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A Detailed Survey of Machine Learning Interpretability through Feature Interactions and Additive Models

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Abstract

Interpretability has gained an immense amount of popularity over the past decade, mostly riding the wake of neural networks' impact on the field of machine learning. The growth in success and application of neural networks, as well as other blackbox machine learning approaches, in everyday life has led to a revitalized interest in understanding the blackbox models making those decisions. In this survey, we give a holistic coverage of the current state of the interpretability literature, focusing on a detailed coverage only for machine learning tasks and feature interaction methods like SHAP explanations, functional ANOVA, and the generalized additive model. We achieve this by first mapping out the many different subareas and paradigms under the larger umbrella of the *Interpretability* or *XAI* literature. We next isolate the scope of this survey and provide a detailed account of historical developments leading to the modern convergence of interpretability through feature interactions and interpretability through additive models. Finally, we conclude with a discussion of specific domains of application and with future directions for interpretability.

Keywords: interpretability, explainability, XAI, IML, feature interactions, additive model, generalized additive model, Shapley value, SHAP, ANOVA, functional ANOVA, functional decomposition, interactions, higher-order interactions

1. Introduction

Blackbox algorithms, developed using a variety of deep learning and machine learning techniques, have quickly become an integral part of daily life in the 21st century as AI applications continue to propagate throughout scientific, industrial, and commercial applications. As these machine learning approaches continue to deliver on their promise of accurate predictions in exchange for big data, the question of *how* a blackbox algorithm makes its decisions or predictions has only grown in importance and frequency. Despite the considerable attention on the problem of how blackbox models transform large datasets into predictive insights, there remain no universal solutions to explain the behavior of these models.

Interpretability is the field born out of studying this question of interpreting, explaining, and understanding the how and the why of predictions made by blackbox models. Although

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interpretation has always been in the background of statistical modeling and was even acknowledged as important in previous decades as model complexity began to grow from linear regression into increasingly opaque nonparametric models, the field would not see more dedicated study until mid 2010s. By this time, the incredible power of deep learning systems had already been demonstrated on audio, vision, and language tasks (Mohamed et al., 2011; Krizhevsky et al., 2012; Bahdanau et al., 2015), cementing these newest blackbox models as more capable at learning from raw features than any previous methods.

Given the diversity of blackbox applications and the difficulty of the blackbox question, there is, unsurprisingly, a wide variety of stylistic approaches, research cultures, and different subfields which are all working on answering the challenging questions of what to explain, how to explain, when to explain, etc. Over the past decade, there have also been many attempts to standardize, rigorize, unify, and qualify what the goals, definitions, and techniques of interpretability are. In this work, we attempt to provide an in-depth survey of a vast swath of this literature without completely disregarding other related branches within the field of interpretability. We accomplish this by narrowing our scope in two key ways. First, we restrict our attention throughout to what we will broadly call *machine learning interpretability*. Second, we focus on those methods which are related to non-additive *feature interactions*, centering our discussion on the duality between GAM and SHAP.

By first restricting our attention to “machine learning interpretability" instead of “deep learning interpretability", we mainly divide along the implicit assumption that the input features themselves are interpretable. This is sometimes referred to as the divide between “structured data" (data with interpretable features) and “unstructured data" (data without interpretable feature representations). This mostly excludes mechanistic interpretability, outside of classical mechanistic methods like gradient saliency and attention maps, due to its primary focus on vision and language data. By second focusing our attention on “feature interactions”, we will dedicate most of our time to those methods focusing on feature attribution and extensions of feature attribution called interaction attribution. We will proceed by first laying out many of the different approaches existing within interpretability before categorizing them amongst three major categories. The topic of feature interactions which we discuss in more detail will be centered around the ‘pillar’ of additive interpretability which incorporates GAM interpretations and SHAP explanations.

In Section 2, we begin by providing a high-level overview of the field of interpretability and some of the various techniques and styles used throughout the literature. By the end of the section we provide a map of the current interpretability landscape and point to exactly where we plan to focus our attention for the rest of the survey. In Section 3, we go into great detail on the explainability approach of feature interactions. In Section 4, we go into great detail on the interpretability approach of additive models. In Section 5, we detail the many applications of feature interaction approaches across vision, language, time series, graphs, and the natural sciences, also mentioning approaches beyond feature interactions when appropriate. Finally, in Section 6, we conclude with many of the open problems and active research areas both within the subfield of non-additive interactions but also in connection with the wider field of interpretability.

2. The Current Map of Interpretability

Given that the goal of interpretability ('to understand the black box') is extremely broad, the methods which researchers have developed to tackle the problem have become equally broad. We use this section to provide a high-level map of the large and diverse space of interpretability and related fields before clarifying which 'part of the map' we will explore in the greatest detail throughout the course of this survey.

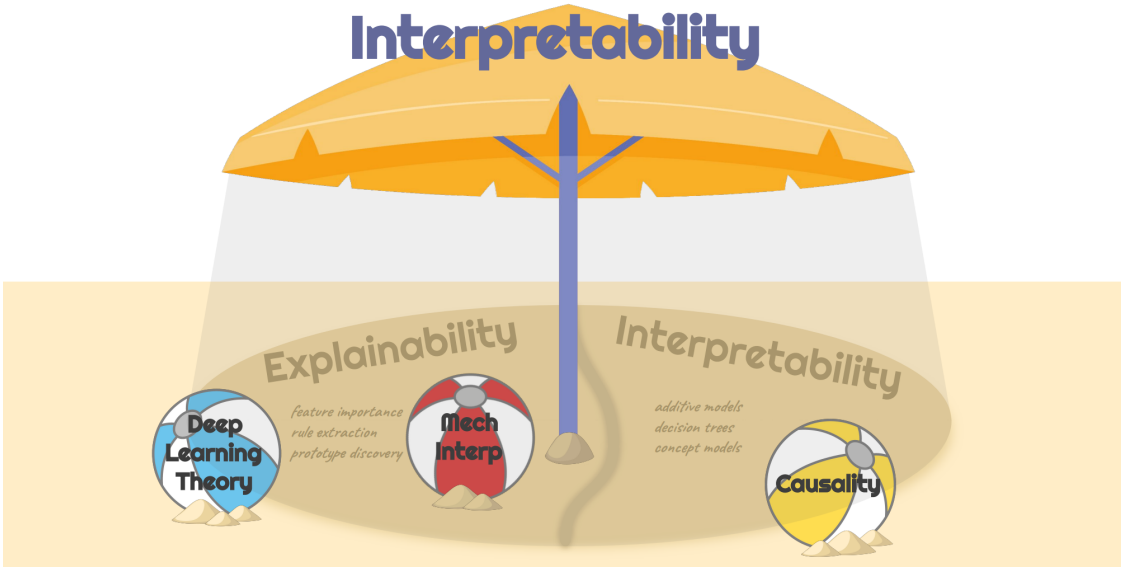

Figure 1: A high-level view of the umbrella of Interpretability research. There is a large line in the sand to distinguish the subgoals of interpretability and explainability. Fields like mechanistic interpretability fall entirely under the umbrella of interpretability, whereas fields like deep learning theory and causality only partially intersect with the goals of interpretability.

2.1 Areas Related to Interpretability

Explainability vs. Interpretability We begin by recalling the key distinction within interpretability research which is rarely known outside of the field: that is the distinction between explanation approaches and interpretation approaches. Of course, in natural language, these two words are nearly synonymous.

In Figure 1, we depict the larger field of Interpretability as the umbrella field which covers many approaches related to interpreting and understanding blackbox models. Underneath the umbrella, we see both interpretability and explainability as subcategories. In this case, interpretability is used to mean intrinsically interpretable glassbox models, whereas explainability is used to mean post-hoc explanations of blackbox models. Although seem-

ingly innocuous at first glance, this distinction turns out to be a critical motivation which underlies interpretability research in practice. Throughout this survey, we will commonly use 'interpretability' both for the umbrella class and the low-level meaning. We will try here to avoid saying 'explainability' to mean the umbrella class, although it is also common in the literature to use explainability as the umbrella class, especially in well-established phrases like XAI (meaning eXplainable Artificial Intelligence). Lastly, the field of explainability also takes on a third meaning regarding the psychological and social aspects of explaining (Miller, 2018), which can be necessary to apply in both interpretability and explainability, and which we will broadly ignore for this survey.

Deep Learning Theory vs. Deep Learning Interpretability As can be seen below in Figure 2, the questions of deep learning interpretability and deep learning theory are very intimately related. Nevertheless, there are some very key nuances between the goals and approaches of the two which mostly separate them. In particular, deep learning theory mostly deals with understanding *how* neural networks learn what they learn, usually beginning from first principles and mathematically studying the effect of gradient descent algorithms. In contrast, (deep learning) interpretability instead often deals with understanding *what* a particular neural network has learned. Typically, this is done by fixing a trained model and applying a variety of counterfactual perturbations in order to ascertain some additional information about the blackbox system.

Both confusingly and excitingly, there are many details in the specifics of how these what/why/how questions are asked within different subfields which impact the flavor of the research questions. For instance, traditional interpretability methods are often concerned with understanding *why* a network has made its prediction, usually in the form of understanding which *input features* 'contributed' to the output prediction. In contrast, mechanistic interpretability methods are more concerned with understanding *how* a network has made its prediction, often in the form of understanding which *substructures* inside the neural network 'control' or 'cause' the final prediction. For this reason, one of the main identifiers between traditional interpretability and mechanistic interpretability is the former's goal of model-agnostic understanding and the latter's goal of model-specific understanding. To summarize, deep learning theory asks *how* the model learns *what* it learns, mechanistic interpretability asks *how* the model predicts *what* it learned, and traditional interpretability asks *why* the model predicts *what* it learned.

Beyond these what/why/how distinctions, there are many different stylistic aspects of each subarea that affect which objectives are targeted and which interpretability methods are used. For example, another subfield of interpretability is the literature focusing on gaining causal insights through interpretability (also related to the recent push for *actionable* interpretability). Here, the goal is to distill information from the model all the way back to the real-world, gaining some causal knowledge about the real world. This is distinct from the causal language which is used inside of mechanistic interpretability. There, one first assumes that the studied network is the 'true process' and then uses tools from causality to causally explain the behavior. In contrast, causal interpretability uses the explanation of model behavior and questions whether the true process of the world (outside of the model) is explained in the same way. These distinctions between 'true-to-the-data' and 'true-to-

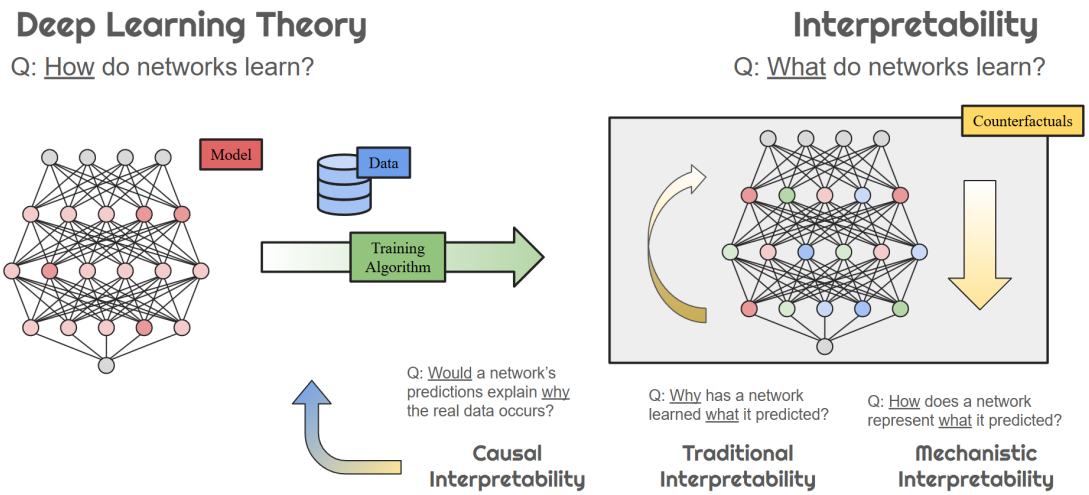

Figure 2: Deep Learning Theory vs. Deep Learning Interpretability

the-model' have been the source of endless confusion and of many unnecessary debates on the topic (Sundararajan and Najmi, 2020; Chen et al., 2020b; Frye et al., 2021).

Causality vs. Interpretability As just alluded to, another key clarification worth discussing is the distinction between causal insights and interpretable insights, especially given the importance of interpretability for causality and the importance of causality for interpretability. This often subtle nuance is only made worse by (a) people's natural inclination to treat explanations as causal, as well as (b) initiatives from the mechanistic interpretability community to explain models exclusively using causal language (Geiger et al., 2025).

The unfortunate truth, however, is that causal claims require causal reasoning and causal assumptions, which are broadly lacking in the interpretability literature. Although there have been attempts to directly incorporate causal reasoning into feature explainability, it is often a careful balance between making too many causal assumptions (Heskes et al., 2020; Biparva and Materassi, 2024) and making unrealistic assumptions (Janzing et al., 2020). Given the rising popularity of interpretability, this is only further confused by causality research using tools coming from interpretability (Jung et al., 2022; Parafita et al., 2025).

Whereas the vast majority of interpretability focuses on the typical 'X to Y' problems of regression or classification (taking $\hat{Y} = f_\theta(X)$), causal insight instead requires a full understanding of the structure between the X variables and between the X and Y. Presupposing the availability of a causal model on the variables hence precludes the need for the blackbox function f_θ in the first place, begging the question of why interpretability methods would even be needed at all. Furthermore, explaining Y and explaining $\hat{Y}$ represent two completely different objectives. A satisfactory middle ground here still seems to be absent from the literature. Accordingly, it is important for the practitioner to always take extra precautions when jumping from interpretable insights to causal claims (and vice versa).

2.2 A Taxonomy of Interpretability Approaches

Over the years, there have been many developments in interpretability methods, leading to a constantly expanding toolkit for understanding model behavior. Despite the constantly evolving landscape of interpretability, there have also been many good summaries of the available interpretability methods for explaining blackbox models, each making their own choices for the taxonomization of the available methods. One of the earliest syntheses of interpretability methods, the 'Interpretability Book' (Molnar, 2019), takes there to be the following classes of methods:

1. Intrinsically Interpretable Methods (GAM-type methods and rule-based methods)
2. Model-agnostic Methods (PDP, ICE, ALE; feature attribution, feature interaction, global surrogate, local surrogate, LIME, SHAP)
3. Example-based Approaches (counterfactual examples, adversarial examples, prototypes/ criticisms, influential instances)
4. Deep Learning Specific Approaches (feature visualization)

The latest version (Molnar, 2025) instead takes the following classes of methods:

1. Intrinsically Interpretable Methods (GAM-type methods and rule-based methods)
2. Local XAI (ICE; LIME, counterfactual examples, anchors, SHAP)
3. Global XAI (PDP, ALE; feature interaction, functional decomposition, leave-one-out, surrogate models, prototypes and criticisms)
4. Deep Learning Methods (learned features; saliency maps; detecting concepts; adversarial examples; influential examples)

Other more recent surveys take a broadly similar approach to categorizing the many different classes of interpretability methods. Zhang et al. (2021) suggests four main explanation types: example-based, attribution-based, hidden semantics, and rule-based. Ji et al. (2025) suggests five main styles: attribution-based, function-based, concept-based, prototype-based, and rule-based self-interpretation.

Herein, we consider there to be three main styles of explanation: concept-based, rule-based, and additive-based. In Figure 3, we depict how many classical interpretability methods fall into these three categories. We find that unlike previous taxonomizations, using three main categories allows for a single interpretable model to be a quintessential representative of the interpretation style, depicted at the base of each pillar. The additive pillar is supported by the interpretable additive model. The reasoning pillar is supported by the interpretable decision tree. Finally, the concept pillar is supported by the k-NN algorithm, which is very often granted the same status as an interpretable model. We expand on this characterization further in Section 2.4.

