach of marginalizing out the removed features from a single model f.

The latter paper is ambiguous about the specific distribution used to marginalize out held out features (Štrumbelj and Kononenko, 2010). Lundberg and Lee (2017) view that features are marginalized out using their distribution from the training dataset (i.e., the marginal distribution). In contrast, Merrick and Taly (2019) view IME as marginalizing out features using a uniform distribution. Upon a close reading of the paper, we opt for the uniform interpretation, but the specific interpretation of IME's choice of distribution does not impact any of our conclusions.

#### A.12 SHAP

SHAP (Lundberg and Lee, 2017) explains individual predictions by decomposing them with the game-theoretic Shapley value (Shapley, 1953), similar to IME (Štrumbelj et al., 2009; Štrumbelj and Kononenko, 2010) and QII (Datta et al., 2016). The original work proposed marginalizing out removed features with their conditional distribution but remarked that the joint marginal provided a practical approximation (see Section 8.2 for a similar argument). Marginalizing using the joint marginal distribution is now the default behavior. KernelSHAP is an approximation approach based on solving a weighted linear regression problem (Lundberg and Lee, 2017).

#### A.13 TreeSHAP

TreeSHAP uses a unique approach to handle held out features in tree-based models (Lundberg et al., 2020). It accounts for missing features using the distribution induced by the underlying trees, and, since it exhibits no dependence on the held out features, it is a valid extension of the original model. However, it cannot be viewed as marginalizing out features using a simple distribution.

Given a subset of features, TreeSHAP makes a prediction separately for each tree and then combines each tree's prediction in the standard fashion. But when a split for an unknown feature is encountered, TreeSHAP averages predictions over the multiple paths in proportion to how often the dataset follows each path. This is similar but not identical to the conditional distribution because each time this averaging step is performed, TreeSHAP conditions only on coarse information about the features that preceded the split.

#### A.14 LossSHAP

LossSHAP is a version of SHAP that decomposes the model's loss for an individual prediction rather than the prediction itself. The approach was first considered in the context of TreeSHAP (Lundberg et al., 2020), and it has been discussed in more detail as a local analogue to SAGE (Covert et al., 2020).

## A.15 Shapley Net Effects

Shapley Net Effects (Lipovetsky and Conklin, 2001) was originally proposed for linear models that use MSE loss, but we generalize the method to arbitrary model classes and arbitrary loss functions. Unfortunately, Shapley Net Effects quickly becomes impractical with large numbers of features or non-linear models.

### A.16 Shapley Effects

Shapley Effects analyzes a variance-based measure of a function's sensitivity to its inputs, with the goal of discovering which features are responsible for the greatest variance reduction in the model output (Owen, 2014). The cooperative game described in the paper is:

$$u(S) = \operatorname{Var} \Big( \mathbb{E} \big[ f(X) \mid X_S \big] \Big).$$

We present a generalized version to cast this method in our framework. In the appendix of Covert et al. (2020), it was shown that this game is equal to:

$$u(S) = \operatorname{Var}\left(\mathbb{E}[f(X) \mid X_S]\right)$$

$$= \operatorname{Var}(f(X)) - \mathbb{E}\left[\operatorname{Var}(f(X) \mid X_S)\right]$$

$$= c - \mathbb{E}\left[\ell\left(\mathbb{E}[f(X) \mid X_S], f(X)\right)\right]$$

$$= c - \mathbb{E}\left[\ell\left(F(X_S), f(X)\right)\right].$$
Dataset loss w.r.t. output

This derivation assumes that the loss function  $\ell$  is MSE and that the subset function F is  $F(x_S) = \mathbb{E}[f(X) \mid X_S = x_S]$ . Rather than the original formulation, we present a cooperative game that is equivalent up to a constant value and that provides flexibility in the choice of loss function:

$$w(S) = -\mathbb{E}\Big[\ell\big(F(X_S), f(X)\big)\Big].$$

## Appendix B. LIME Proofs

LIME calculates feature attribution values by fitting a weighted regularized linear model to an *interpretable representation* of the input (Ribeiro et al., 2016). If we consider that the interpretable representation is binary, then the model is effectively represented by a set function  $u: \mathcal{P}(D) \mapsto \mathbb{R}$  when we take an expectation over the distribution of possible feature imputations. LIME is therefore equivalent to fitting a linear model to a set function, which means solving the optimization problem

$$\min_{b_0,\ldots,b_d} L(b_0,\ldots,b_d) + \Omega(b_1,\ldots,b_d),$$

where we define L as follows:

$$L(b_0, \dots, b_d) = \sum_{S \subseteq D} \pi(S) \left( b_0 + \sum_{i \in S} b_i - u(S) \right)^2.$$
 (46)

Here, we show that several familiar attribution values can be derived within the LIME framework by selecting different weighting kernels  $\pi$  and removing the regularization term (i.e., setting  $\Omega = 0$ ).

## **B.1** Include individual

Consider the weighting kernel  $\pi_{\text{Inc}}(S) = \mathbb{1}(|S| \leq 1)$ , which puts weight only on coalitions that have no more than one player. With this kernel, the weighted least squares problem reduces to:

$$a_1, \dots a_d = \underset{b_0, \dots, b_d}{\operatorname{arg \, min}} \left( b_0 - u(\{\}) \right)^2 + \sum_{i=1}^d \left( b_0 + b_i - u(\{i\}) \right)^2.$$

It is clear that the unique global minimizer of this function is given by the following solution:

$$a_0 = u(\{\})$$
  
 $a_i = u(\{i\}) - u(\{\}).$ 

LIME will therefore calculate the attribution values  $a_i = u(\{i\}) - u(\{\})$ , which is equivalent to how Occlusion, PredDiff and CXPlain calculate local feature importance and how permutation tests and feature ablation (LOCO) summarize global feature importance (Breiman, 2001; Strobl et al., 2008; Zeiler and Fergus, 2014; Zintgraf et al., 2017; Lei et al., 2018; Schwab and Karlen, 2019).

### **B.2** Remove individual

Consider the weighting kernel  $\pi_{\text{Ex}}(S) = \mathbb{1}(|S| \ge d-1)$ , which puts weight only on coalitions that are missing no more than one player. With this kernel, the weighted least squares problem reduces to:

$$a_1, \dots, a_d = \underset{b_0, \dots, b_d}{\operatorname{arg \, min}} \left( b_0 + \sum_{j \in D} b_j - u(D) \right)^2 + \sum_{i=1}^d \left( b_0 + \sum_{j \in D \setminus \{i\}} b_j - u(D \setminus \{i\}) \right)^2.$$

It is clear that the unique global minimizer of this function is given by the following solution:

$$a_0 = u(D) - \sum_{i \in D} a_i$$
$$a_i = u(D) - u(D \setminus \{i\}).$$

LIME will therefore calculate the attribution values  $a_i = u(D) - u(D \setminus \{i\})$ , which is equivalent to how the univariate predictors approach summarizes global feature importance (Guyon and Elisseeff, 2003).

#### B.3 Banzhaf value

Consider the weighting kernel  $\pi_B(S) = 1$ , which yields an unweighted least squares problem. This version of LIME's optimization problem has been analyzed in prior work, which showed that the optimal coefficients are the Banzhaf values (Hammer and Holzman, 1992).

As an alternative proof to this work, we demonstrate that a solution that uses the Banzhaf values is optimal by proving that its partial derivatives are zero. To begin, consider the following possible solution, which uses the Banzhaf values  $a_i = \psi_i(u)$  for i = 1, ..., d and a carefully chosen intercept term  $a_0$ :

$$a_0 = \frac{1}{2^d} \sum_{S \subseteq D} u(S) - \frac{1}{2} \sum_{j=1}^d a_j$$

$$a_i = \frac{1}{2^{d-1}} \sum_{S \subseteq D \setminus \{i\}} \left( u(S \cup \{i\}) - u(S) \right) = \psi_i(u).$$

We can verify whether this is a solution to the unweighted least squares problem by checking if the partial derivatives are zero. We begin by verifying the derivative for the intercept  $a_0$ :

$$\frac{\partial}{\partial b_0} L(a_0, \dots, a_d) = 2 \sum_{S \subseteq D} \left( a_0 + \sum_{j \in S} a_j - u(S) \right)$$
$$= 2 \left( 2^d a_0 + 2^{d-1} \sum_{j=1}^d a_j - \sum_{S \subseteq D} u(S) \right)$$
$$= 0.$$

Next, we verify the derivatives for the other parameters  $a_i$  for i = 1, ..., d:

$$\frac{\partial}{\partial b_i} L(a_0, \dots, a_d) = 2 \sum_{T \supseteq \{i\}} \left( a_0 + \sum_{j \in T} a_j - u(T) \right)$$

$$= 2 \left( 2^{d-1} a_0 + 2^{d-2} \sum_{j=1}^d a_j + 2^{d-2} a_i - \sum_{T \supseteq \{i\}} u(T) \right)$$

$$= 2^{d-1} a_i + \sum_{S \subseteq D \setminus \{i\}} \left( u(S) - u(S \cup \{i\}) \right)$$

$$= 0$$

Since the gradient is zero and the problem is jointly convex in  $(b_0, \ldots, b_d)$ , we conclude that the solution given above is optimal. The optimal coefficients  $(a_1, \ldots, a_d)$  are precisely the Banzhaf values  $(\psi_1(u), \ldots, \psi_d(u))$  of the cooperative game u (Dubey and Shapley, 1979).

### **B.4** Shapley value

LIME's weighted least squares problem is optimized by the Shapley value when we use the following weighting kernel:

$$\pi_{\rm Sh}(S) = \frac{d-1}{\binom{d}{|S|}|S|(d-|S|)}.$$

Since this connection has been noted in other model explanation works, we direct readers to existing proofs (Charnes et al., 1988; Lundberg and Lee, 2017).

#### Appendix C. Shapley Axioms for Other Approaches

Here, we describe which Shapley axioms or Shapley-like axioms apply to other summarization approaches.

### C.1 LIME Axioms

By fitting a regularized weighted least squares model to a cooperative game, LIME is effectively an explanation mapping of the form  $E: \mathcal{U} \to \mathbb{R}^d$ . We can show that this mapping satisfies certain Shapley axioms. To do so, we make the following assumptions about  $\pi$  and  $\Omega$ :

- 1. The weighting kernel  $\pi$  is non-negative and finite for all  $S \subseteq D$  except for possibly the sets  $\{\}$  and D.
- 2. The weighting kernel  $\pi$  satisfies the inequality

$$(\mathbf{1} \quad X)^T W (\mathbf{1} \quad X) \succeq 0,$$

where  $X \in \mathbb{R}^{2^d \times d}$  contains an enumeration of all subsets  $S \subseteq D$  and  $W \in \mathbb{R}^{2^d \times 2^d}$  is a diagonal matrix containing an equivalent enumeration of  $\pi(S)$  for  $S \subseteq D$ . This ensures that the part of the LIME objective represented by L is strictly convex (Eq. 46).