2.3 Mechanistic?

As alluded to before, in this survey we will mainly ignore approaches from mechanistic interpretability in favor of more established approaches to interpretability, especially model-agnostic interpretability; however, we still find it important to review the major developments and techniques coming from this subfield.

Mechanistic approaches to neural network interpretability have existed just as long as neural networks themselves. Beginning in computer vision, one of the simplest early methods was *gradient saliency* (Simonyan et al., 2014), originally applied to those deep convolutional

networks which were able to achieve stunning accuracy on the ImageNet challenge. This method simply takes the gradient of the class logit with respect to the input pixels. Later follow-ups like Layer-wise Relevance Propagation (LRP) (Bach et al., 2015), GradCAM (Selvaraju et al., 2017), DeepLIFT (Shrikumar et al., 2017), and Integrated Gradients (IG) (Sundararajan et al., 2017) provided extensions to the simple gradient approach which gave it increased stability or convenient properties. Unfortunately, later work (Adebayo et al., 2018) called into question how useful these saliency maps are, providing sanity checks showing most saliency methods provided little information beyond edge detection. It was argued that these approaches most likely hijack our human intuition to make researchers feel as though we were understanding the predictions of the neural networks. Despite these major limitations, it often remains the dirty go-to throughout many areas of computer vision research.

Another popular method in mechanistic interpretability approaches is the *attention mechanism* (Bahdanau et al., 2015), coming directly from the neural architecture in its application to machine translation in natural language. Its usage as an interpretability approach eventually became widespread enough that a work summarizing its limitations called "Attention is not Explanation" (Jain and Wallace, 2019) was published. This led to a retort called "Attention is not not Explanation" (Wiegreffe and Pinter, 2019) which claimed attention was at least 'doing something', as well as works like Attention Flow (Abnar and Zuidema, 2020) which instead tried to correct some of its shortcomings. Although attention is also commonly used throughout NLP applications as a quick approximation of importance, concerns regarding the faithfulness of such explanations persist into the current day (Lyu et al., 2024).

The final key mechanistic explanation approach is the method of *feature visualization* (Erhan et al., 2009). Originating again in computer vision research and even earlier than the simple gradient saliency approach, the earliest iterations of this approach simply find the solution to a maximization problem for each of the class labels, usually maximizing the logit activation through a gradient descent algorithm. Later interpretation works (Simonyan et al., 2014) would also include this approach; however, this direction picked up greater steam after Google's DeepDream visualization (Mordvintsev et al., 2015) on the state-of-the-art Inception network (Szegedy et al., 2015). Later works like Olah et al. (2017) and Bau et al. (2017) would continue to build towards a larger-scale analysis of entire convolutional networks (and ultimately form the basis for modern mechanistic approaches).

More modern versions of mechanistic interpretability (also MI or mech interp) continue further down the path trailblazed by Chris Olah and coauthors, mainly through the approaches of feature visualization (Carter et al., 2019b; Schubert et al., 2020) and circuit decomposition (Olah et al., 2020), later pivoting to primarily focus on researching large language models. This push has been integrated with many 'call to action's motivated by concerns surrounding AI safety, which have been bolstered further by the creation of companies like Anthropic specifically with these goals and values in mind. This has led to the explosive growth of mechanistic interpretability as a subfield in recent years, focusing on a wide array of approaches trying to understand the feature representations of large language models and trying to understand the algorithmic computations run by deep neural networks, including: linear probes (Alain and Bengio, 2017), nonlinear probes (Li et al., 2023), sparse autoencoders (Huben et al., 2024), sparse circuits (Marks et al., 2025), causal mediation analysis (Vig et al., 2020), model editing (Meng et al., 2022), and causal abstraction (Geiger

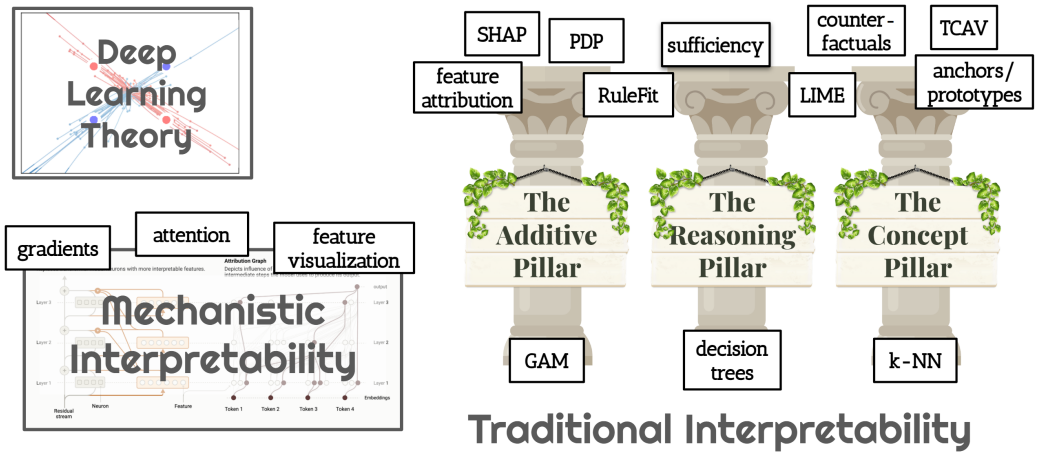

Figure 3: Taxonomization of the Classical Approaches to Interpretability

et al., 2025). As was already mentioned, this is often done in a manner which is both empirical and applied, distinguishing it from the sometimes similar works in deep learning theory.

2.4 Pillars of Interpretability

We now discuss the three pillars of interpretability as depicted in Figure 3 and how they are representative of interpretability research which we will herein call *traditional interpretability*, to better distinguish it from mechanistic interpretability. Each of these pillars is supported at the base by an intrinsically interpretable model, and at the top of each pillar we list many classical explainability approaches which are related to that interpretability style. Supported by the generalized additive model (GAM), we have the additive pillar. Supported by the decision tree model, we have the reasoning pillar. Supported by the k-nearest neighbor model (k-NN), we have the concept pillar.

There is near-complete consensus throughout the interpretability community that additive models and decision trees are interpretable models (of course to varying degrees in various situations), so many readers will be comfortable with these choices for the first two pillars. It is slightly less standard to make the same claim that the k-NN model is interpretable; however, in contexts like data attribution, it is the simplest possible model for understanding the influence of individual data points. Additionally, this choice aligns well with previous attempts to categorize the field which instead keep prototypes and concepts as separate approaches. We discuss this decision further in its respective paragraph.

The Additive Pillar is centered around the generalized additive model (Hastie and Tibshirani, 1990; Lou et al., 2012) which additively incorporates the influences of individual features into a final prediction. These separate contributions are implicitly understood to independently contribute towards the final prediction, allowing them to be interpreted individually. Extensions to models with pairwise interactions (Lou et al., 2013) or higher-order interactions (Enouen and Liu, 2022) provide a spectrum of gradually increasing complexity which can ultimately represent any function, at the expense of deteriorated interpretability.

On the explainability side, feature attribution approaches (Smilkov et al., 2017; Sundararajan et al., 2017) primarily use the same feature-based reasoning as generalized additive models. Although beginning in the gradient saliency literature measuring local sensitivity, progress slowly developed towards smoother, model-agnostic measurements of local influence like SmoothGrad (Smilkov et al., 2017) and Integrated Gradients (IG) (Sundararajan et al., 2017). Further developments into feature perturbation approaches (Breiman, 2001a; Aaron Fisher, 2019; Hooker and Mentch, 2019) and feature removal approaches (Lei et al., 2018; Covert et al., 2021) helped standardize progress. Specific cases like the SHAP approach (Lundberg and Lee, 2017) greatly unified interest in the field, now known to be directly dual to GAM interpretations (Bordt and von Luxburg, 2023; Enouen and Liu, 2025).

One of the earliest interpretability approaches, the partial dependence plot (PDP) (Friedman, 2001), works on the exact same intuition as the shape functions of the additive model, marginalizing the effect of an individual feature on the blackbox model across the entire dataset. Later work called the individual conditional expectation (ICE) (Goldstein et al., 2015) instead considered the individual curves of each data point together in a single plot. Although these two approaches implicitly consider the marginal distribution, it is often preferable to consider the conditional distribution instead. Although these conditionally marginalized plots are typically difficult to compute, the accumulated local effects (ALE) plot (Apley and Zhu, 2020) attempts to balance the local influence of the gradient with the global influence of the conditional distribution.

The Logical Pillar is focused on the logical, mechanical steps taken to arrive at a final decision. Even simpler than the decision *tree* (Hastie et al., 2001) is the decision *list* (Chen and Rudin, 2018) which allows for a deterministic list of decisions to be sequentially followed until a particular condition is met. The decision tree instead allows for a flow chart to be followed depending on the previous set of logical conditions. Taking this complexity further, the decision *circuit* (Oliver, 1993; Kohavi, 1994; Kohavi and Li, 1995; Darwiche and Marquis, 2002) allows for even more compact representations, potentially at the expense of a more entangled reasoning process.

Although practical extensions to decision trees have mainly been the additive ensemble of the random forest (Breiman, 2001a), it is folk knowledge that this immediately destroys the interpretability. Broadly, this seems to be due to the 'incompatibility' of mixing additive interpretability and logical interpretability in this particular way. Alternatives to extend the complexity of the decision process while remaining interpretable have instead considered a large set of near-optimal decision trees called the *Rashomon set* (Xin et al., 2022). These small decision trees are designed to be interpreted individually and then chosen based on alternative objectives like fairness, robustness, or simply preference by domain experts. RuleFit (Friedman and Popescu, 2008) is an additive combination of rules which uses *sparsity* to ensure that few rules will be added together, allowing each individual rule to still be interpreted.

On the explanation side, the sufficient input subset (SIS) method (Carter et al., 2019a) aligns heavily with the logical reasoning of decision processes, providing the input features which were sufficient for the model to be certain about its decision. The closely related notion of necessity (Darwiche and Hirth, 2020; Watson et al., 2022) describes which input features cannot be changed to maintain the same prediction. These logic-based notions of

explanation often have formal origins coming from causal reasoning (Pearl, 2009; Halpern, 2016), abductive reasoning (Peirce, 1903; Josephson and Josephson, 1994), and earlier.

The closely related approach of counterfactual explanations (Wachter et al., 2017) proposes alternative feature values which are sufficient to change the prediction or decision. When focusing on the features which were changed to arrive at the new prediction, these can be related to the notions of sufficiency and necessity (Kommiya Mothilal et al., 2021). Counterfactual examples are another popular method, but these approaches are closer to the prototype-based reasoning of the third pillar. The method of LIME (Ribeiro et al., 2016) uses a local surrogate around a data point, typically either a decision tree or linear model, which then applies the additive reasoning or logical reasoning to a local region around the data point. Anchors (Ribeiro et al., 2018) provide local logical explanations in a similar fashion using a different algorithm.

The Conceptual Pillar is about the construction of new features or concepts, allowing for greater abstraction and simpler higher-level reasoning. Interpretable works like Prototypical Part Network (ProtoPNet) (Chen et al., 2019) and the Concept Bottleneck Model (CBM) (Koh et al., 2020) extend the reasoning style of the k-NN which makes determinations based on similarity with previously seen examples.

Previous survey hierarchies (Zhang et al., 2021; Ji et al., 2025) have argued that *concept-based* and *prototype-based* interpretability represent fundamentally different categories. Although we agree that there are key stylistic differences between concept approaches and prototype approaches, we believe that their overall reasoning styles are fundamentally the same, with both being represented by the k-NN model. Although k-NN models and prototype-based regression make predictions directly from distance-based similarity using a prespecified distance, more general CBMs extend the similarity metric across a multidimensional array of concepts and accordingly complexify the final prediction step. Nonetheless, the prediction is only due to the similarity computed according to a 'blackbox distance' and the interpretability is instead coming from our ability to inductively reason from similar examples which we have seen before.

While ProtoPNet and CBM push example-based reasoning to its extremes, achieving decent computer vision performance while maintaining an intermediary layer which is mostly interpretable, there is also work on the side of post-hoc explanation. TCAV (Kim et al., 2018) uses a set of training data samples which are labeled as obeying or disobeying a concept to be able to find a vector direction within the latent space which points in the direction of the concept. As previously mentioned, methods like LIME (Ribeiro et al., 2016) and Anchors (Ribeiro et al., 2018) which take a local perspective in a small region around the data point are partially a prototype-style explanation. Even moreso are direct prototype-based explanations (Fix and Hodges, 1951; Cover and Hart, 1967; Hart, 1968) which find explanatory samples nearby in input space or latent space, and counterfactual explanations (Wachter et al., 2017) which find explanatory samples which are nearby but with different predictions. Moreover, this goal of finding an appropriate set of concepts is related to notions of compressibility (Tishby et al., 2000; Hutter, 2005) and sparse coding (Donoho, 2006; Rubinstein et al., 2010), with notions from mechanistic interpretability trying to extend these to notions of algorithmically or mechanically compressible (Geiger et al., 2025).

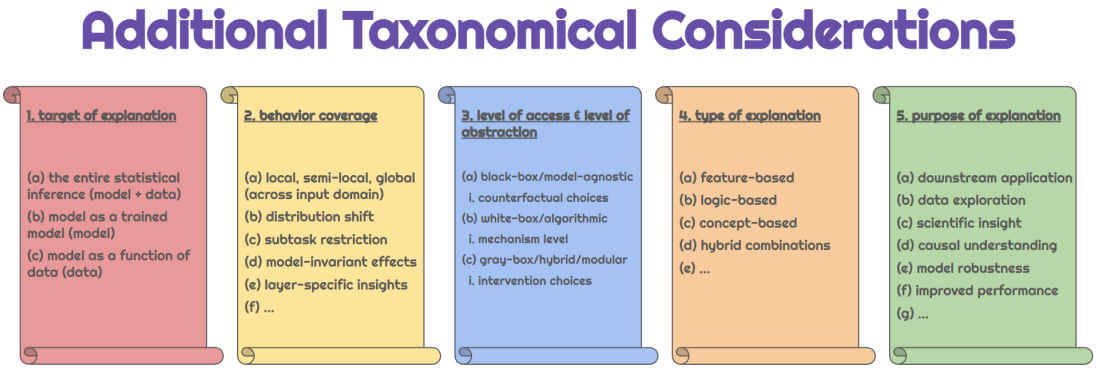

Figure 4: Additional Axes of an Interpretability Taxonomy.

2.5 Further Jargon and Taxonomical Aspects

Finally, for completeness, we will briefly go over some other taxonomical aspects of the interpretability literature before moving into surveying the main topics of additive explainability and additive interpretability. We provide a brief summarization of some of the main considerations in Figure 4 below.

We begin by noting that the majority of interpretability work takes the model-based perspective that the goal is to explain a trained blackbox model as depicted in the right-hand side of Figure 2, and this accordingly frames a lot of the discussion about and previous taxonomies of the field; however, there are emerging areas considering data valuation (Ghorbani and Zou, 2019; Jia et al., 2019b) or even explanations of the entire statistical inference (Bordt et al., 2025). One of the main taxonomizations of explainability methods is whether or not they are local, semi-local, or global (Zhang et al., 2021). This refers to whether an XAI method is supposed to explain the behavior of the model only in a local area near the data point, in a larger region around the data point, or across the entire input manifold. This local vs. global question can be seen as a special case (although the most common case) of the larger question: how much of the model behavior is covered by my explanation method? Further examples of this question include: Am I explaining this behavior only on the training distribution? Am I explaining this behavior only for a certain subtask?

Another key distinction is between black-box explanations and white-box explanations. Note that this is different from blackbox vs. glassbox which refers to the lack of transparency in these models from an interpretability perspective, whereas black box vs. white box refers to the level of access to the actual model mechanisms, regardless of the complexity in interpreting those mechanisms. Historically, there was a push to move away from early gradient-based and attention-based methods (gray box) towards model-agnostic interpretability methods which could be applied to any blackbox model; however, there has also been the more recent push for methods specifically designed to understand neural network layers and transformer mechanisms given their widespread successes. Obviously the level of access restricts the lowest level of abstraction which is possible; however, researchers often choose a higher level of abstraction than the lowest available. Immediately, one is then faced with the questions about what counterfactual queries are possible for the questions

of feature removal, data point removal, model type change, mechanism perturbation, etc. These are critical questions related to the explanation target and explanation purpose.