3. The regularizer  $\Omega$  is convex (e.g., it is either the Lasso or ridge penalty).

We now address each property in turn:

- (Efficiency) LIME satisfies the efficiency property only when the weighting kernel is chosen such that  $\pi(\{\}) = \pi(D) = \infty$ . These weights are equivalent to constraints that the optimization variables satisfy  $b_0^* = u(\{\})$  and  $\sum_{i \in D} b_i^* = u(D) u(\{\})$ . In cooperative game theory, linear models with these constraints have been referred to as faithful linear approximations (Hammer and Holzman, 1992).
- (Symmetry) LIME satisfies the symmetry axiom as long as the weighting kernel  $\pi$  and the regularizer  $\Omega$  are permutation-invariant (i.e.,  $\pi$  is a function of the subset size, and  $\Omega$  is invariant to the ordering of parameters). To see this, consider an optimal solution with parameters  $(b_0^*, \ldots b_d^*)$ . Swapping the coefficients  $b_i^*$  and  $b_j^*$  for features with identical marginal contributions gives the same objective value, so this is optimal, as well. The strict convexity of the objective function implies that there is a unique global optimum, so we conclude that  $b_i^* = b_j^*$ .
- (Dummy) The dummy property holds for the Shapley and Banzhaf weighting kernels  $\pi_{\rm B}$  and  $\pi_{\rm Sh}$ , but it does not hold in the general case for arbitrary  $\pi, \Omega$ .
- (Additivity) The additivity property holds when the regularizer is set to  $\Omega = 0$ . This can be seen by considering how the solution to a weighted least squares problem is a linear function of the response variables (Kutner et al., 2005).
- (Marginalism) Given two games u, u' where players have identical marginal contributions, we can see that u' = u + c for some  $c \in \mathbb{R}$ . LIME satisfies the marginalism property because it learns identical coefficients  $b_1^*, \ldots, b_d^*$  but different intercepts of the form  $b_0^*(u') = b_0^*(u) + c$ .

#### C.2 Feature Selection Axioms

The feature selection summarizations (MP, MIR, L2X, EP, MM) satisfy properties that are analogous to the Shapley value axioms. Each method outputs an optimal coalition  $S^* \subseteq D$  rather than an allocation  $a \in \mathbb{R}^d$ , so the Shapley value axioms do not apply directly. However, we note that each optimization problem satisfies the following analogous properties:

- (Symmetry) If there are two players i, j with identical marginal contributions and there exists an optimal coalition  $S^*$  that satisfies  $i \in S$  and  $j \notin S$ , then the coalition  $(S^* \cup \{j\}) \setminus \{i\}$  is also optimal.
- (Dummy) For a player i that makes zero marginal contribution, there must be an optimal solution  $S^*$  such that  $i \notin S^*$ .

• (Marginalism) For two games u, u' where all players have identical marginal contributions, the coalition  $S^*$  is optimal for u if and only if it is optimal for u'.

The feature selection explanations do not seem to satisfy properties that are analogous to the efficiency or additivity axioms. And, unlike the attribution case, these properties are insufficient to derive a unique method.

# Appendix D. Consistency Proofs

Here, we restate and prove the results from Section 8.1, which relate to extensions of a model  $f \in \mathcal{F}$  that are consistent (Definition 5) with a probability distribution q(X). Both results can be shown using simple applications of basic probability laws.

**Proposition 6** For a classification model  $f \in \mathcal{F}$  that estimates a discrete Y's conditional probability, there is a unique extension  $F \in \mathfrak{F}$  that is consistent with q(X). It is given by

$$F(x_S) = \mathbb{E}_{q(X_{\bar{S}}|X_S = x_S)}[f(x_S, X_{\bar{S}})],$$

where  $q(X_{\bar{S}} \mid X_S = x_S)$  is the conditional distribution induced by q(X).

**Proof** We begin by assuming the existence of a subset function  $F \in \mathfrak{F}$  that satisfies q(Y|X=x)=F(x)=f(x) for all  $x \in \mathcal{X}$  and consider how the probability axioms can be used to compute the conditional probability  $q(Y|X_S=x_S)$  given only q(X) and q(Y|X=x).

For this proof we consider the case of discrete X, but a similar argument can be used to prove the same result with continuous X. Below, we provide a step-by-step derivation of  $q(Y|X_S=x_S)$  that indicates which axioms or definitions are used in each step. (Axiom 1 refers to the countable additivity property and Axiom 2 refers to Bayes rule.)

$$q(y \mid x_S) = \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} q(y, x_{\bar{S}} \mid x_S)$$
 (Axiom 1)

$$= \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} \frac{q(y, x_S, x_{\bar{S}})}{q(x_S)}$$
 (Axiom 2)

$$= \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} q(y \mid x_S, x_{\bar{S}}) \frac{q(x_S, x_{\bar{S}})}{q(x_S)}$$
(Axiom 2)

$$= \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} f(x_S, x_{\bar{S}}) \cdot q(x_{\bar{S}} \mid x_S)$$
 (Definition of  $f$ , Axiom 2)

$$= \mathbb{E}_{q(X_{\bar{S}}|X_S = x_S)} \big[ f(x_S, X_{\bar{S}}) \big]$$
 (Definition of expectation)

This derivation shows that in order to be consistent with q(X) according to the probability laws, F must be defined as follows:

$$F(x_S) \equiv \mathbb{E}_{q(X_{\bar{S}}|X_S = x_S)} [f(x_S, X_{\bar{S}})]. \tag{47}$$

To complete the proof, we consider whether there are other ways of deriving F's behavior that may demonstrate inconsistency. The only other case to consider is whether we can

derive a unique definition for  $F(x_{S\setminus T})$  when beginning from F(x) and when beginning from  $F(x_S)$  for  $T\subset S\subset D$ . The first result is given by Eq. 47, and we derive the second result as follows:

$$\begin{split} F(x_{S\backslash T}) &= q(y\mid x_{S\backslash T}) \\ &= \sum_{x_T \in \mathcal{X}_T} q(y, x_T \mid x_{S\backslash T}) \\ &= \sum_{x_T \in \mathcal{X}_T} \frac{q(y, x_T, x_{S\backslash T})}{q(x_{S\backslash T})} \\ &= \sum_{x_T \in \mathcal{X}_T} \frac{q(y\mid x_T, x_{S\backslash T})}{q(x_{S\backslash T})} \\ &= \sum_{x_T \in \mathcal{X}_T} q(y\mid x_T, x_{S\backslash T}) \frac{q(x_T, x_{S\backslash T})}{q(x_{S\backslash T})} \\ &= \sum_{x_T \in \mathcal{X}_T} q(y\mid x_T, x_{S\backslash T}) \cdot q(x_T\mid x_{S\backslash T}) \\ &= \sum_{x_T \in \mathcal{X}_T} F(x_T, x_{S\backslash T}) \cdot q(x_T\mid x_{S\backslash T}) \\ &= \sum_{x_T \in \mathcal{X}_T} \mathbb{E}_{q(X_{\bar{S}} \mid X_S = x_S)} \big[ f(x_T, x_{S\backslash T}, X_{\bar{S}}) \big] \cdot q(x_T\mid x_{S\backslash T}) \\ &= \sum_{x_T \in \mathcal{X}_T} \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} f(x_T, x_{S\backslash T}, x_{\bar{S}}) \cdot q(x_{\bar{S}} \mid x_T, x_{S\backslash T}) \cdot q(x_T\mid x_{S\backslash T}) \\ &= \sum_{x_T \in \mathcal{X}_T} \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} f(x_T, x_{S\backslash T}, x_{\bar{S}}) \cdot q(x_T, x_{\bar{S}} \mid x_{S\backslash T}) \\ &= \mathbb{E}_{q(X_T, X_{\bar{S}} \mid X_{S\backslash T} = x_{S\backslash T})} \big[ f(X_T, x_{S\backslash T}, X_{\bar{S}}) \big] \end{aligned} \tag{Axiom 2}$$

This result shows that deriving  $F(x_{S\setminus T})$  from F(x) or from  $F(x_S)$  yields a consistent result. We conclude that our definition of F, which marginalizes out missing features with the conditional distribution induced by q(X), provides the unique extension of f that is consistent with q(X).

**Proposition 7** For a regression model  $f \in \mathcal{F}$  that estimates Y's conditional expectation, there is a unique extension  $F \in \mathfrak{F}$  that is consistent with q(X). It is given by

$$F(x_S) = \mathbb{E}_{q(X_{\bar{S}}|X_S = x_S)}[f(x_S, X_{\bar{S}})],$$

where  $q(X_{\bar{S}} \mid X_S = x_S)$  is the conditional distribution induced by q(X).

**Proof** Unlike the previous proof, F does not directly define some  $q(Y|X_S = x_S)$ . However, F represents an estimate of the conditional expectation  $\mathbb{E}[Y|X_S = x_S]$  for each  $S \subseteq D$ , so we can assume the existence of conditional distributions  $q(Y \mid X_S = x_S)$  that satisfy

$$F(x_S) = \mathbb{E}_{q(Y|X_S = x_S)}[Y].$$

We show that our probability laws are sufficient to constrain the conditional expectation represented by F to have a unique definition for each  $S \subset D$ .

Consider how the probability laws can be used to compute  $q(Y|X_S = x_S)$  given only q(X) and the assumed q(Y|X = x). For this proof, we consider the case of discrete X and Y, but a similar argument can be used to prove the same result for continuous X and Y. Below, we provide a step-by-step derivation of  $q(Y|X_S = x_S)$  that indicates which axioms or definitions are used in each step. (Axiom 1 refers to the countable additivity property and Axiom 2 refers to Bayes rule.)

$$q(y \mid x_S) = \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} q(y, x_{\bar{S}} \mid x_S)$$
 (Axiom 1)

$$= \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} \frac{q(y, x_S, x_{\bar{S}})}{q(x_S)} \tag{Axiom 2}$$

$$= \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} q(y|x_S, x_{\bar{S}}) \frac{q(x_S, x_{\bar{S}})}{q(x_S)}$$
(Axiom 2)

$$= \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} q(y \mid x_S, x_{\bar{S}}) \cdot q(x_{\bar{S}} \mid x_S)$$
 (Axiom 2)

$$= \mathbb{E}_{q(X_{\bar{S}} \mid X_S = x_S)} \big[ q(y \mid x_S, X_{\bar{S}}) \big] \tag{Definition of expectation}$$

This derivation shows that in order to be consistent with q(X), the conditional distribution  $q(Y|X_S=x_S)$  must be defined as follows:

$$q(Y \mid X_S = x_S) = \mathbb{E}_{q(X_{\bar{S}} \mid X_S = x_S)}[q(x_S, X_{\bar{S}})].$$

Since F represents the expectation of these distributions, it can be derived as follows:

$$F(x_S) = \mathbb{E}_{q(Y \mid X_S = x_S)}[Y]$$
 (Definition of  $F$ )
$$= \sum_{y \in \mathcal{Y}} y \cdot q(y \mid x_S)$$
 (Definition of expectation)
$$= \sum_{y \in \mathcal{Y}} \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} y \cdot q(y \mid x_S, x_{\bar{S}}) \cdot q(x_{\bar{S}} \mid x_S)$$
 (Previous derivation)
$$= \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} \mathbb{E}[Y \mid x_S, x_{\bar{S}}] \cdot q(x_{\bar{S}} \mid x_S)$$
 (Interchanging order of sums)
$$= \sum_{x_{\bar{S}}} f(x_S, x_{\bar{S}}) \cdot q(x_{\bar{S}} \mid x_S)$$
 (Definition of  $f$ )
$$= \mathbb{E}_{q(X_{\bar{S}} \mid X_S = x_S)}[f(x_S, X_{\bar{S}})]$$
 (Definition of expectation)

According to this result, the probability laws imply that F must be defined as follows:

$$F(x_S) \equiv \mathbb{E}_{q(X_{\bar{S}}|X_S = x_S)} [f(x_S, X_{\bar{S}})]. \tag{48}$$