Finally, there are the aspects of the type of explanation, which we taxonomized in much greater detail in the previous sections, and can also be very much entangled with these other questions about model type and behavior coverage. Also worth mentioning is the model's task (decision-making, prediction-making, or generative) which can be seen as a subquestion of the first question on the target of the explanation. Lastly, we have the all-important question about the downstream purpose of the explanation itself. Although this does not always make its way into the papers creating XAI methods, it is an undeniable part of XAI application, and thus must be considered as part of how to interpret and integrate the explanation. This again gets into the challenging questions of causality, social explanation, and broader context (Miller, 2018).

Contents

1 Introduction **1**

2 The Current Map of Interpretability **3**
2.1 Areas Related to Interpretability . . . 3
2.2 A Taxonomy of Interpretability Approaches . . . 6
2.3 Mechanistic? . . . 6
2.4 Pillars of Interpretability . . . 8
2.5 Further Jargon and Taxonomical Aspects . . . 11

3 Additive Explainability (Feature Interactions) **14**
3.1 A History of Feature Interaction Detection . . . 14
3.2 A History of the Shapley Value (Additive Explanations) . . . 16
3.3 Applying the Shapley Value to Data Valuation . . . 27
3.4 Extending the Shapley Value to Feature Interactions . . . 28
3.5 Connections to Global Explainability . . . 32

4 Additive Interpretability (Additive Models) **36**
4.1 A History of Generalized Additive Models . . . 36
4.2 A History of Sparse Additive Models . . . 38
4.3 Modern Additive Models . . . 40
4.4 Feature Interaction Selection . . . 47
4.5 Modern Topics . . . 49

5 Application Areas **55**
5.1 Vision . . . 56
5.2 Language . . . 57
5.3 Vision-Language . . . 58
5.4 Longitudinal and Time Series . . . 59
5.5 Graphical and Natural Sciences . . . 59

6 Future Directions **60**
6.1 Building up the Pillars . . . 60
6.2 Compositionality . . . 62
6.3 Generative Interpretability . . . 63

7 Conclusion **64**

3. Additive Explainability (Feature Interactions)

In this section we go into great detail on the study of feature interactions and related additive explainability approaches. If you are not already sold on the importance of feature interactions and additive interpretability, we recommend skimming the historical details or visiting Section 5 to see applications, returning to the relevant topics as necessary.

3.1 A History of Feature Interaction Detection

In order to have a detailed understanding of the history of feature interactions, we must begin at nearly the very beginning of statistics and start by first discussing the Design of Experiments (DOE).

First DOE Wave (Agricultural) A discussion of the history of feature interactions must undoubtedly start with Ronald A. Fisher's work on the analysis of variance (ANOVA) in 1925 (Fisher, 1925), which built upon decades of agricultural data collected by John Lawes and Joseph Gilbert at the Rothamsted Experimental Station, originally established in 1843. The goal was to measure the effect of crop treatments against the background randomness of different plots of land. This research was continued by Frank Yates of the same institution, furthering the work on ANOVA (Yates, 1935). A major clarification on the assumptions which were required for this approach was later provided in 1947 by Churchill Eisenhart (Eisenhart, 1947). ANOVA was then developed further by John W. Tukey who in 1949 helped isolate the key property of a feature interaction as the non-additivity between the two independent variables of the contingency table (Tukey, 1949). Despite the focus on interactions, this was still a time where running experiments was extremely costly and accordingly higher-order feature interactions (interactions of three or more variables) were often completely ignored or explicitly assumed to be zero in order to minimize the number of required experiments. Further developments continued on factorial designs such as those taken by M. B. Wilk in 1955 to extend to the generalized randomized block design (Wilk, 1955) and by B. V. Shah in 1960 for balanced factorial experiments (Shah, 1960).

Second DOE Wave (Industrial) Around this time, the experimental design literature saw a second revitalization with G. E. P. Box and K. B. Wilson's work on applying similar ideas to industrial applications (Box and Wilson, 1951). It is here where we see the clear introduction of continuous variables and a notation much more similar to the modern approaches. Specifically, a set of experimental variables, which are measurable and controllable, are chosen and then an experiment is 'run', leading to a functional *response surface* in the observed outcome variable, often with some potential error or confounding due to factors beyond the control of the experimenter. Despite these many modernizations, the focus remained on minimizing the required number of costly experiments, thus discarding higher-order effects. Later improvements by Box and Hunter (Box and Hunter, 1957) and Box and Behnken (Box and Behnken, 1960) continued to refine the response surface approach, still focusing on optimizing performance with minimal experiments. Developments continued with the treatment of experiments with material mixtures like in the production of rubber or alloys (Scheffe, 1958) as well as extensions to more complex time-confounded errors (Geisser and Greenhouse, 1958; Huynh and Feldt, 1970). Industrial applications in the post-war era expanded over the next decades beyond chemistry into tool-life, foodstuffs,

biology, ecology, and manufacturing (Myers et al., 1989). This later evolved into the 'quality assurance' era, mimicking the Japanese industrial boom which used statistical methods pioneered by researchers like Taguchi (Taguchi, 1986), and ultimately evolving into the Total Quality Management (TQM) and Continuous Quality Improvement (CQI) approaches which came to define American industrial management by the end of the century.

Third DOE Wave (Informational) Although the industrial experimentation era would go on to become majorly corporatized, the design of experiments would see what could be described as two spiritual successors. The first successor which emphasized the focus on experimental design is the modern research of AB experimental design, as now used liberally by tech companies to quickly gain insight into user behavior (Quin et al., 2024). With the digitization of many user experiences, large-scale tech companies are able to receive near-instantaneous feedback, both direct and indirect, allowing for rapid quality improvements in distributed software. Further discussion on this direction will mostly be out of scope for this survey. The second successor which emphasized the focus on the response surface methodology is better represented by the literature on Sensitivity Analysis (SA). Also fueled by the modern digitization, or more specifically the proliferation of computerized simulation, the modern researcher may have access to a much greater number of experiment runs. It is here where we finally see the exploration of higher-order feature interactions. Earlier works like (McKay et al., 1979) and (Sacks et al., 1989) set the stage for computer-based experiments, and sensitivity analysis ultimately developed around the modern techniques centered on Sobol' analysis (Sobol', 1990; Chan et al., 1997; Saltelli et al., 2000; Santner et al., 2003). We will discuss this direction of sensitivity analysis in much greater detail in Sections 3.5.1 and 4.5.3.

Feature Interaction Detection (Decision Trees) During this time, the precursors to the modern decision tree like Automatic Interaction Detection (AID) (Belson, 1959; Morgan and Sonquist, 1963) and the Chi-squared Automatic Interaction Detection (CHAID) (Kass, 1980) were already under development. These methods were novel approaches for determining how to best combine features to interact within a decision tree. These approaches would later culminate into the famous CART algorithm (Breiman et al., 1984) and ultimately modern decision trees and random forests (Ho, 1995; Breiman, 2001a). By the turn of the century, it was already clear that the major interest in feature interactions would be in the context of accurate prediction models and machine learning.

Feature Interaction Detection (Premodern) Although many works at this time would already use the occasional interaction term (most often polynomial cross terms or tensor product splines), the detection of more general feature interactions remained uncommon (Aiken et al., 1991). Some preliminary works like Ai and Norton (2003) proposed extracting interactions from logit and probit models via mixed partial derivatives and Gevrey et al. (2006) followed up by proposing mixed partial derivatives to extract interactions from shallow neural networks. An important change in perspective occurred after two nearly concurrent papers showed how to leverage the powerful decision tree models to detect meaningful interactions, with Friedman and Popescu (2008) and Sorokina et al. (2008) both restricting the features to be included in the trees of a random forest and a similar statistic to measure the strength of an interaction between two or more features. Of major importance was the nonparametric setup which did not necessarily require the use of a specific choice of

ML model, enabling the use of the powerful random forest model. Later works provided clarification of the sparse selection problem and the strong heredity principle (Bien et al., 2013) as well as formulating the screening problem for high-dimensional statistics (Hao and Zhang, 2014). These developments into feature interactions continued into the present day; however, they become increasingly intertwined with related areas like explainability, sensitivity analysis, and additive models as this survey highlights. Accordingly, we will pause in this timeline to introduce these other research areas, first focusing on blackbox explanations, which later become almost indistinguishable from interaction detection itself.

Additional details on the topics of experimental design and feature interaction detection are available in the surveys Dean et al. (2015), Rosenberger (2019), and Tsang et al. (2021). We will pick up our discussion on feature interactions in Section 3.4 with the introduction of interaction-based generalizations of the Shapley value.

3.2 A History of the Shapley Value (Additive Explanations)

The Shapley value itself was introduced in 1953 by Lloyd Shapley (Shapley, 1953), devised to equally distribute the rewards of some collaborative project amongst its constituent players. It was a fundamental concept in collaborative game theory, inspiring many extensions we will later discuss. It was brought into popularity for the machine learning interpretability literature much later in 2017 (Lundberg and Lee, 2017). Generally, we will use the Shapley value to refer to the game-theoretic concept and SHAP to refer to the ML explainability concept; however, we will occasionally use Shapley to describe the latter (e.g. conditional Shapley). Although the Shapley value does not focus on interactions, either in its original conception or its ML revitalization, it has become a centerpiece or a rallying cry for these research directions which focus on interpretable features, including the study of feature interactions. Accordingly, we will center our discussion in the next sections as if Shapley were the unifying force behind all of these areas, even if for nearly all these areas, Shapley played no part in the origin of the field.

3.2.1 The Shapley Value

The Shapley value was designed to solve the problem of fair attribution amongst a set of d players under a fixed *value function*, v. This function (originally assumed to be superadditive in the spirit of cooperation) maps a coalition of players to the value generated by their collaborative efforts, $v : \mathcal{P}([d]) \to \mathbb{R}$ where $\mathcal{P}([d])$ denotes the power set of $[d] := \{1, \dots, d\}$. That is, for each coalition (subset) of players $S \subseteq [d]$, we write their combined value as $v(S)$.

In Lloyd Shapley's original formulation of his solution concept, he used three axioms: the symmetry axiom, the carrier axiom, and the additivity axiom. These are now more commonly decomposed into four axioms, dividing the carrier axiom into the dummy axiom and the efficiency axiom. We write the four Shapley axioms in the operator notation as follows:

1. **Dummy** If $[\delta_i \circ v](S) = c \in \mathbb{R}$ for all S, then $[\phi_i \circ v] = c$.
2. **Symmetry** $\phi_{\pi(i)} \circ (\pi \circ v) = \phi_i \circ v, \quad \forall \pi \in \Pi_d$
3. **Efficiency** $\sum_{i \in [d]} (\phi_i \circ v) = v([d]) - v(\emptyset)$

4. **Additivity** $\phi \circ (v + w) = \phi \circ v + \phi \circ w$

where we define $[\delta_i \circ v](S) := v(S+i) - v(S-i)$ as the difference in value of a coalition with and without player i, $\pi \in \Pi_d$ is a permutation of d elements, $(\pi \circ v)$ is the game where player i is relabelled as player $\pi(i)$, and $(v + w)$ is the game defined as $(v + w)(S) := v(S) + w(S)$.

Theorem 1 *(Shapley, 1953) There is a unique solution concept obeying these axioms, now called the Shapley value, obeying the equation below.*

$$\phi_i^{Sh}(v) := \sum_{S \subseteq ([d]-i)} \frac{1}{d} \binom{(d-1)}{|S|}^{-1} \cdot \Big[v(S+i) - v(S) \Big] \tag{1}$$

Although this is a closed form directly in terms of the value function, it obscures the nature of Shapley's solution. Instead, let us first decompose the value function into its composite 'unanimity games', also called the synergy functions, the purified value function, the Mobius function, or the discrete derivative.

$$\tilde{v}(S) := \sum_{T \subseteq S} (-1)^{|S|-|T|} \; v(T) \tag{2}$$

We may then write the Shapley value in a form which exactly describes its approach. The Shapley value takes all of the unique synergies amongst each set of players, and for each synergy divides it equally amongst all those players.

$$\phi_i^{\text{Sh}}(v) := \sum_{S \ni i} \frac{\tilde{v}(S)}{|S|} \tag{3}$$

Another relevant definition is the Shapley value in its permutation form. Here it becomes very clear how the Shapley value obeys both its symmetry and its efficiency axioms. Unlike what is sometimes erroneously claimed, this was not the original definition in (Shapley, 1953) and was perhaps more likely solidified through collaboration with Martin Shubik on the Shapley variant designed for voting games (Shapley and Shubik, 1954), see below. The Shapley can also be defined as:

$$\phi_i^{\text{Sh}}(v) := \frac{1}{d!} \sum_{\pi \in \Pi_d} \Big[v(S_i^\pi + i) - v(S_i^\pi) \Big] \tag{4}$$

where the sum is taken over all permutations/ orderings of the players, and the set S_i^π is the set of predecessors of i given the permutation π, i.e. $S_i^\pi := \{j \in [d] : \pi(j) < \pi(i)\}$. This definition is often used as the basis for Monte Carlo sampling via random permutations, now commonly referred to as *PermSHAP*.

Another important formula is the realization that the Shapley value is the average over marginal contributions where all sizes of subsets are weighted equally. This is easy to imagine given the permutation definition, and can be written as:

$$\phi_i^{\text{Sh}}(v) := \sum_{k=0}^{d-1} \frac{1}{d} \cdot \sum_{\substack{S \subseteq ([d]-i) \\ \text{s.t. } |S|=k}} \binom{d-1}{k}^{-1} \cdot \Big[v(S+i) - v(S) \Big] \tag{5}$$

where k is 'uniformly distributed' over the set $\{0, \ldots, d-1\}$ and S is 'uniformly distributed' over subsets of size k. From this definition it is clearest to see that we may equally write this sum as over S s.t. $\{i\} \subseteq S \subseteq [d]$ or S s.t. $\emptyset \subseteq S \subseteq [d]$ instead of the original S s.t. $\emptyset \subseteq S \subseteq ([d] - i)$ (with the appropriate adjustments).

Finally, the last important definition is the variational definition, which defines the Shapley value as the solution to a minimization problem. This alternate definition was discovered much later than the original formulation of the Shapley value.

Theorem 2 *(Charnes et al., 1988) The Shapley value can be written as:*

$$\phi^{Sh} := \underset{\phi \in \mathbb{R}^d}{\operatorname{argmin}} \left\{ \sum_{S \subseteq [d]} m^{\mathrm{Sh}}(|S|) \cdot \left[v(S) - \phi_\emptyset - \sum_{i \in S} \phi_i \right]^2 \right\} \tag{6}$$

$$s.t. \quad v(\emptyset) = \phi_\emptyset \;\; and \;\; v([d]) = \phi_\emptyset + \sum_{i=1}^{d} \phi_i$$

where $m^{\mathrm{Sh}}(s)$ *is taken equal to* $m^{\mathrm{Sh}}(s) = \binom{d-2}{s-1}^{-1}$.

In other words, we can define the Shapley value as the least squares solution to the 'additive approximation' of the true value function, under some specific distribution over S, now often called the *Shapley kernel* (sometimes Shapley kernel measure or Shapley kernel distribution) because of its connection to KernelSHAP discussed below.

It is equivalent to scale the measure $m^{\mathrm{Sh}}(s)$ by any positive constant without changing the optimization problem, so a natural version of the measure is the one normalized to be a probability measure (to enable random sampling of S). However, the normalizing constant is not available in a simple closed form, so there are many reasonable rescalings of the Shapley kernel. Moreover, it is now popular to use a measure closer to the one independently discovered by Lundberg decades later in the SHAP paper (Lundberg and Lee, 2017). This is the measure defined as $m^{\mathrm{Sh}}(s) = \frac{d-1}{s \cdot (d-s)} \binom{d}{s}^{-1} = \frac{1}{d} \binom{d-2}{s-1}^{-1}$. A strong reason to prefer this version is that it reminds us more explicitly that when $s = 0$ or $s = d$ that the measure is implicitly infinite, corresponding to the constraints of the system in Equation 6. A reason to further prefer $m^{\mathrm{Sh}}(s) = \frac{1}{s \cdot (d-s)} \binom{d}{s}^{-1}$ over $m^{\mathrm{Sh}}(s) = \frac{d-1}{s \cdot (d-s)} \binom{d}{s}^{-1}$ is its even greater simplicity (although the renormalization constant of the former scales almost linearly where the latter scales only logarithmically). In this case, one only needs to recall that all S of size s receive a total weight of $\frac{1}{s(d-s)}$, split equally amongst all $\binom{d}{s}$ of them. Let us now move on to discuss the ML application of Shapley by Lundberg and Lee (2017) in more detail, including how they leveraged this variational formulation.

3.2.2 The SHAP Value

The SHAP value, introduced in 2017 by Lundberg and Lee (2017), was an effort to unify several recent explainability methods under the roof of 'additive explanations' and then provide an axiomatic characterization of their introduced additive explanation, the SHAP value. Although predated by other approaches incorporating the Shapley value into machine learning explanations, this framing would go on to see the greatest amount of follow-up work. It is important to note that this was around the dawn of the push for 'model-agnostic'

approaches, meaning they treated the ML model entirely as a black box after abstracting how to remove the features from the model. This would allow them to directly import the set functions from the original Shapley and would continue to influence subsequent developments, not least of which can be seen in the modern notation used throughout this survey.

Definition 3 *(**Additive Explanation**) The umbrella class which was studied by Lundberg and Lee (2017) was the additive explanation, defined as:*

$$v(S) := \phi_\emptyset + \sum_{i=1}^{d} \mathbb{I}(i \in S) \cdot \phi_i \tag{7}$$

Their originally proposed axioms for what a 'good' explanation should satisfy were presented in a now-outdated notation which is related to the baseline method of feature removal. We write them in an updated notation:

1. **Local Accuracy** $v([d]) = \phi_\emptyset + \sum_{i=1}^{d} \phi_i$ and $v(\emptyset) = \phi_\emptyset$
2. **Missingness** $v(S+i) - v(S) = 0$ for all $S \implies \phi_i = 0$.
3. **Consistency** $v(S+i) - v(S) \geq v'(S+i) - v'(S)$ for all $S \implies \phi_i \geq \phi_i'$.

Theorem 4 *(Lundberg and Lee, 2017) The only additive explainer of the form $w(S) := \phi_\emptyset + \sum_{i=1}^{d} \mathbb{I}(i \in S) \cdot \phi_i$ which obeys Local Accuracy, Missingness, and Consistency is the Shapley value.*

Although these alternative axiomatizations of the Shapley value were already known from the literature below on cooperative game theory, the critical development was to bring these notions into the language of blackbox (i.e. model-agnostic) explainability. It is worth noting that the original missingness condition had the different requirement that $\phi_i = 0$ whenever the feature value $x_i = 0$, since 0 was taken as the baseline value. We extend this meaning beyond the baseline approach to interpret that no change would occur for the value function.

Again, much of the original language was limited to the then popular baseline removal method; however, the paper alluded to more general perturbations. In particular, the paper writes:

$$\begin{aligned} v(S) := \mathbb{E}[f(X_S, X_{-S}) | X_S = x_s] &= \mathbb{E}_{p(X_{-S}|x_s)}\Big[f(x_S, X_{-S})\Big] && (8) \\ &\approx \mathbb{E}_{p(X_{-S})}\Big[f(x_S, X_{-S})\Big] && (9) \\ &\approx f(x_S, \mathbb{E}_{p(X_{-S})}\big[X_{-S}\big]) && (10) \end{aligned}$$

where the first line (Equation 8) corresponds to Equations 9 and 10 of (Lundberg and Lee, 2017). The second line (Equation 9) corresponds to their Equation 11, achieved by assuming that the input features are independent. The third line (Equation 10) corresponds to their Equation 12, achieved by assuming the function is linear in the features. As a reminder, one would typically center their input features so that the third line could be evaluated via $f(x_S, 0_{-S})$. Although these are clearly very heavy assumptions, these are the same

simplifications which allowed for SHAP to be relatively computable at the time. Each line of this equation now corresponds to a different 'flavor' of Shapley value discussed in the next section, namely conditional, marginal, and baseline (Sundararajan and Najmi, 2020).

Beyond its clear formulation, another major advantage of the paper was its ease of computation and strong code support. In particular, the previously mentioned optimization formulation from Equation 6 was used for approximating the Shapley value without inheriting the exponential complexity required to compute the Shapley value exactly.

$$\hat{\phi}^{\text{KernelSHAP}} = \underset{\phi \in \mathbb{R}^d}{\text{argmin}} \left\{ \sum_{S \in \mathcal{S}} m(|S|) \cdot \left[v(S) - \phi_\emptyset - \sum_{i \in S} \phi_i \right]^2 \right\} \tag{11}$$
$$\text{s.t.} \quad v(\emptyset) = \phi_\emptyset \;\text{ and }\; v([d]) = \sum_{i=1}^{d} \phi_i$$

where $m(s) = \frac{d-1}{\binom{d}{s} \cdot s \cdot (d-s)}$. This algorithmic approach was called *KernelSHAP* because of its use of the Shapley kernel. Once again, we use modern notation instead of the original. The key difference from the exact equation is the use of an approximating set of subsets $\mathcal{S} \subseteq \mathcal{P}([d])$, instead of measuring the blackbox function on all 2^d possible subsets as in Equation 6. Algorithmically, there was also a choice to always include the smallest and biggest subsets inside $\mathcal{S}$ (i.e. S where $|S| = 1, 2, d-1, d-2$) and there was a small L1 penalty applied to encourage slightly sparser explanations.

This quickly attracted attention from many different perspectives and is currently the most popular and well-studied explainability approach.

3.2.3 Variants of SHAP

As was quickly realized, however, the Shapley value depends critically on how the machine learning problem is translated into a choice of value function. The 'many Shapley values' paper (Sundararajan and Najmi, 2020) was among the first to clearly articulate this point.

They begin by noting how several works prior to the SHAP paper have made attempts to apply the Shapley value solution concept to machine learning applications. Lindeman et al. (1980) and Kruskal (1987) apply Shapley to linear regression's R^2 values, averaging across all orderings of the input features (not realizing the connections with the Shapley value); Owen (2014) and Owen and Prieur (2017) apply the Shapley value to the variance explained for a general function (not just a linear function); and Strumbelj et al. (2009), Strumbelj and Kononenko (2010), Strumbelj and Kononenko (2014), and Datta et al. (2016) all apply Shapley to model explanations in a very similar way to SHAP for the goal of model explainability (Lundberg and Lee, 2017).

In addition, the work makes connections with existing methods like Integrated Gradients (IG) (Sundararajan et al., 2017) were made with a variant of the Shapley value, the Aumann-Shapley value (Aumann and Shapley, 1974), and mentions follow-up works like (Lundberg et al., 2018) continuing to develop Shapley applications. Alongside soon-to-be-published works like (Lundberg et al., 2020; Covert et al., 2020), this begged the question of what is the right Shapley value, with (Sundararajan and Najmi, 2020) giving the first attempt at setting up the question.

Although a definitive answer to the 'many Shapley values' question itself was not necessarily provided, Covert et al. (2021) also gave a careful characterization and catalogue of the many published works on the topic, emphasizing the choice of:

1. summary technique
2. captured model behavior
3. feature removal technique

We delay a more detailed discussion of alternate summarization techniques besides the Shapley value until Section 3.2.4. For the captured model behavior, the paper mostly considered two possibilities: (i) the case of explaining an individual prediction; or (ii) the case of total loss of the method. In the second case, this is highly connected to global feature explainability and feature importance measures which we discuss in Section 3.5.2. These approaches try to explain how important a feature is *overall* for the model. For now, we instead focus on the first case which focuses on how a feature impacted a particular prediction, called its *local attribution*.

Finally, the critical choice of feature removal technique generally resulted in three main approaches: replace by a baseline feature, marginalize out a feature by its marginal distribution, or marginalize out a feature by its conditional distribution. In the context of explaining a prediction, this results in:

$$v^{\text{base}}(S) := \mathcal{M}_S^{\text{base}} \circ f := f(x_S, \bar{x}_{-S}) \tag{12}$$

$$v^{\text{marg}}(S) := \mathcal{M}_S^{\text{marg}} \circ f := \mathbb{E}_{\bar{X}_{-S} \sim p(X_{-S})}\Big[f(x_S, \bar{X}_{-S})\Big] \tag{13}$$

$$v^{\text{cond}}(S) := \mathcal{M}_S^{\text{cond}} \circ f := \mathbb{E}_{\bar{X}_{-S} \sim p(X_{-S} | X_S = x_S)}\Big[f(x_S, \bar{X}_{-S})\Big] \tag{14}$$

These are the baseline value function, marginal value function, and conditional value function, which in turn result in the baseline Shapley, marginal Shapley, and conditional Shapley. Discussion on some of the methods used for approximating these values is provided at length in Covert et al. (2021). There are also additional methods for removing features within certain application domains. Some vision-specific examples include image blurring (Fong and Vedaldi, 2017; Fong et al., 2019) and conditional VAEs/ GANs (Chang et al., 2019). There are also notions of causally setting a feature to a certain value, such as following Pearl's *do*() operator framework (Heskes et al., 2020). They show how there can be sensitive and counter-intuitive results if one believes Shapley represents a causal influence without understanding the underlying causal structure.

Debate over the choice of how to reduce to the value function continues into the present day. Despite Lundberg and Lee (2017) and predecessors making it explicit that the choice of marginal and baseline are only a simplifying choice for computational reasons, there are several researchers who argue for the use of the marginal value with different motivations. A major argument is that of (Janzing et al., 2020) which argues that under a causal independence assumption, this leads to a causal interpretation, calling it the interventional Shapley instead of the marginal Shapley.

Another major discomfort coming from those supporting the marginal approach is regarding the apparent paradox that a model which exclusively uses X_1 (and not X_2) can be

found to have importance for both features X_1 and X_2 if they are heavily correlated (Merrick and Taly, 2020). Although this is perfectly reasonable from a statistical perspective since X_1 and X_2 contain the same information content, making models which use X_1 or use X_2 fundamentally similar in their decision-making process (Adler et al., 2018), researchers finding this fact paradoxical claim to want to better understand the algebraic structure of the blackbox model, rather than the statistical structure.

Frye et al. (2021) instead provides a convincing argument for why researchers should never use the baseline or marginal approaches for correlated features, namely that when making queries to the model 'off the manifold' of where it saw training data, this leads to the classic 'garbage in, garbage out' issue and leads to unpredictable behavior from the model. This sentiment has been further echoed by other researchers working on feature-based explanations (Hooker and Mentch, 2019).

Accordingly, we implore those authors who sympathize with the name of 'interventional Shapley' to justify which of their favorite datasets have independent features and hereafter we only consider the name 'marginal Shapley'. Nevertheless, many researchers continue to be attracted to this style of explanation, either due to a belief in its computational simplicity or due to being interested in a more mechanistic and causal explanation of how changing inputs will change the output prediction. Although completely ignoring the data manifold can only lead to catastrophically irrelevant explanations, conditional Shapley is not insulated from producing counterintuitive results.

Finally, before moving on to the next section, we also discuss some of the model-specific variants of estimating SHAP. Generally, these are approaches which are specially designed for certain architectures and thereby have some computational advantages. The most major of these should be the approach of TreeSHAP (Lundberg et al., 2018) which was one of the earliest approaches to have a computationally easy way to calculate the SHAP value for the specific architecture of decision trees or random forests. Although it was not well understood at its origin, it is now better understood that this algorithm requires the assumption of independent input features to calculate the conditional SHAP value, and otherwise computes a model-specific version of the SHAP value which is neither the marginal nor conditional Shapley (Amoukou et al., 2022; Filom et al., 2024). Nevertheless, due to its great popularity at the time, several extensions to enhance the algorithm exist, including GPU Tree SHAP (Mitchell et al., 2022b) and Fast Tree SHAP (Yang, 2022).

Another major class of interesting machine learning algorithms are those of kernel machines. This includes the method RKHS SHAP (Chau et al., 2022) for reproducing kernel Hilbert spaces. Then there is the extension from RKHS SHAP to GP SHAP (Chau et al., 2023) which extends to Gaussian Processes. There they also consider the method of Bayes-GP-SHAP as an attempt to integrate both the GP posterior uncertainty and the SHAP approximation uncertainty into the same approach. Unfortunately, both of these kernel-based approaches are restricted to the assumption of independent features by nature of the tensor product structural assumption on the Hilbert spaces. One class of models which has been able to overcome the assumption of independence is the generalized additive model (GAM), which has seen specific algorithms due to its similar additive structure to SHAP (Bordt and von Luxburg, 2023; Enouen and Liu, 2025).

In addition to these model-specific enhancements, there have also been many works focusing on faster and more efficient approximation of the Shapley value, especially extending the two major approximation algorithms of permutation sampling and the kernel approximator. This includes empirical studies of permutation sampling (PermSHAP) (Mitchell et al., 2022a), functional extensions of kernel estimation (FastSHAP) (Jethani et al., 2022), approximating without marginal contributions (SVARM) (Kolpaczki et al., 2024), and many more.

3.2.4 Probabilistic Values: Extensions of the Shapley Value

The cooperative game theory literature did not stop advancing after the introduction of Shapley's 1953 method, with many further extensions of the Shapley value being developed in the half a century which it took for the ML community to discover it. In alternate contexts, many of the defining axioms of the Shapley value may be important to get rid of. Many of these extensions and related approaches have also been incorporated into the ML interpretability literature.

The largest class of these are the *probabilistic values* which are generally defined as solutions which only obey the linearity axiom and the dummy axiom (dropping symmetry and efficiency). These are further categorized as efficient probabilistic values, called *quasivalues*, which obey every axiom except for symmetry, and symmetric probabilistic values, called *semivalues*, which obey every axiom except for efficiency.

Definition 5 *(Weber, 1988) A* ***probabilistic value*** *can be defined as those values which, for each i, obey:*

$$\phi_i(v) = \sum_{S \subseteq ([d]-i)} p^i(S) \cdot \Big[v(S+i) - v(S) \Big] \tag{15}$$

for some probability distribution $p^i(S)$ over all of the coalitions without i, namely $S \in \mathcal{P}([d]-i)$. In other words, a probabilistic value can be defined by an averaging over its marginal contributions for some specified averaging scheme which depends on i.

Theorem 6 *(Weber, 1988) A solution is a probabilistic value iff it obeys the additivity (linearity) axiom and dummy axiom.*

This covers a fairly wide number of solution concepts of interest, including the Banzhaf value, Owen value, and Myerson value. Of course lifting both of the symmetry and efficiency axioms is potentially unnecessary, and it is commonly of interest to lift only one of symmetry or efficiency, giving the semivalue and the random order value (quasivalue).

Definition 7 *(Weber, 1988) A* ***random order value*** *(or quasivalue) can be defined as those values which, for each i, obey:*

$$\phi_i(v) = \sum_{\pi \in \Pi_d} p(\pi) \cdot \Big[v(S_i^\pi + i) - v(S_i^\pi) \Big] \tag{16}$$

for some distribution p over all permutations of $[d]$, namely $\pi \in \Pi_d$.

Theorem 8 *(Weber, 1988) A solution is a random order value iff it obeys additivity, dummy, and efficiency.*

It becomes clear why this is a random order value because we order the players according to a random ordering drawn from some distribution, and then take their marginal contribution according to that ordering. This extends Shapley's weighted value (Shapley, 1953; Kalai and Samet, 1987) and the more general *path value* (Owen, 1972). Another specific random-order value of interest is the Owen value (Owen, 1977) with developments and extensions by (Hart and Kurz, 1983) and (Winter, 1989).