To complete the proof, we consider whether there are other ways of deriving F's behavior that may demonstrate inconsistency. The only other case to consider is whether we can derive a unique definition for  $F(x_{S\setminus T})$  when beginning from F(x) and when beginning from F(x) for  $T \subset S \subset D$ . The first result is given by Eq. 48, and we now derive the second result. To begin, we derive  $q(Y|X_{S\setminus T})$  from  $q(Y|X_S)$ :

$$q(y \mid x_{S \setminus T}) = \sum_{x_T \in \mathcal{X}_T} q(y, x_T \mid x_{S \setminus T})$$
(Axiom 1)

$$= \sum_{x_T \in \mathcal{X}_T} \frac{q(y, x_T, x_{S \setminus T})}{q(x_{S \setminus T})}$$
 (Axiom 2)

$$= \sum_{x_T \in \mathcal{X}_T} q(y \mid x_T, x_{S \setminus T}) \frac{q(x_T, x_{S \setminus T})}{q(x_{S \setminus T})}$$
(Axiom 2)

$$= \sum_{x_T \in \mathcal{X}_T} q(y \mid x_T, x_{S \setminus T}) \cdot q(x_T \mid x_{S \setminus T})$$
 (Axiom 2)

$$= \mathbb{E}_{q(X_T \mid X_{S \setminus T} = x_{S \setminus T})} [q(y \mid x_T, x_{S \setminus T})]$$
 (Definition of expectation)

We can now derive  $F(x_{S\setminus T})$  by taking the expectation of this distribution:

$$\begin{split} F(x_{S\backslash T}) &= \mathbb{E}_{q(Y|X_{S\backslash T} = x_{S\backslash T})}[Y] & \text{(Definition of } F) \\ &= \sum_{y \in \mathcal{Y}} y \cdot q(y \mid x_{S\backslash T}) & \text{(Definition of expectation)} \\ &= \sum_{y \in \mathcal{Y}} \sum_{x_T \in \mathcal{X}_T} y \cdot q(y \mid x_T, x_{S\backslash T}) \cdot q(x_T \mid x_{S\backslash T}) & \text{(Previous derivation)} \\ &= \sum_{x_T \in \mathcal{X}_T} \mathbb{E}[Y \mid x_T, x_{S\backslash T}] \cdot q(x_T \mid x_{S\backslash T}) & \text{(Interchanging order of sums)} \\ &= \sum_{x_T \in \mathcal{X}_T} F(x_T, x_{S\backslash T}) \cdot q(x_T \mid x_{S\backslash T}) & \text{(Definition of } F) \\ &= \sum_{x_T \in \mathcal{X}_T} \sum_{x_{\bar{S}} \in \mathcal{X}_{\bar{S}}} f(x_T, x_{S\backslash T}, x_{\bar{S}}) \cdot q(x_{\bar{S}} \mid x_T, x_{S\backslash T}) \cdot q(x_T \mid x_{S\backslash T}) & \text{(Definition of } F) \\ &= \mathbb{E}_{q(X_T, X_{\bar{S}} \mid X_{S\backslash T} = x_{S\backslash T})} \big[ f(X_T, x_{S\backslash T}, X_{\bar{S}}) \big] \big] & \text{(Definition of expectation)} \end{split}$$

This result shows that deriving  $F(x_{S\backslash T})$  from F(x) or from  $F(x_S)$  yields a consistent result. We conclude that our definition of F, which marginalizes out missing features with the conditional distribution induced by q(X), provides the unique extension of f that is consistent with q(X).

## Appendix E. Conditional Distribution Approximations

We now describe how three approaches to removing features can be understood as approximations of marginalizing out missing features according to their conditional distribution.

## E.1 Separate models

Shapley Net Effects (Lipovetsky and Conklin, 2001) and the original version of IME (Štrumbelj et al., 2009) require training models for each subset of features. We denote these models as  $\{f_S: S\subseteq D\}$ . Similarly, the univariate predictors approach requires training models with individual features, and feature ablation requires training models with individual features held out. These models are used to make predictions in the presence of missing features, and they can be represented using the subset function  $F(x_S) = f_S(x_S)$ .

Note that this F satisfies the necessary properties to be an extension of  $f_D$  (invariance to missing features and agreement with  $f_D$  in the presence of all features) despite the fact that its predictions with held out features do not explicitly reference  $f_D$ . However, under the assumption that each  $f_S$  optimizes the population risk, each  $f_S$  can be understood in relation to  $f_D$ .

For a regression task where each model  $f_S$  is trained with MSE loss, the model that optimizes the population risk is the conditional expectation  $f_S(x_S) = \mathbb{E}[Y|X_S = x_S]$ . Similarly, if the prediction task is classification and the loss function is cross entropy (or another strictly proper scoring function; see Gneiting and Raftery, 2007) then the model that optimizes the population risk is the conditional probability function  $f_S(x_S) = p(Y|X_S = x_S)$ . In both cases, if each  $f_S$  for  $S \subseteq D$  optimizes the population risk, then we observe the following relationship between F and  $f_D$ :

$$F(x_S) = f_S(x_S) = \mathbb{E}[f_D(X) \mid X_S = x_S].$$

This is precisely the approach of marginalizing out missing features from  $f_D$  with their conditional distribution.

### E.2 Missingness during training

Learning to explain (L2X, Chen et al., 2018a) is not a post hoc explanation method; it is based on a model learned with missingness introduced during training. L2X (Chen et al., 2018a) and INVASE (Yoon et al., 2018) are based on a model learned with missingness during training. These methods train a model where zeros (or potentially other values) take the place of removed features, so that the model can recognize these as missing values and make the best possible prediction given the available information.

We show here how this approach can be understood as an approximation of marginalizing out features with their conditional distribution. First, we note that replacing features with a default value is problematic if that value is observed in the dataset because the model then faces ambiguity about whether the value is real or represents missingness. This issue can be resolved either by ensuring that the replacement value does not occur in the dataset or by providing a mask vector  $m \in \{0,1\}^d$  indicating missingness as an additional input to the model.