Definition 9 *(Weber, 1988) A* ***semivalue*** *can be defined as those values which, for each i, obey:*

$$\phi_i(v) = \sum_{S \subseteq ([d]-i)} p^i(|S|) \cdot \Big[v(S+i) - v(S) \Big] \tag{17}$$

for some 'distribution' $p^i(s)$ over the possible sizes of S, i.e. $\sum_{s=0}^{d-1} [\binom{d-1}{s} \cdot p^i(s)] = 1$.

Here, the Banzhaf value (Banzhaf, 1965) is the greatest representative here, also with integral extensions in a similar fashion to path values providing a bijection with possible semivalues (Dubey and Weber, 1977; Dubey et al., 1981).

Definition 10 ***(Banzhaf value)*** *The Banzhaf value may be defined in its 'closed form' solution in terms of using each $v(S)$ only once as:*

$$\phi_i^{Bz}(v) = \sum_{S \subseteq ([d]-i)} \frac{1}{2^{d-1}} \cdot \Big[v(S+i) - v(S) \Big], \tag{18}$$

but this can easily be seen to be equal to taking the same sum over all 2^d possibilities or by grouping by marginal size, making the semivalue formula, Equation 16, clear:

$$\phi_i^{Bz}(v) = \sum_{k=0}^{d-1} \frac{1}{2^{d-1}} \cdot \sum_{\substack{S \subseteq ([d]-i) \\ s.t.\ |S|=k}} \Big[v(S+i) - v(S) \Big] \tag{19}$$

Lastly, the Banzhaf value can also be put into its purified form in terms of the purified contributions:

$$\phi_i^{Bz}(v) := \sum_{S \ni i} \frac{\tilde{v}(S)}{2^{(|S|-1)}} \tag{20}$$

Important extensions which do not obey either of the original symmetry or efficiency axioms originally often incorporate some alternative structure: the AD value (Aumann and Dreze, 1974) respects a partition of the players (obeying partition-symmetry and partition-efficiency) and the Myerson value (Myerson, 1977) respects graphical connections between the players. The Owen-Winter value (Owen, 1977; Winter, 1989) also respects hierarchical partitioning, but obeys normal efficiency. Additionally, there is the von-Neumann-Morgenstern solution (von Neumann et al., 1944), the core (Gillies, 1959; Shapley, 1965), the least core (Maschler et al., 1979), and the nucleolus (Schmeidler, 1969).

Important topics related to these approaches but not providing individual methods are the potential function (Hart and Mas-Colell, 1989), the Harsanyi dividend (Harsanyi, 1963), and monotonic solutions (Kalai and Samet, 1985). A great resource for starting to explore these topics in greater depth is (Winter, 2002; Monderer and Samet, 2002).

Simple Monotone Games In the machine learning language, we have so far focused on games which are dealing with the case of regression problems rather than classification problems. But, these game-theoretic axioms and solutions have also been quite extensively studied in the context of what are called simple monotonic games or voting games. Here, the input features are players voting for a final (discrete) decision, rather than contributing to an overall valuation. These games are defined as those which are both *simple* and *monotone*.

Definition 11 *(Simple)* $v : \mathcal{P}([d]) \to \{0, 1\}$

Definition 12 *(Monotone)* *If* $v(S) = 1$ *and* $R \supseteq S$*, then* $v(R) = 1$.

where v takes the interpretation of describing a coalition S as 'winning' (1) or 'losing' (0). It is very often in the context of voting, where a coalition represents the voters willing to vote for the bill.

It is here actually, where the Banzhaf value (Banzhaf, 1965), or more specifically the Penrose-Banzhaf power index (Penrose, 1946), actually predates the Shapley value, or more specifically in this context the Shapley-Shubik power index (Shapley and Shubik, 1954), in its original 1946 conception. In this new context of voting games, many axioms need to be slightly reinterpreted. For these reasons, these values are also usually called an 'index of power' instead of a 'value' to refer to the voting power held, rather than the monetary value distributed.

In this context, the concept of the 'minimal winning coalition' also becomes a more critical aspect of the definition.

Definition 13 *(Winning Coalition) A set* S *is a winning coalition if* $v(S) = 1$*. Due to monotonicity, this implies* $v(R) = 1$ *for all* $R \supseteq S$*.*

Definition 14 *(Minimal Winning Coalition) A set* S *is a minimal winning coalition if it is a winning coalition containing no other winning coalition.* $v(S) = 1$*, but* $v(S - i) = 0$ *for all* $i \in S$*.*

These are necessary to define the Deegan-Packel index (Jr. and Packel, 1978), which weights each MWC S as $\frac{1}{|S|}$ to all $i \in S$ and averages this amount over all MWCs, $\mathcal{I}_{\text{MWC}} = \{S : S \text{ is MWC}\}$.

Definition 15 ***(Deegan-Packel index)***

$$\phi_i^{DP} := \frac{1}{|\mathcal{I}_{MWC}|} \sum_{S \in \mathcal{I}_{MWC}} \frac{\mathbb{1}(i \in S)}{|S|} \tag{21}$$

Relatedly, we will call a player i *critical* for coalition S if removing i results in a losing vote, we will call a set's *critical number* the number of critical players, and we will call a set critical if it has critical number greater than zero. Write $\mathcal{I}_{\text{crit}} = \{S : S \text{ is critical}\}$.

Definition 16 *(Critical Player) A player i is critical for S if S is winning but $S-i$ is not: $v(S)=1$ and $v(S-i)=0$.*

Definition 17 *(Critical Number) A set S has critical count, $Crit(S)=|\{i\in S : i \text{ is critical in } S\}|$.*

These are necessary to define the Johnston index (Johnston, 1977), which replaces the Banzhaf uniform scoring across critical votes with a balanced score based on the number of players which criticality is shared with.

Definition 18 ***(Johnston Index)***

$$\phi_i^{Js} := \frac{c_i^{Js}}{\sum_j c_j^{Js}} \qquad where \qquad c_i^{Js} := \sum_{S\in\mathcal{I}_{crit}} \frac{\mathbb{1}(i \text{ is critical in } S)}{Crit(S)} \tag{22}$$

Theorem 19 ***(Banzhaf Power Index)*** *The Banzhaf index of power is equal to*

$$\phi_i^{Bz} = \frac{c_i^{Bz}}{\sum_j c_j^{Bz}} \qquad where \qquad c_i^{Bz} := \sum_{S\in\mathcal{I}_{crit}} \mathbb{1}(i \text{ is critical in } S) \tag{23}$$

A third renormalization of the Banzhaf value is the Coleman index (Coleman, 1971), which in addition to providing the typical 'power to initiate voting action' also provides a measure of 'power to prevent voting action'.

Definition 20 ***(Banzhaf–Coleman Index)***

$$\phi_i^{Cl\text{-}init} = \frac{\sum_{S\not\ni i}[v(S+i)-v(S)]}{\sum_{S\not\ni i} \quad [1-v(S)]} \tag{24}$$

$$\phi_i^{Cl\text{-}prev} = \frac{\sum_{S\ni i}[v(S)-v(S-i)]}{\sum_{S\ni i} \quad [v(S)]} \tag{25}$$

The former again counts all sets which i is critical in, this time normalizing by the total number of coalitions without i where there is inaction. The latter counts all sets which i is 'reverse-critical' in, normalizing by the total number of coalitions with i which have already achieved action. There are also further extensions which deal with the case of each player being able to explicitly vote for or against the bill, resulting in ternary values instead of the binary subset representation (Felsenthal and Machover, 1997, 2001).

This already gives a taste for the much greater complexity afforded when making the application to even the simplest machine learning problems with binary inputs and one binary output. The differences between explaining a decision of 1 or a decision of 0 are already poorly captured by many of the existing approaches. For instance, treating the same boolean function in a computer science context requires the dual concepts of *satisfiability* and *unsatisfiability* which each provide distinct notions of hardness. Applying to more realistic classification problems with hundreds or thousands of output classes and mixed-type input features only further complicates this connection (Krizhevsky et al., 2012; Bahdanau et al., 2015). Beyond classification, additive modeling applied to more complex scenarios like ordinal regression (Kook et al., 2022) or hazard regression (Cox, 1972) is also not guaranteed to align with game-theoretic solutions to the same problem.

It is here where we emphasize that the commonly abused phrase 'game-theoretic explainability' in reference to the Shapley value is an injustice to the field. In particular, although the Shapley value has its roots in cooperative game theory, extending the analogy beyond superadditive value functions and monotone voting functions where these game-theoretic approaches draw their conceptual origins really strains this analogy. Hopefully, it can be seen how these ϕ^{DP} and ϕ^{Js} indices provide a first look at the type of indices which require more than the set-theoretic 'Mobius' structure and begin to focus on the non-cooperative game-theoretic aspects of the problem.

Some additional values in this direction are the Holler-Packel index (Holler, 1978; Holler and Packel, 1983; Napel, 1999; Holler and Napel, 2004) and the shift minimal winning coalition index (Alonso-Meijide and Freixas, 2010; Alonso-Meijide et al., 2012). A great resource for an introduction into the measurement of voting power is (Felsenthal and Machover, 1998).

3.3 Applying the Shapley Value to Data Valuation

As discussed thoroughly in the previous section, a major effort of defining the Shapley value for a certain problem is in the setup of the value function, which is to then be summarized by the Shapley solution. The previous section focused entirely on how the *removal of a feature* would affect an individual prediction; however, this section will instead look at the *removal of a data point*. Many of these works focus on explaining the total loss rather than the individual prediction (although feature-based loss explanations and dataset-based prediction explanations do also exist, see Section 3.5 for the former). This is another key set of value functions to explore for interpreting machine learning models and has helped further spark research in the direction of data attribution and data valuation.

Although *influence functions* had already been classically proposed for this problem (Cook, 1977; Cook and Weisberg, 1980, 1982) and later modernized for the modern machine learning era (Koh and Liang, 2017), there was much greater interest into researching the topic after the introduction of the unifying view of the Data SHAP method (Ghorbani and Zou, 2019; Jia et al., 2019b).

$$V(S) := \mathbb{E}_{\hat{\theta}\sim p_{S,\mathcal{A}}(\hat{\theta})}\Big[\mathcal{L}_{\text{test}}(f_{\hat{\theta}})\Big] \quad \text{s.t.} \quad \hat{\theta} \approx \underset{\theta}{\text{argmin}}\left\{\mathcal{L}_{\text{trn},S}(f_\theta)\right\} \tag{26}$$

where $\mathcal{A}$ denotes the specific algorithm chosen to minimize the empirical risk $\mathcal{L}_{\text{trn},S}$ over the subset $S \subseteq [n]$ of the full n training data points. $p_{S,\mathcal{A}}(\hat{\theta})$ denotes the distribution over the approximately optimal $\hat{\theta}$ returned by algorithm $\mathcal{A}$ when trained on data subset $(x^{(\alpha)}, y^{(\alpha)})_{\alpha\in S}$. For a deterministic algorithm $\mathcal{A}$, this will be a Dirichlet distribution with 100% of its mass on the returned parameters. For simplicity, let us also write $z := (x, y) \in \mathcal{Z} := \mathcal{X} \times \mathcal{Y}$ with training dataset $Z_{\text{trn}} = \{z^{(\alpha)}\}_{\alpha=1}^n = \{(x^{(\alpha)}, y^{(\alpha)})\}_{\alpha=1}^n$.

The complexity of retraining a model for each coalition of data points (a requirement for computing this value function at each S) is extremely costly, even for moderately sized ML models. This is the huge disadvantage of this formulation and has been a challenge of data valuation research since the beginning. This is also why alternative approaches like TracIn (Pruthi et al., 2020) and representer points (Yeh et al., 2018) have been introduced which avoid retraining entirely, instead choosing to use gradient approximations or representer theorems, respectively.

Despite these many challenges, the allure of an approach for fairly dividing value amongst the different data points has resulted in continuing developments of this research direction. First, (Ghorbani et al., 2020) removes the dependence on a specific dataset context and reframes the data SHAP value from a dataset-dependent value to a distributionally-dependent value. The original data SHAP can be written like Equation 5 as:

$$\phi_\alpha^{\text{DataSHAP}} = \sum_{k=0}^{n-1} \frac{1}{n} \cdot \sum_{\substack{S \subseteq ([n]-\alpha) \\ \text{s.t. } |S|=k}} \binom{n-1}{k}^{-1} \cdot \Big[V(S+\alpha) - V(S) \Big] \Big] \tag{27}$$

where it becomes more clear that from the perspective of data point i, S serves the role of a random data subset of size k. The distributional Shapley value (Ghorbani et al., 2020) makes this clear by actually sampling the $z_S = (x_S, y_S)$ randomly from a distribution, $\mathcal{D}$, instead of subsampling from a fixed dataset, $(x^{(\alpha)}, y^{(\alpha)})_{\alpha \in S}$ for $S \subseteq [n]$.

$$\phi_{z^{(\alpha)}}^{\text{DistSHAP}} := \sum_{k=0}^{n-1} \frac{1}{n} \cdot \mathbb{E}_{Z \sim \mathcal{D}^k} \Big[V(Z + z^{(\alpha)}) - V(Z) \Big] \tag{28}$$

where Z is a random dataset of size k, sampled i.i.d. according to distribution $\mathcal{D}$. We also abuse the notation of V, allowing it to take data points instead of the subsets which represented those data points, extended in the obvious way.

Although very similar to the original definition, this definition no longer has an explicit dependence on the fixed dataset which was drawn, much like how the influence of a random algorithm was already averaged out directly in the definition. Both of these choices abstract away details of the implementation process while maintaining the critical details to define an axiomatically sound data valuation process.

Similar to the 'model-specific' SHAP variants, model-specific DataSHAP variants have also emerged. Unsurprisingly, the data influence of a hard-label k-NN model is relatively easy to compute (Jia et al., 2019a). Further calculations were done for the distributional SHAP on linear models, logistic models, and kernel density estimators (Kwon et al., 2021). Follow-up work continued to improve the efficiency of DataSHAP estimation for weighted k-NN classifiers (Wang et al., 2024b).

Further developments continued, introducing variations of the Shapley value for explaining the value functions. In particular, removing the efficiency axiom results in a 'semivalue' as discussed previously, with approaches like Beta Shapley (Kwon and Zou, 2022), Least Core for data attribution (Yan and Procaccia, 2021), and Data Banzhaf (Wang and Jia, 2023). Follow-up works have also contextualized the limitations of Data SHAP and variants for downstream tasks like data selection (Wang et al., 2024c). Other works have managed to come full circle, reframing gradient approximations back within the Shapley framework (Wang et al., 2025). Further details on data valuation can be found in Hammoudeh and Lowd (2024).

3.4 Extending the Shapley Value to Feature Interactions

Although we have already established the long history of studying the detection of feature interactions, in the modern context of explainability for machine learning, we here find it

convenient to group all of the interaction-based explanations as though they were motivated by SHAP, even though this is not necessarily the case.