We assume for simplicity that this binary vector is provided as an additional input, and we let  $x \odot m$  (the element-wise product) represent feature masking and  $f(x \odot m, m)$  denote the model's prediction. This can be viewed as a technique for parameterizing a subset function  $F \in \mathfrak{F}$  because it ensures invariance to the features that are not selected. If we let M denote a random mask variable, then the loss is:

$$\mathbb{E}_{MXY}\Big[\ell\big(f(X\odot M,M),Y\big)\Big].$$

If M is independent from (X,Y), then we can decompose the loss as follows:

$$\mathbb{E}_{MXY}\Big[\ell\big(f(X\odot M,M),Y\big)\Big] = \mathbb{E}_{M}\mathbb{E}_{XY}\Big[\ell\big(f(X\odot M,M),Y\big)\Big]$$
$$= \sum_{m} p(m) \cdot \mathbb{E}_{XY}\Big[\ell\big(f(X\odot m,m),Y\big)\Big].$$

For each value of m, we can regard  $f(x \odot m, m)$  as a separate function on the specified subset of features  $\{x_i : m_i = 1\}$ . Then, for classification tasks using cross entropy loss, the objective is optimized by  $f^*$  such that

$$f^*(x \odot m, m) = p(Y|X_S = x_S),$$

where  $S = \{i : m_i = 1\}$ . A similar result holds for regression tasks trained using MSE. In both cases, the result is equivalent to marginalizing out missing features according to their conditional distribution.

One issue with L2X and INVASE is that the mask variable M is dependent on X. Intuitively, this means that the selected features communicate information about the held out features, which then inform the model's prediction about the response variable. The L2X and INVASE models therefore may not approximate  $p(Y|X_S=x_S)$ , potentially invalidating their interpretation in terms of mutual information maximization (Chen et al., 2018a) or KL divergence minimization (Yoon et al., 2018).

Nonetheless, it is possible to learn a model with missingness introduced at training time that approximates marginalizing out features using their conditional distribution. It suffices to sample masks during training independently from the model input, e.g., by sampling masks uniformly at random or according to the distribution described in Appendix E.3.

#### E.3 Surrogate models

Rather than learning a model with missingness at training time, we can train a surrogate model to match an existing model's predictions when features are held out. This technique, described by Frye et al. (2020), also approximates marginalizing out features using their conditional distribution.

Similar to the model trained with missingness (see above), we require a model that removes the original features using a mask variable  $m \in \{0,1\}^d$ . Frye et al. (2020) suggest replacing held out features with a value that does not occur in the training set, but we can instead provide the mask as an additional input to the model. By ensuring invariance to the removed features, this is equivalent to parameterizing a subset function  $F \in \mathfrak{F}$ .

We denote the original model's predictions as f(x) and the surrogate's predictions as  $g(x \odot m, m)$ . If we let M denote a random mask variable that is independent from (X, Y), then we can train the surrogate using the following objective function:

$$\min_{q} \mathbb{E}_{X} \Big[ \mathbb{E}_{M} \Big[ \ell \big( g(X \odot M, M), f(X) \big) \Big] \Big]. \tag{49}$$

To show that optimizing this objective is equivalent to marginalizing out features using their conditional distribution, we point to a result from Covert et al. (2020) that is specific to MSE loss:

$$\min_{h} \mathbb{E}_{X} \left[ \left( f(X) - h(X_{S}) \right)^{2} \right] = \mathbb{E}_{X} \left[ \left( f(X) - \mathbb{E}[f(X) \mid X_{S}] \right)^{2} \right].$$

This shows that if we view  $g(x \odot m, m)$  as a separate function for each  $m \in \{0, 1\}^d$ , or  $h(x_S)$  for  $S = \{i : m_i = 1\}$ , then the objective function (Eq. 49) is optimized by a model that marginalizes out features according to their conditional distribution.

While Frye et al. (2020) focused on MSE loss, we opt to use a cross entropy loss rather than MSE for classification tasks. Covert et al. (2020) proved another result that is specific to cross entropy loss, which we denote here as H(a,b) for two discrete probability distributions:

$$\min_{h} \mathbb{E}_{X} \Big[ H \big( f(X), h(X_{S}) \big) \Big] = \mathbb{E}_{X} \Big[ H \big( f(X), \mathbb{E}[f(X) \mid X_{S}] \big) \Big].$$

This shows that if we train the surrogate to match the original model's predictions using cross entropy loss, then the surrogate approximates marginalizing out features according to their conditional distribution. Our experiments use this approach because they all analyze classification models.

The only detail left to specify is the distribution for M in Eq. 49. Any distribution that places mass on all  $m \in \{0,1\}^d$  should suffice, at least in principle. One natural choice is to sample masks uniformly at random, similar to applying dropout with probability 0.5. However, for models with large numbers of features, this places nearly all the probability mass on subsets with approximately half of the features included. We therefore opt to use a distribution that samples the *subset size* uniformly at random. In our experiments, we sample masks m as follows:

- 1. Sample  $k \in \{0, 1, \dots, d\}$  uniformly at random.
- 2. Sample k indices  $(i_1, \ldots, i_k)$  from  $\{1, 2, \ldots, d\}$  at random and without replacement.
- 3. Set m such that  $m_i = \mathbb{1}(i \in \{i_1, \ldots, i_k\})$ .

# Appendix F. Information Theory Connections in Regression

Here, we describe probabilistic interpretations of each explanation method's underlying set function (Section 5) in the context of regression models rather than classification models (Section 8.3). We assume that the models are evaluated using MSE loss, and, as in the main text, we assume model optimality. The different set functions have the following interpretations.

• The set function  $v_x(S) = F(x_S)$  quantifies the response variable's conditional expectation:

$$v_x(S) = \mathbb{E}[Y \mid X_S = x_S]. \tag{50}$$

This set function lets us examine each feature's true relationship with the response variable.