We begin by recalling the purified form of the game by the Mobius transform from Equation 2:

$$\tilde{v}(S) := \sum_{T \subseteq S} (-1)^{|S|-|T|} \; v(T) \tag{29}$$

We also define the discrete derivative operator, δ_S, by writing $w = \delta_S \circ v$ as:

$$w(T) = [\delta_S \circ v](T) := \sum_{R \subseteq S} (-1)^{|S|-|R|} \cdot v(T - S + R) \tag{30}$$

It can be noticed that this definition of $[\delta_S \circ v]$ on all $T \subseteq [d]$ is an extension of the common definition only on $T \subseteq ([d] - S)$, because for any such T, $w(T) = w(T + Q)$ for all $Q \subseteq S$. This is similar to how Shapley values and probabilistic values are commonly only defined over $([d] - i)$. Further, it can also easily be seen that:

$$\tilde{v}(S) = [\delta_S \circ v](\emptyset) \tag{31}$$

We may now define the simplest feature interaction explanations which are the inclusion and removal values, ϕ^{inc} and ϕ^{rem}, in terms of the discrete derivative, δ_S:

$$\phi_S^{\text{inc}}(v) := [\delta_S \circ v](\emptyset) = \sum_{R \subseteq S} (-1)^{|S|-|R|} \cdot v(R) \tag{32}$$

$$\phi_S^{\text{rem}}(v) := [\delta_S \circ v]([d]) = \sum_{Q \subseteq S} (-1)^{|Q|} \cdot v([d] - Q) \tag{33}$$

From this it can be seen that:

$$\phi_S^{\text{inc}}(v) = \tilde{v}(S) \qquad \phi_S^{\text{rem}}(v) = \sum_{T \supseteq S} \tilde{v}(T) \tag{34}$$

The line of research from the cooperative game theory literature, despite the large variety of solution concepts for value allocation and voting power, would not study the interaction strength between two players until 1999. Measuring the strength of a pair of players rather than their individual strengths first appeared in the work of (Grabisch and Roubens, 1999) which extended the Shapley axioms to be able to apply to this different situation. Solution concepts for this scenario are generally called interaction indices instead of values based off this first solution being called the Shapley Interaction Index. The solution was obtained by combining the two players i and j together into a joint player and then applying the Shapley value, comparing that against the individualized contributions of those same players. The typical definition is given as

$$\phi_S^{\text{SII}}(v) = \sum_{T \subseteq [d]-S} \frac{(d - |S| - |T|)!|T|!}{(d - |S| + 1)!} \sum_{L \subseteq S} (-1)^{|S|-|L|} v(L + T), \tag{35}$$

which can be shown to be equal to

$$\phi_S^{\text{SII}}(v) = \frac{1}{d - |S| + 1} \sum_{T \subseteq [d]-S} \binom{d - |S|}{|T|}^{-1} \sum_{R \subseteq T} \tilde{v}(S + R), \tag{36}$$

and with just a little more work is equal to

$$\phi_S^{\text{SII}}(v) = \sum_{R \subseteq [d]-S} \frac{1}{(|R|+1)} \tilde{v}(S+R), \tag{37}$$

which is nearly the same as the purified version of the Shapley value from Equation 3.

Modern attempts to create another Shapley interaction index would not appear until two decades later within the explainability literature: the Shapley-Taylor Interaction Index (Sundararajan et al., 2020), the Faithful Shapley Interaction Index (Tsai et al., 2023), and the k-Shapley Interaction Index (Bordt and von Luxburg, 2023).

Accordingly, it is here where our story of feature interaction detection picks back up as the historical approaches bleed together with the modern approaches working on interaction detection from the perspective of explainability. As we left off in the end of Section 3.1, the problem of interaction detection was beginning to gain traction in high-dimensional statistics with (Bien et al., 2013) and (Hao and Zhang, 2014) using heredity to ensure detection of interactions even in the presence of high-dimensional data and few available samples. Follow-up works continued to look at selecting from all pairwise interactions without having to face the full quadratic complexity in terms of the input dimension (Lim and Hastie, 2015; Bien et al., 2015; Kong et al., 2017).

Around this time, the importance of interactions for the interpretability literature was starting to become increasingly well-known. Existing tools like LIME and SHAP were ill-equipped for handling or describing the interaction between inputs like in word negation in natural language and part hierarchies in computer vision. Early works like NID (Tsang et al., 2018a) and CD (Murdoch et al., 2018) gave architecture-specific approaches for understanding the nonlinear interactions occurring within neural networks.

Important follow-up works use model-agnostic approaches for the detection of interactions. The Shapley-Taylor interaction index (Sundararajan et al., 2020) uses a Taylor-series-like expansion which gives all interactions of degree less than k exactly their purified contribution and splits the remaining contributions amongst those interactions of degree k.

$$\phi_S^{\text{ShapleyTaylor-}k}(v) = \begin{cases} \tilde{v}_S, & \text{if } |S| < k \\ \sum_{T \supseteq S} \binom{|T|}{|S|} \cdot \tilde{v}_T, & \text{if } |S| = k \end{cases} \tag{38}$$

which is designed to satisfy efficiency when considering the entire set of singles and pairs $\mathcal{I}^{\leq 2} := \{S : S \subseteq [d], |S| \leq 2\}$.

The approach of Archipelago (Tsang et al., 2020b) also took a model-agnostic approach to define the importance of an interaction

$$\phi_S^{\text{ArchDetect}}(v) = \frac{1}{2}\phi_S^{\text{inc}}(v)^2 + \frac{1}{2}\phi_S^{\text{rem}}(v)^2 \tag{39}$$

$$\phi_S^{\text{ArchAttrib}}(v) = v(S) - v(\emptyset) \tag{40}$$

where we write the definition in terms of the inclusion and removal values, ϕ^{inc} and ϕ^{rem}, defined above in Equation 33. Note that the $\phi^{\text{ArchDetect}}$ score is designed to be positive to measure the strength of an interaction, whereas $\phi^{\text{ArchAttrib}}$ can be positive or negative to

measure the overall effect of the feature set S. Follow-up works also consider the Archipelago defined as an interaction index to fit within the Mobius game:

$$\phi_S^{\text{Archipelago}}(v) = \frac{1}{2}\phi_S^{\text{inc}}(v) + \frac{1}{2}\phi_S^{\text{rem}}(v), \tag{41}$$

but note that not only $\phi_S^{\text{Archipelago}} \neq \phi_S^{\text{ArchAttrib}}$, but also $\phi_S^{\text{ArchDetect}} \neq (\phi_S^{\text{Archipelago}})^2$.

Not too long after, further attempts at defining a 'correct' interaction index extending the Shapley value would be developed from the interpretability literature. The Faithful Shapley Interaction Index (Tsai et al., 2023) or Faith-SHAP would be introduced by extending the variational formulation of Shapley from Equation 6. Equation 6 is first reformulated as Equation 42 and then extended to the definition in Equation 43.

$$\phi^{\text{SHAP}} = \underset{\phi \in \mathbb{R}^d}{\text{argmin}} \left\{ \sum_{S \subseteq [d]} m^{\text{Sh}}(|S|) \cdot \left[v(S) - \phi_\emptyset - \sum_{i=1}^{d} \mathbb{I}\big(\{i\} \subseteq S\big) \cdot \phi_i \right]^2 \right\} \tag{42}$$
$$\text{s.t.} \quad v(\emptyset) = \phi_\emptyset \;\text{ and }\; v([d]) = \phi_\emptyset + \sum_{i=1}^{d} \phi_i,$$

$$\phi^{\text{FaithSHAP-}k} := \underset{\phi \in \mathbb{R}^{d_k}}{\text{argmin}} \left\{ \sum_{S \subseteq [d]} m^{\text{Sh}}(|S|) \cdot \left[v(S) - \sum_{T \in \mathcal{I}^{\leq k}} \mathbb{I}\big(T \subseteq S\big) \cdot \phi_T \right]^2 \right\} \tag{43}$$
$$\text{s.t.} \quad v(\emptyset) = \phi_\emptyset \;\text{ and }\; v([d]) = \sum_{T \in \mathcal{I}_{\leq k}} \phi_T,$$

where $m^{\text{Sh}}(s) = [\binom{d}{s} \cdot s \cdot (d-s)]^{-1}$, $\mathcal{I}_{\leq k} := \{S \subseteq [d] : |S| \leq k\}$, and $d_k = |\mathcal{I}_{\leq k}|$. This definition simply takes the one-dimensional additive model and extends it to the k-dimensional additive model which is trying to capture the 'best approximation' to the true value function $v(S)$, under the masking distribution defined by m^{Sh}.

Around the same time, the k-Shapley interaction index (Bordt and von Luxburg, 2023) was defined as the correction to the SII value which additionally obeys the efficiency axiom. This is achieved by setting the largest subsets with $|S| = k$ as the SII value and recursively defining lower-order values such that they obey efficiency:

$$\phi_S^{k\text{-SII}}(v) = \begin{cases} \phi_S^{\text{SII}}(v), & \text{if } |S| = k \\ \phi_S^{(k-1)\text{-SII}}(v) + B_{k-|S|} \cdot \sum_{R \supseteq S, |R|=k}^{R \text{ s.t.}} \phi_R^{\text{SII}}(v), & \text{if } |S| < k \end{cases} \tag{44}$$

where B_n are the Bernoulli numbers (which can be defined as the sequence obeying $B_0 = 1$ otherwise $\sum_{i=0}^{n} \binom{n+1}{i} B_i = 0$). These numbers simply show up as the combinatorial coefficients required to balance the interaction index to obey the efficiency condition across all subsets $S \in \mathcal{I}^{\leq k}$.

Although there are several more approaches to explaining interactions in the literature, many of these approaches are model-specific or tied to a specific application domain. We discuss many of these in Section 5 on applications. Accordingly, this already covers the majority of model-agnostic approaches to understanding interactions, besides their connections

to global interpretability. Before finishing the section on feature interactions, we discuss the all-important connection to the classical approach of sensitivity analysis from the 1990s. This area uses the tool of the functional ANOVA to provide a link between the local feature attribution and the global feature importance, or equally the local interaction attribution and the global interaction importance. It does this through the Sobol indices which measure the variation of the local attribution. In the case of independent variables, it provides an exact link between these two views and thus a link between local attribution explanations and global importance explanations for a large majority of existing explainability approaches. The techniques from functional ANOVA help to cement these interrelated areas of generalized additive models, feature interaction detection, and Shapley explanations as fundamentally the same.

3.5 Connections to Global Explainability

In this section, we discuss the connections between the local methods of feature attribution and interaction attribution and the global methods of feature importance and interaction importance. This is done mainly through the connections to the literatures of *sensitivity analysis* and *feature importance*, related also to the study of feature selection and variable importance.

3.5.1 Relationship with Sensitivity Analysis

It has become increasingly popular to understand the connections with the functional ANOVA decomposition or what is often called the Mobius transform in XAI literature (Herren and Hahn, 2022; Fumagalli et al., 2025). In this section, we take a first look at this connection between the Shapley value and other related explainability approaches, before a deeper analysis of the three-way connection between feature interactions, additive models, and sensitivity analysis is further explored in Section 4.5.3.

Variance-based sensitivity analysis, sometimes called the method of Sobol', is based on the functional ANOVA decomposition

$$f(x) = \sum_{S \subseteq [d]} \tilde{f}_S(x_S) \tag{45}$$

where as before we have the purified functions as

$$\tilde{f}_S(x_S) = \sum_{T \subseteq S} (-1)^{|S|-|T|} \cdot (\mathcal{M}_T^{\text{cond}} \circ f)(x_T). \tag{46}$$

Note that because the original application was to simulated experiments (Sobol', 1990), this allowed researchers to easily make the assumption that all input variables are independent. Accordingly, using $\mathcal{M}^{\text{cond}}$ or $\mathcal{M}^{\text{marg}}$ is equivalent in the definition and modern extensions have considered both approaches, although $\mathcal{M}^{\text{cond}}$ is more popular.

As pointed out in Herren and Hahn (2022); Bordt and von Luxburg (2023); Enouen and Liu (2025), it can be seen fairly immediately that this allows for a correspondence between the SHAP functional applied to a machine learning model and the functional ANOVA

decomposition, extending the form in Equation 3:

$$\phi_i^{\text{SHAP}}(x) = [\Phi_i^{\text{SHAP}} \circ f](x) = \sum_{S \ni i} \frac{\tilde{f}(x_S)}{|S|} \tag{47}$$

The functional decomposition itself is only part of the story for sensitivity analysis. The key object of study for the sensitivity analysis approach is mostly the set of Sobol indices (Sobol', 1990) defined from these functions as:

$$\sigma_S^2 := \mathbb{V}\text{ar}_{X_S}\left[\tilde{f}_S(X_S)\right] \tag{48}$$

Please note again that this definition is also worth scrutinizing because there are multiple equivalent formulations in the independent variable case and there is no 100% consensus on how to extend the original techniques.

The major property of the Sobol' indices is the ***decomposition of variance*** formula which states that:

$$\sigma^2 = \mathbb{V}\text{ar}_X\left[f(X)\right] = \sum_{S \subseteq [d]} \mathbb{V}\text{ar}_{X_S}\left[\tilde{f}_S(X_S)\right] =: \sum_{S \subseteq [d]} \sigma_S^2, \tag{49}$$

meaning that the total variance of the function f decomposes into a measure of how much variance there is across each of the different interactions S. Critically, this formula *only* holds in the case of independent input variables and completely breaks down for correlated variables. Nevertheless, let us make this assumption for the rest of the section.

There is also the 'total-effect' index, defined in a somewhat dualistic fashion to the Sobol index, which is designed to measure how S interacts with all of the other features:

$$\varphi_S^{\text{Sobol-total}} := \mathbb{E}_{x_{-S}}\left[\mathbb{V}_{X_S \sim p(X_S | X_{-S} = x_{-S})}\left[f(X_S, x_{-S})\right]\right] \tag{50}$$

$$\sigma_S^2 := \mathbb{V}_{x_S}\left[\mathbb{E}_{X_{-S} \sim p(X_{-S} | X_S = x_S)}\left[f(x_S, X_{-S})\right]\right] \tag{51}$$

which is equal to $\varphi_S^{\text{Sobol-total}} = \sum_{T \subseteq [d] \text{ s.t. } T \cap S \neq \emptyset} \sigma_T^2$ for independent variables. Because of the decomposition of variance formula, it is also common to consider the Sobol index as the percentage of the variance explained, as in $\sigma_S^2 / \mathbb{V}[f]$. The same can be done for the total index, $\varphi_S^{\text{Sobol-total}} / \mathbb{V}[f]$.

Other work had already made a connection between this global variance sensitivity and the Shapley value (Owen, 2014), writing the Shapley of the variance game $\varphi_i^{\text{Shapley}} := [\Phi_i^{\text{SHAP}} \circ v^{\text{var}}]$ where $v^{\text{var}}(S) := \mathbb{V}\text{ar}_X\left[f_S(X_S)\right]$. By then leveraging the following lower and upper bounds, it was possible to bound this new Shapley explanation between known values based on the Sobol coefficients.

$$\varphi_S^{\text{Sobol-lower}} = \sum_{T \subseteq S} \sigma_T^2, \qquad \varphi_S^{\text{Sobol-upper}} = \sum_{T \subseteq [d] \text{ s.t. } T \cap S \neq \emptyset} \sigma_T^2, \tag{52}$$

$$\varphi_{\{i\}}^{\text{Sobol-lower}} \leq \varphi^{\text{Shapley}} \leq \varphi_{\{i\}}^{\text{Sobol-upper}}. \tag{53}$$

This is again only true in the case of independent variables and is straightforward to see from Equation 3 and the fact that $\sigma_S^2 \geq 0$.

It is worth noting how the Shapley of the variance (Owen, 2014) is different from the variance of the Shapley value, even for independent variables.

$$\Phi_i^{\text{SHAP}} \circ v^{\text{var}} = \sum_{S \ni i} \frac{\sigma_S^2}{|S|} \tag{54}$$

$$\mathbb{V}\left[\phi_i^{\text{SHAP}}\right] = \sum_{S \ni i} \frac{\sigma_S^2}{|S|^2} \tag{55}$$

From here, we hold off an saying much more on functional ANOVA until a further discussion on additive models. Hopefully, these results already begin to demonstrate how intimately tied different research areas of feature interactions, Shapley values, and sensitivity analysis truly are. We revisit the discussion on functional ANOVA connections in Section 4.5.3. For now, we further connect this global perspective with other variable importance and feature importance measures beyond those found in sensitivity analysis like the Sobol indices (Sobol', 1990) and shapley of variance (Owen, 2014).