• The set function  $v_{xy}(S) = -\ell(F(x_S), y)$  quantifies the squared distance between the model output and the correct label:

$$v_{xy}(S) = -\left(\mathbb{E}[Y \mid X_S = x_S] - y\right)^2. \tag{51}$$

Under the assumption that the response variable's conditional distribution is Gaussian, this represents the pointwise mutual information between  $x_S$  and y up to factors that depend on S:

$$I(y; x_S) = -\log p(y) - \frac{1}{2} \log 2\pi - \frac{1}{2} \log \text{Var}(Y \mid X_S = x_S) - \frac{1}{2} \underbrace{\left(\mathbb{E}[Y \mid X_S = x_S] - y\right)^2}_{v_{xy}(S)} / \text{Var}(Y \mid X_S = x_S).$$
 (52)

• The set function  $w_x(S) = -\mathbb{E}_{p(Y|X=x)}[\ell(F(x_S),Y)]$  quantifies the squared difference of the conditional expectation from the model output, up to a constant value:

$$w_x(S) = -\left(\mathbb{E}[Y \mid X = x] - \mathbb{E}[Y \mid X_S = x_S]\right)^2 + c.$$
 (53)

Under the assumption that the response variable's distribution conditioned on X = x and  $X_S = x_S$  are both Gaussian, this quantity has a relationship with the negative Kullback-Leibler divergence between p(Y|X = x) and  $p(Y|X_S = x_S)$ :

$$D_{\mathrm{KL}}\left(p(Y\mid X=x)\mid\mid p(Y\mid X_{S}=x_{S})\right)$$

$$=\frac{1}{2}\log\frac{\mathrm{Var}(Y\mid X_{S}=x_{S})}{\mathrm{Var}(Y\mid X=x)} - \frac{1}{2}$$

$$+\left(\mathrm{Var}(Y\mid X=x) + \underbrace{\left(\mathbb{E}[Y\mid X=x] - \mathbb{E}[Y\mid X_{S}=x_{S}]\right)^{2}}_{w_{x}(S)}\right)/\left(2\cdot\mathrm{Var}(Y\mid X_{S}=x_{S})\right).$$
(54)

• The set function  $v(S) = -\mathbb{E}_{XY} \Big[ \ell \big( F(X_S), Y \big) \Big]$  quantifies the explained variance in the response variable Y, up to a constant value:

$$v(S) = \operatorname{Var}(Y) - \mathbb{E}[\operatorname{Var}(Y \mid X_S)] + c. \tag{55}$$

Using the entropy maximizing property of the Gaussian distribution (Cover and Thomas, 2012), we see that the explained variance has the following relationship with the mutual information between  $X_S$  and the response variable Y:

$$I(Y; X_S) = H(Y) - \mathbb{E}[H(Y \mid X_S)]$$

$$\geq H(Y) - \frac{1}{2} \mathbb{E}\Big[\log (2\pi e \cdot \text{Var}(Y \mid X_S))\Big]$$

$$\geq H(Y) - \frac{1}{2} \log 2\pi e - \frac{1}{2} \log \underbrace{\mathbb{E}[\text{Var}(Y \mid X_S)]}_{v(S)}.$$
(56)

Equality is achieved in the first bound if the distribution  $p(Y|X_S = x_S)$  is Gaussian. The second bound is due to Jensen's inequality.

• The set function  $w(S) = -\mathbb{E}_{XY} \Big[ \ell \big( F(X_S), f(X) \big) \Big]$  quantifies the explained variance in the model output, up to a constant value:

$$w(S) = \operatorname{Var}(f(X)) - \mathbb{E}\left[\operatorname{Var}(f(X) \mid X_S)\right] + c. \tag{57}$$

Using the same entropy maximizing property of the Gaussian distribution, we can see that the explained variance is related to the mutual information with the model output, which can be viewed as a random variable f(X):

$$I(f(X); X_S) = H(f(X)) - \mathbb{E}[H(f(X) \mid X_S)]$$

$$\geq H(f(X)) - \frac{1}{2} \mathbb{E}\Big[\log (2\pi e \cdot \text{Var}(f(X) \mid X_S))\Big]$$

$$\geq H(f(X)) - \frac{1}{2} \log 2\pi e - \frac{1}{2} \log \underbrace{\mathbb{E}\Big[\text{Var}(f(X) \mid X_S)\Big]}_{w(S)}$$
(58)

Equality is achieved in the first bound if f(X) has a Gaussian distribution when conditioned on  $X_S = x_S$ . The second bound is due to Jensen's inequality.

These results are analogous to the results from the classification case, and they show that each explanation method's set function has an information-theoretic interpretation even in the context of regression tasks. However, the regression case requires stronger assumptions about the data distribution to yield these information-theoretic links. The assumptions do not hold in the general case, but they do hold in the special case where p(X,Y) is a multivariate Gaussian distribution. To avoid strong distributional assumptions, it is more conservative to interpret these quantities in terms of Euclidean distances (Eqs. 51, 53) and conditional variances (Eqs. 55, 57).

# Appendix G. Experiment Details

### G.1 Hyperparameters

The original models used for each dataset are:

- For the census income dataset, we trained a LightGBM model with a maximum of 10 leaves per tree and a learning rate of 0.05 (Ke et al., 2017).
- For MNIST, we trained a 14 layer CNN consisting of convolutional layers with kernel size 3, max pooling layers, and ELU activations (Clevert et al., 2015). The output was produced by flattening the convolutional features and applying two fully connected layers, similar to the VGG architecture (Simonyan and Zisserman, 2014). We trained the model with Adam using a learning rate of 0.001 (Kingma and Ba, 2014).
- For the BRCA dataset, we trained a  $\ell_1$  regularized logistic regression model and selected the regularization parameter using a validation set.

For the BRCA dataset, we randomly selected a subset of 100 genes to analyze out of 17,814 total. To ensure that a sufficient number BRCA-associated genes were selected, we tried 10 random seeds for the gene selection step and selected the seed whose 100 genes achieved the best performance. The selected genes are shown in Table 6. A small portion of missing expression values were imputed with their mean. The data was centered and normalized prior to fitting the regularized logistic regression model.

When generating explanations using feature removal approaches that required sampling multiple values for the missing features (marginalizing with uniform, product of marginals, or joint marginal), we used 512 samples for the census income and MNIST datasets and 372 for the BRCA dataset (the size of the train split).

As described in the main text (Section 10) and in Appendix E.3, we trained surrogate models to represent marginalizing out features according to the conditional distribution. Our surrogate models were trained as follows:

- For the census income data, the surrogate was a MLP with a masking layer and four hidden layers of size 128 followed by ELU activations. During training, the mask variable was sampled according to the procedure described in Appendix E.3. Our masking layer replaced missing values with -1 (a value that did not occur in the dataset) and also appended the mask as an additional set of features, which improved its ability to match the original model's predictions.
- For MNIST, the surrogate was a CNN with an identical architecture to the original model (see above) except for a masking layer at the input. The masking layer replaced missing values with zeros and appended the mask along the channels dimension.
- For the BRCA data, the surrogate was an MLP with two hidden layers of size 64 followed by ELU activations. The masking layer replaced missing values with their mean and appended the mask as an additional set of features.

Genes 1-17	Genes 18-34	Genes 35-51	Genes 52-68	Genes 69-85	Genes 86-100
OSTbeta	NBR2	TSHR	HPS4	GRINA	C20orf111
STATH	CCDC64	C7	ZFPM1	YTHDF3	OMA1
MAPK10	NUP210	CRYBB2	OAS2	TMCC1	NCAPH2
PLEKHG5	HEMGN	PPAPDC3	TUBA1C	UBE1DC1	GPX2
ERO1L	SLC25A3	TXNL4B	OR8K5	C6orf15	BPY2C
ZNF711	LEF1	CHST9	THSD3	PDE6A	ZNF324
ZNF385	MVD	HACE1	ATP6V0C	PEO1	CDC27
OR52E8	OTUD3	AYTL1	RAB22A	TMEM52	CCNB2
SLC5A11	KIAA1949	PRSS35	AP1B1	PARP1	CNOT7
P4HA3	SLC44A3	ZNF408	CTAGE6	GSS	BIRC3
LHFPL4	ZNF775	DDC	C6orf26	RDH11	GAL3ST3
MGC33657	THY1	CSTL1	ESR1	STXBP1	PLEKHM1
CAPZB	DYNC1I2	OR2F1	UPK3B	ACLY	SPOCD1
RBM15B	CYP1A1	C12 orf 50	ROBO4	TMSB10	PENK
C1orf176	SPTA1	SH3YL1	TMEFF1	TUBB	TAS2R9
KLF3	CLEC4M	SNUPN	KIAA1279	LIPK	
OLFM4	RXFP3	COL25A1	ZFP36L1	HRC	

Table 6: List of genes analyzed.

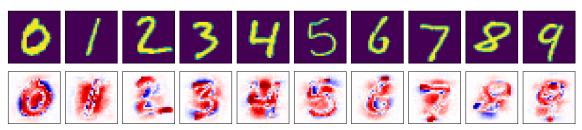


Figure 11: More MNIST prediction loss explanations using LossSHAP (feature removal with the conditional distribution and summary with the Shapley value).

### G.2 Additional results

We present two supplementary results for the experiments described in Section 10. Figure 11 shows more examples of MNIST explanations using the combination of the conditional distribution and Shapley value (i.e., LossSHAP). These explanations consistently highlight important pixels within the digit as well as empty regions that distinguish the digit from other possible classes (e.g., see 3, 4, 9).

Figure 12 quantifies the similarity between dataset loss explanations for the BRCA dataset using their correlation (top) and Spearman rank correlation (bottom). We see patterns in these explanations that are similar to the census explanations (Figure 6); explanations that remove individual features or use the mean when included or Banzhaf value summary are often strongly correlated. Explanations generated by removing features using different marginalizing strategies are less similar than in the census dataset, which suggests

the presence of strong feature correlations. Interestingly, the Shapley value explanations are more strongly correlated across different removal strategies than they are to other explanations that remove features in the same way (see bottom row of Figure 12).

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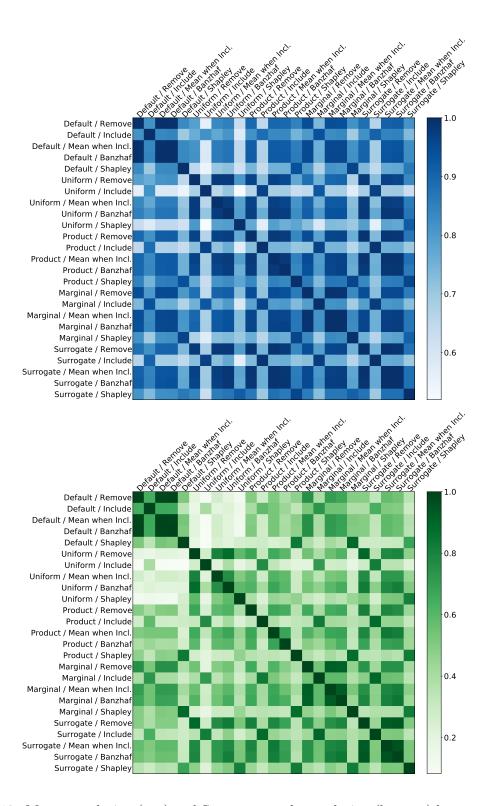


Figure 12: Mean correlation (top) and Spearman rank correlation (bottom) between different explanation methods on the BRCA dataset.

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