3.5.2 Relationship with Global Feature Importance

Explainability approaches have also been applied directly to the global level by explaining which features are important to a given model. This is of particular relevance for feature screening and feature selection, especially in the case of high-dimensional data where it is cumbersome to consider all input variables and it is preferable to only consider a few. In the Shapley and ANOVA framework, there are a few key value functions which get used as a global summarizing statistic, the *total variance*, the *total loss*, and the *total score*:

$$v^{\text{var}}(S) := \quad \mathbb{V}\text{ar}_X\left[f_S(X_S)\right] \tag{56}$$

$$v^{\text{loss}}(S) := -\mathbb{E}_{X,Y}\left[\ell(Y, f_S(X_S))\right] \tag{57}$$

$$v^{\text{score}}(S) := \quad \mathbb{E}_{X,Y}\left[s(Y, f_S(X_S))\right] \tag{58}$$

Note that the loss is negated such that more important features which correspond to large reductions in the loss are still assigned large and positive values. Typical choices of loss function are mean squared error and KL divergence, $\ell(y, f) = \|y - f\|^2$ and $\ell(y, f) = -\sum_{c=1}^{C} y_c \cdot \log(y_c/f_c)$. Typical choices of score function are R^2 and classification accuracy, $s(y, f) = 1 - \|y-f\|^2/\mathbb{V}\text{ar}[Y]$ and $s(y, f) = \mathbb{1}(y_c = 1 \text{ for } c = \text{argmax}_{c'} f_{c'})$. Also write $\mathcal{L}(f_S) := \mathbb{E}_{X,Y}[\ell(Y, f_S(X_S))]$ and $\mathcal{S}(f_S) := \mathbb{E}_{X,Y}[s(Y, f_S(X_S))]$ as the expected loss and expected score. The MSE loss function is highly related to the variance explained under simplifying assumptions about the residual error. For instance, assuming $Y = f(X) + \varepsilon$ for independent noise $\varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2)$ and taking f_S as the natural $\mathcal{M}_S^{\text{cond}} \circ f$ gives

$$v^{\text{loss}}(S) = v^{\text{var}}(S) - \mathbb{V}\text{ar}_{X,Y}[Y] \tag{59}$$

meaning that the loss explanation and variance explanation value functions are only a constant shift away from each other, something which almost always never affects the final explanation. This remains true under more general conditions, but not for alternate choices of loss function. Many approaches to global feature importance are surveyed in Covert

et al. (2021), but these approaches were also predated by some more classical methods to measuring variable importance which we mention first.

An early measure of importance during the early days of random forests and boosting was the impurity reduction measure (Breiman et al., 1984; Friedman, 2001) which calculated the reduction in loss after a tree split, assigning the reduction to the feature which was split. This approach is not as relevant in the context of additive explanations (being more related to reasoning-based explanations), but also suffers from many other empirical limitations (Strobl et al., 2006; Sandri and Zuccolotto, 2008). Another early measure was permutation feature importance or marginal feature importance (MFI) (Breiman, 2001a) which measures the importance as the decrease in score (or increase in loss) coming from replacing each feature x_j with a random one coming from the marginal distribution (i.e. one coming from permuting the rows of the data matrix), $\varphi_j^{\text{MFI}} := \mathcal{S}(f) - \mathcal{S}(\mathcal{M}^{\text{marg}}_{[d]-\{j\}} \circ f)$. This of course suffers the previously discussed 'off-the-manifold' problem. This was later corrected by the measure of conditional feature importance (Strobl et al., 2008) defined as $\varphi_j^{\text{CFI}} := \mathcal{S}(f) - \mathcal{S}(\mathcal{M}^{\text{cond}}_{[d]-\{j\}} \circ f)$ and originally approximated with related permutation techniques. The Shapley value was applied early on to linear regression models by taking the Shapley explanation of the R^2 score, called Shapley Value Net Effects (Lipovetsky and Conklin, 2001), $\varphi_j^{\text{SVNE}} = \Phi_j^{\text{Sh}} \circ v^{\text{score}}$. There is also the classical approach of computing univariate predictors and measuring their R^2 score $\varphi_j^{\text{univariate}} := \mathcal{S}(\mathcal{M}^{\text{cond}}_{\{j\}} \circ f)$ (Guyon and Elisseeff, 2003), which has the benefit of easily avoiding off-the-manifold predictions, but at the expense of missing features which interact together. Similar approaches can be used for discrete Y by calculating the univariate mutual information (Guyon and Elisseeff, 2003).

More modern importance methods also generally follow the set-valued interpretations laid out in Equations 56, 57, and 58. Shapley of variance (also, Shapley effects) (Owen, 2014; Owen and Prieur, 2017) apply the Shapley value functional to the variance game as discussed in the previous section on sensitivity analysis, $\varphi_j^{\text{Sh}} = \Phi_j^{\text{Sh}} \circ v^{\text{var}}$. Leave one covariate out (LOCO) (Lei et al., 2018), computes the conditional feature importance score, but does this by explicitly retraining new models on the subset of features, $\varphi_j^{\text{CFI}} := -[\mathcal{L}(f) - \mathcal{L}(\mathcal{M}^{\text{cond}}_{[d]-\{j\}} \circ f)]$. They also provide statistical tests and related measures therein. Shapley Population Variable Importance Measure (SPVIM) (Williamson and Feng, 2020) generalizes previous global Shapley aggregates Lindeman et al. (1980); Lipovetsky and Conklin (2001) beyond linear models and R^2 score metrics, $\varphi_j^{\text{SPVIM}} = \varphi_j^{\text{SVNE}} = \Phi_j^{\text{Sh}} \circ v^{\text{score}}$. Shapley Additive Global Importance (SAGE) (Covert et al., 2020) applies the Shapley value to the loss game, $\varphi_j^{\text{SAGE}} := \Phi_j \circ v^{\text{loss}}$. In addition to these global explanations, there are also several explainers which operate on the pointwise loss instead of the global loss v^{loss} (Chen et al., 2018; Schwab and Karlen, 2019; Lundberg et al., 2020; Jethani et al., 2021), also focusing on explainers beyond the simplest choices of Shapley, inclusion, and removal.

As mentioned previously, much of the work in feature importance is directly relevant for feature selection, which we discuss in Section 4.2 in connection with high-dimensional statistics. There, sparse linear models and sparse additive models can additionally be considered as measures of feature importance in and of themselves. This somewhat dualistic model-fitting perspective is explored further in the next section on additive models where we again begin with a historical overview before detailing modern approaches to the topic.

4. Additive Interpretability (Additive Models)

4.1 A History of Generalized Additive Models

Let us once again turn to the very beginning of statistics with the advent of linear regression. One of the first clear publications on the topic is A.M. Legendre's 1805 work (Legendre, 1805) on the method of least squares for applications in astronomy (claimed also by Gauss (Gauss, 1809) for the same application). This was done in the background of earlier work on dataset averaging by Isaac Newton in 1700 and Tobias Mayer in 1750, and overcame the computational difficulties of least absolute deviation from Roger Joseph Boscovich's 1757 work and P.S. Laplace's 1793 developments. Not so long after Legendre's and Gauss's work, Francis Galton, beginning in 1875, applied the same technique to problems which are more statistical in nature, like predicting the height of a sweet pea plant from the height of its parent (Galton, 1889). Galton continued his studies onto human height and other heredity questions, seeming to incidentally give the name 'regression' around this time (Galton, 1886). After his death, Karl Pearson later picked up his mentor's work on sweet peas and genetics, ultimately synthesizing his works on linear regression and providing much greater mathematical rigor (e.g. Pearson's correlation coefficient, chi-square test, method of moments) (Pearson, 1914). Further developments in the beginning of the twentieth century like those of Ronald Fisher (Fisher, 1935) as well as those of Jerzy Neymann and Egon Pearson (Neyman and Pearson, 1933) finalized statistics as its own independent field of study.

Picking back up with the rapid developments in statistics near the end of the 20th century, the linear regression model had already seen ubiquitous use in statistics for decades at this point. A major development relevant for our discussion on the generalized additive model is the invention of the generalized linear model (Nelder and Wedderburn, 1972; McCullagh and Nelder, 1989).

$$\mathbb{E}[Y|X = x] \approx \hat{f}(x) = g^{-1}(\beta^T x) \tag{60}$$

Via the introduction of a link function, g, this framework unified the learning of a variety of distributions using a simplified linear model. Originally for the important logistic regression as well as Poisson regression and Gamma regression, and later to density estimation and other exponential families, this framework comprehensively unified many linear models.

Other critical precursors to GAMs are the development of splines as a nonparametric approach (Schoenberg, 1964; Casteljau, 1986; Bézier, 1972; Birkhoff and De Boor, 1965; De Boor, 1978) and their subsequent application to scatterplot smoothing (Reinsch, 1967; Kimeldorf and Wahba, 1970, 1971; Wold, 1974; Wahba and Wold, 1975; Craven and Wahba, 1978; Golub et al., 1979; Rice and Rosenblatt, 1983; Silverman, 1984; Eubank, 1985)

Application of these one-dimensional techniques to multivariate data required usage of the more complex surface splines (Duchon, 1977) or the choice of a particular direction to linearly project the multidimensional data (Friedman and Tukey, 1974). Building on the idea of projection, Friedman and Stuetzle (1981) instead suggested the ability to project onto multiple directions and add up the total influences, leading to the additive modeling assumption. Additionally, the potential merits of projecting onto the coordinate directions

were also suggested (but not exclusively focused on):

$$\hat{f}(x) = \sum_{i=1}^{d} f_d(x_d) \tag{61}$$

This work not only introduced the nonparametric additive model to the literature, but also introduced the backfitting algorithm for iteratively fitting the shape functions of the additive model (Friedman and Stuetzle, 1981).

This original idea was taken further by Stone (1985) to give some theoretical developments and Breiman and Friedman (1985) to develop the ACE algorithm. At the same time, other works doing semiparametrics were giving special attention to reducing the nonparametric estimation to as few components as possible (Green et al., 1985; Engle et al., 1986). It was around this time that the Generalized Additive Model (GAM) combining the nonparametric additive structure with the generalized link function allowing for regression, classification, etc. to be incorporated together. First combined as a 1984 technical report (Hastie and Tibshirani, 1984), then into a 1986 paper (Hastie and Tibshirani, 1986), and finally into a full book in 1990 (Hastie and Tibshirani, 1990), the generalized additive model proposed an extremely flexible nonparametric modeling structure which still overcame practical considerations like the curse of dimensionality.

By the time of the final book, the additive model had already been popularized and seen some attention from many other researchers (Stone, 1982; Friedman et al., 1983, 1984; Burman, 1985; Stone, 1986; Buja et al., 1989; Chen et al., 1989; Gu and Wahba, 1991b). Moreover, extensions to interaction models (mostly in the form of interaction splines) had been studied, chiefly by Wahba and her students (Barry, 1986; Wahba, 1986; Gu et al., 1989; Chen, 1987, 1991a). Indeed, just months later, a book focusing entirely on smoothing splines would be published by Wahba (Wahba, 1990).

Continued developments would improve on existing works like interaction models (Stone, 1985) and MARS (Friedman, 1991) to combine tensor product splines and thin plate splines (which were previously viewed as separate approaches) under the same framework called *Smoothing Spline ANOVA* (Gu and Wahba, 1991a, 1993b) as in Equation 62:

$$f(x) = C + \sum_{\alpha=1}^{d} f_\alpha(x_\alpha) + \sum_{\alpha<\beta} f_{\alpha\beta}(x_\alpha, x_\beta) + \sum_{\alpha<\beta<\gamma} f_{\alpha\beta\gamma}(x_\alpha, x_\beta, x_\gamma) + \dots \tag{62}$$

This nonparametric description already provided the precursors for the functional ANOVA perspective which we will see connects with the approaches from sensitivity analysis. Many refinements of this approach continued (Chen, 1991a; Gu and Wahba, 1991b, 1993a,b), ultimately culminating into Wahba's 1995 memorial lecture (Wahba et al., 1995), with later extensions to 'generalized' applications like density estimation and hazard estimation (Gu, 1995, 1996, 1998) ultimately culminating into Gu's 2002 book on SS-ANOVA (Gu, 2002). Although older works like this one make explicitly clear that higher-order interactions are excluded in practice, the ingredients for a functional ANOVA perspective connecting with sensitivity analysis can already be seen.

Another key era of interest in the GAM was its indirect attention due to the success and popularity of boosting. At the time, it was very surprising that a set of boosted tree

stumps could achieve good performance on classification tasks (Freund and Schapire, 1997; Schapire and Singer, 1998). Shortly after, it was realized that the choice of tree stumps as the weak learner automatically led to an additive modeling assumption (due to each stump's dependence on only a single input feature) (Friedman et al., 2000). Thus, a large subset of researchers were training additive models without even realizing that is what they were doing. Further developments on boosting emphasized this functional perspective, re-envisioning a round of boosting a weak learner as a gradient step in a functional optimization problem (Friedman, 2001, 2002; Bühlmann and Yu, 2003).

Other work at the turn of the century focused on increasing the practical usefulness of generalized additive models, with many practitioners remaining wary of the many nuisance parameters which must be fit in a nonparametric method like smoothing spline ANOVA (spline knots and smoothing parameter). Of great significance is the line of work by Wood making developments on the splines including better basis functions and efficient multiple smoothing (Wood, 2003, 2004, 2006b) which culminated into an R package (`mgcv`) and associated book (Wood, 2006a). Theoretical and practical developments on these approaches continue into the modern day (Schmid and Hothorn, 2008; Lee and Durbán, 2011; Marra and Wood, 2011; Lee et al., 2013; McLean et al., 2014; Wood et al., 2015).

Although the history of the additive model does not end here, we take a break to discuss another important and emerging field, high-dimensional statistics, which ends up being of great significance to additive models. We will then come back to discuss recent additive models after their modern revitalization due to their interpretability properties.

4.2 A History of Sparse Additive Models

High-dimensional statistics is an area of statistics focused on describing the statistical behavior when classical asymptotic results break down. Although classical results in statistics, such as those on the central limit theorem and likelihood ratio tests, take the number of feature dimensions d to be fixed and take the number of samples n to infinity, in many empirical situations these asymptotic predictions turn out to be completely inadequate. This is where high-dimensional statistics comes in, ultimately evolving to describe the regime when $n \ll d$ or more broadly when n is somehow comparable to d (Wainwright, 2019).

Early works identified hints of these potential problems while working with large-scale datasets, like Rao (1949) and Deev (1970). Around the same time, works on inverse problems for integral equations also ran into the same issues for similar reasons (and came up with similar solutions (Tikhonov, 1943; Phillips, 1962; Tikhonov, 1963)). Rigorous progress was first made in the field of random matrix theory, which was forced to contend with $n \approx d$ in the calculation of eigenvalues of infinite random matrices (Wigner, 1955, 1958; Marčenko and Pastur, 1967; Pastur, 1972). Soon after, other works brought the same ideas directly into statistical applications like robust regression, with Huber (1973) introducing the 'high-dimensional limit' which takes $c = {}^{d}/_{n}$ fixed as constant before an asymptotic approach is employed. In a bit more technical detail, a sequence like $d_n = \lfloor cn \rfloor$ is taken such that $\lim_{n\to\infty} \frac{d_n}{n} = c$ holds, and then the statistic $\hat{\theta}_{n,d_n}$ is studied as $n \to \infty$.

In later years, the topic only grew in importance in response to factors like the increasing availability of high-dimensional data (Breiman, 1995; Tibshirani, 1996) and the increasing complexity of recovery in signal processing applications (Mallat and Zhang, 1993; Pati et al.,

1993). A quintessential example is the LASSO (Tibshirani, 1996), which uses L1 regularization to shrink the coefficients towards sparse estimates via control of the λ_1 hyperparameter:

$$\hat{\beta}^{\text{LASSO}} := \underset{\beta_\emptyset,\beta}{\text{argmin}} \left\{ \left\| Y - (\beta_\emptyset + X\beta) \right\|_2^2 + \lambda_1 \|\beta\|_1 \right\} \tag{63}$$

$$= \underset{\beta_\emptyset,\beta}{\text{argmin}} \left\{ \sum_{i=1}^{n} \left(y^{(i)} - \beta_\emptyset - \sum_{j=1}^{d} \beta_j x_j^{(i)} \right)^2 + \lambda_1 \cdot \sum_{j=1}^{d} |\beta_j| \right\} \tag{64}$$

Developments of these original approaches like matching pursuit (Mallat and Zhang, 1993) and orthogonal matching pursuit (Pati et al., 1993) would continue to be enhanced with basis pursuit (Chen et al., 2001) and sparse dictionaries (Donoho and Huo, 2001; Elad and Bruckstein, 2002). Further development on the linear problem of the garrote (Breiman, 1995) or lasso (Tibshirani, 1996) would be taken on by LARS (Efron et al., 2004), ElasticNet (Zou and Hastie, 2005), and the Dantzig selector (Candes and Tao, 2007), providing better methods of solving Equation 63 and further improvements to the solution itself. These works would continue to develop the practical usefulness and empirical understanding of shrinkage-based sparsity approaches. Further works would continue to develop a better theoretical understanding of when these approaches succeed in the context of signal recovery (Candes and Tao, 2005; Donoho, 2006; Candes and Tao, 2007; Bickel et al., 2009).

$$\hat{\beta}^{\text{ElasticNet}} := \underset{\beta_\emptyset,\beta}{\text{argmin}} \left\{ \left\| Y - (\beta_\emptyset + X\beta) \right\|_2^2 + \lambda_2 \|\beta\|_2 + \lambda_1 \|\beta\|_1 \right\} \tag{65}$$

$$\hat{\beta}^{\text{Dantzig}} := \underset{\beta_\emptyset,\beta}{\text{argmin}} \left\{ \|\beta\|_1 \qquad \text{s.t.} \qquad \|X^T(y - \beta_\emptyset - X\beta)\|_\infty \leq C\sigma\sqrt{\log d} \right\} \tag{66}$$

Some of the earliest methods transitioning these insights into the more nonparametric approaches of kernel-based learning were SUPANOVA (Gunn and Brown, 1999; Gunn and Kandola, 2002) and likelihood basis pursuit (LBP) (Zhang et al., 2004).

$$\hat{\beta}^{\text{SUPANOVA}} := \underset{\beta_\emptyset,\beta}{\text{argmin}} \left\{ \left\| Y - (\beta_\emptyset + \Phi\beta) \right\|_2^2 + \lambda_1 \|\beta\|_1 \right\} \tag{67}$$

$$\hat{\beta}^{\text{LBP}} := \underset{\beta_\emptyset,\beta}{\text{argmin}} \left\{ \left\| Y - (\beta_\emptyset + \Phi\beta) \right\|_2^2 + \lambda_1 \|\beta\|_1 \right\} \tag{68}$$

Although SUPANOVA and LBP focused on the K-ANOVA and SS-ANOVA respectively, they remained treating basis function coefficients as individual terms to be sparse regularized, requiring multiple-stage procedures for ensuring additional sparsity of the ANOVA components. As the ubiquity of high-dimensional principles became clear throughout the 2000s, it was the COSSO model (Lin and Zhang, 2006) and SpAM model (Ravikumar et al., 2009) which reduced to simpler GAM-1 models via a restriction of the functional hypothesis space, but treated a more general nonparametric function with the use of functional norms. These extensions of sparse selection to the additive model would continue with other 'SPAM-class' models: HDAM (Meier et al., 2009), a version for multiple kernel learning (Koltchinskii

and Yuan, 2010) and a version for minimax optimal rates (Raskutti et al., 2012).

$$\hat{f}^{\text{COSSO}} := \underset{f_\emptyset \in \mathbb{R}, f_i \in \mathcal{H}_i}{\text{argmin}} \left\{ \sum_{i=1}^{n} \left(y^{(i)} - f_\emptyset - \sum_{j=1}^{d} f_j(x_j^{(i)}) \right)^2 + \lambda_{1,2} \cdot \sum_{j=1}^{d} \|f_j\|_{\text{Sobolev}} \right\} \tag{69}$$

$$\text{where} \quad \|f_j\|^2_{\text{Sobolev}} := \sum_{\nu=0}^{1} \left(\mathbb{E}\left[D^\nu f_j(X_j) \right] \right)^2 + \mathbb{E}\left[|D^2 f_j(X_j)|^2 \right]$$

$$\hat{f}^{\text{SPAM}} := \underset{f_\emptyset \in \mathbb{R}, f_i \in \mathcal{H}_i}{\text{argmin}} \left\{ \sum_{i=1}^{n} \left(y^{(i)} - f_\emptyset - \sum_{j=1}^{d} f_j(x_j^{(i)}) \right)^2 + \lambda_{1,2} \cdot \sum_{j=1}^{d} \|f_j\| \right\} \tag{70}$$

$$\text{where} \quad \|f_j\|^2 := \mathbb{E}\left[|f_j(X_j)|^2 \right]$$

Around this time, a major innovation in how to include interaction effects in linear models would occur with the hierarchical lasso (Bien et al., 2013). This reintroduction of heredity would become a key development in the study of feature interactions, which remains a central focus for modern approaches to higher-order additive models as discussed further in Section 4.4 on the topic of feature interaction selection.

4.3 Modern Additive Models

Although additive models had remained a useful statistical model in the decades that followed their 1981 invention, their representative power would slowly fade as their main selling point. Indeed, more powerful models like boosted forests (Schapire, 1990; Freund and Schapire, 1997; Breiman, 1998) and eventually deep neural networks (Mohamed et al., 2011; Krizhevsky et al., 2012; Bahdanau et al., 2015) proved themselves as incredibly useful modeling tools across a wide variety of problems (Breiman, 2001b). Accordingly, modern interest in additive models has been due to reasons contrary to their original motivation: they are now chosen mainly due to their *simplicity* compared with the blackbox machine learning and deep learning approaches which have emerged in the past several decades.

Interest in GAMs was once again revitalized when two of its key properties were emphasized: (i) interpretability of the additive influence coming from each input feature; and (ii) near-competitiveness with modern state-of-the-art methods like random forests and boosting (Lou et al., 2012, 2013). The good performance of additive models across many real-world datasets alongside the importance of interpretability for certain tasks like medical applications led to a rekindled interest in the study of GAM models as a solution to the blackbox problem (Caruana et al., 2015). Table 1 provides a summarization of available GAM approaches with a focus on modern research working on interpretability.

Conversations in statistics about the diverging needs of statistical modeling for explanation or statistical modeling for prediction (Breiman, 2001b; Shmueli, 2010) had already begun by the turn of the century, with methods like Partial Dependence Plots (PDPs) already providing the first 'explanations' of blackbox boosting models (Friedman, 2001). Nevertheless, the field of interpretability, specifically dedicated to fighting the blackbox problem, seems to have only accelerated in the wake of deep learning's widespread success across previously untouched domains. As already discussed in the previous sections, this led

to a flurry of research, beginning in the mid 2010s and continuing to the present day, which is focused on *explaining* the complex blackbox models which were being applied across an increasingly wide set of tasks.

This led to an explosion of approaches used for explaining blackbox behavior. It was only later that Rudin (2019) put their foot down and demanded that researchers return to fully *interpretable* models which faithfully represent their decisions, instead of relying on post-hoc *explanations* which only approximate the behavior of a blackbox model. This work pointed out the fundamental gap existing between approximate explanations and the true blackbox model. For example, a good explanation at that time could still 'fail' around 10% of the time. However, those same failures happening 10% of the time could be exactly the critical points where the model behavior needed to be understood and explained in the first place. In this view, the generalized additive model and other intrinsically interpretable models solve this problem by exactly aligning the explanations and the predictions.

Follow-up works have pushed this duality even further, finding explicit duals between XAI explanations and IML interpretations (Enouen and Liu, 2025; Günther et al., 2025), for example the duality between SHAP and GAM emphasized herein. As a consequence of Rudin (2019), there has only been a greater push to focus on intrinsically interpretable approaches. As it currently stands, additive models remain the most well-studied class of interpretable models and seem to be the furthest along at matching SOTA performance (in tabular data), although other methods are following close behind.

After the revitalization of interest in GAMs due to the EBM line of work (Lou et al., 2012, 2013; Caruana et al., 2015), a next major development occurs with the work of SALSA (Kandasamy and Yu, 2016). This work was able to fit k-th order additive models via the use of a specific kernel which allows a computational trick for calculating the value of the kernel in $\mathcal{O}(k^2 d)$ time instead of the naive $\mathcal{O}(d^k)$ time. Kandasamy and Yu (2016) find that by balancing the bias-variance tradeoff (choosing between the high bias of the 1D additive model or the high variance of the fully nonparametric model), the best-performing choice of k depends on the dataset. Unfortunately, the method cannot scale past several thousand samples by nature of being a kernel machine approach (requiring $\mathcal{O}(n^2 k^2 d)$ time to compute the kernel matrix and $\mathcal{O}(n^3)$ time to compute the matrix inverse). SpAM-2 (Tyagi et al., 2016) extended the sparse gradient approach of SpAM to fit the functional forms, using discretized variable domains instead of kernel machines or kernel smoothing.

Neural Interaction Transparency (NIT) (Tsang et al., 2018b) uses a special neural architecture which uses a first layer for enforcing sparsity and disentangling the interactions. The first layer is restricted to a maximal number of nonzero entries per feature node to be k, limiting the maximal degree of feature interactions which are possible to represent. Another early NAM approach which did not intentionally leverage a GAM structure is BagNet (Brendel and Bethge, 2019). Applied to computer vision classification, this approach took the final logits to be a sum of the local logits computed based on a small patch of the image, showing that large enough patches from 10x10 to 30x30 pixels achieved surprisingly competitive performance. Sparse Shrunk Additive Model (SSAM) (Liu et al., 2020b), amongst peers like COSSO and SALSA, focuses on the case of $k = 2$ and tries to incorporate additional sparse selection into SALSA, on both the samples and the features.

The paper taking the name which also came to describe the general class of models, Neural Additive Models (NAM) (Agarwal et al., 2021), simply replaces the nonparametric method with a neural network, but emphasizes the many interpretability benefits of this approach (despite NAMs technically being a neural network). A major change to the neural network architecture is the introduction of the ExU activation function to allow the network to capture the same sharp edges which are possible using tree ensembles. Unfortunately, this also has the effect of greatly destabilizing the neural network training, meaning that an ensemble of around 100 NAM networks is required to achieve good performance. Around the same time, another approach to neural additive models called GAMI-Net (Generalized Additive Model with Interactions Network) (Yang et al., 2021) included pairwise interactions within the neural network structure. Although this had the additional complexity of a stagewise, heredity-based selection procedure to choose relevant pairs, it maintained interpretability by not pushing beyond into higher-order interactions.

Shortly after, a lot of work picked up in this direction. NODE-GAM and NODE-GA2M (Chang et al., 2022) utilize the differentiable tree called NODE (Popov et al., 2019) as the nonparametric approach. This is combined with a clever 'color gating' mechanism to gradually ensure the feature sparsity of each component (which then ensures the overall GAM structure is obeyed), following a similar intuition to the gating used in NIT (Tsang et al., 2018b). Sparse NAM (SNAM) (Xu et al., 2023) attempts to learn a sparse set of 1D shape functions by enforcing a group parameter penalty on each of the subnetworks of a neural additive model. Higher-Order NAM (HONAM) (Kim et al., 2022) uses a very similar trick to SALSA in order to compute symmetric polynomials of the embeddings, using neural network embeddings instead of kernel embeddings.

The Neural Basis Model (NBM) (Radenovic et al., 2022) is a specific type of NAM which uses a bank of shared basis functions which are learned across all features, allowing for repeated shape functions to be learned more easily, while still respecting the additive GAM structure. This was done in close development with Scalable Polynomial Additive Model (ScalPol-AM) (Dubey et al., 2022) which instead generalizes the opposite direction, using the most simple basis function (polynomials) but adding complex higher-order interactions to the model. Instead of the existing kernel ANOVA trick from SALSA, they instead write the polynomial of degree k with weight tensor $W^{(k)} \in \mathbb{R}^{d^{\otimes k}}$ as a low-rank approximation $W^{(k)} \cdot x^{\otimes k} \approx \sum_{i=1}^{r_k} \lambda_i^{(k)} \langle u_i^{(k)}, x \rangle^k$. This polynomial also has the advantage of being easily computable and they further combine this idea with using neural basis functions to compute the input features to the polynomial approach, similar to HONAM. Sparse Interaction Additive Networks (SIAN) (Enouen and Liu, 2022) also consider higher-order neural additive models, but instead focus on the problem of sparse selection of these interactions. This requires a two-stage procedure where interactions are first chosen based on important interactions according to an MLP and then a NAM is fit according to the chosen interactions.

Regionally Additive Models (RAMs) (Gkolemis et al., 2023) combine the GAM structure with the nearest-neighbor simplicity bias, subdividing into patches on which the function structure obeys the simple GAM structure. Generalized Sparse Learning of Additive Models with Interactions (G-SLAMIN) G-SLAMIN (Ibrahim et al., 2023) returns to two-dimensional, tree-based ensembles while incorporating explicit masking variables obeying weak or strong heredity alongside a hard cutoff threshold as chosen by hyperparameters.

AHOFM (Ruegamer, 2024) uses the factorization machine approach discussed further in the subsection below as applied to tensor product splines to limit the consequences of higher-order effects in large dimensions.

Optimized Regularized Stump Forests (ORSF) (Gabidolla and Carreira-Perpiñán, 2025) reverts even further to one-dimensional, tree-based stump ensembles. They show that directly optimizing each stump alongside careful balancing of regularization hyperparameters can outperform existing GAM-1 approaches. PatternGAM (Clark et al., 2025) corrects for the redundancy of correlated input features by adjusting via the Pattern method (Haufe et al., 2014) originally designed for collinearity in linear regression. InstaSHAP (Enouen and Liu, 2025) instead uses a masking-based framework to automatically correct for this redundancy in the additive model shape functions. Tensor-Product Neural Network (TPNN) (Park et al., 2025) combines the tensor-product spline approach with the neural basis approach as in HONAM and ScalPol-AM, while additionally requiring the Hooker purification condition ((Hooker, 2007) to be discussed in Section 4.5.3).

In addition to these works on the 'main' line of research into additive models, there are other key directions of research which are closely related to additive models. We focus here on two. First is the research into uncertainty using GAMs. Although GAMs are typically shown alongside their bagged intervals which already give some notion of a confidence interval, more serious notions of uncertainty exist using Gaussian processes or Bayesian approaches. Second, there is the large amount of research into Factorization Machines (FMs) which are very closely related to additive model structural assumptions. The biggest difference can be seen in the implicit assumption in the FM literature that input features are themselves large and high-dimensional (rather than the number of input features being large as in high-dimensional GAMs).

4.3.1 GAM Uncertainty

Many different approaches have incorporated GAM structure into uncertainty estimation or added uncertainty to GAM predictions. The Generalized Additive Models for Location, Scale, and Shape (GAM-LSS) (Rigby and Stasinopoulos, 2005) is an approach for distribution modeling which makes great use of the 'generalized' aspected of generalized additive models, modeling a wide variety of parametrized distributions from normal and logistic to Box-Cox and Poisson. This approach allows for conditional uncertainty to be directly modeled via the modeling of the target distribution. Follow-up work called gamboostLSS also extended the fitting method to incorporate boosting, enabling high-dimensional fitting through the implicit regularization of boosting (Mayr et al., 2012).

Additive Gaussian Processes (Duvenaud et al., 2011), or the nearly equivalent Additive Kriging (Durrande et al., 2011), followed up on previous works in hierarchical kernel learning (Bach, 2009) and Gaussian process Sobol indices (Marrel et al., 2009), respectively, to deliver the Gaussian process obeying the additive assumption of the GAM. Further works looking at using kernel-based functional ANOVA extensions to additive Gaussian processes and general Gaussian processes (Ginsbourger, 2013; Duvenaud, 2014) as well as specially designed Kernel ANOVA (Ginsbourger et al., 2016) which can further decompose into 4^d terms by nature of each $2^d \cdot 2^d$ cross-terms contributing to the kernel. Although no general selection algorithms are given, small examples are used to illustrate the flexibility of the modeling approach.

Table 1: Tabulation of many GAM methods over the years.

Method	Degree			Generalized			Sparsity Type	Nonparametric Model	Year
	1D	2D	3D+	reg	cls	other			
GAM	✓			✓	✓	✓	✗	kernel smoothing	1990
SS-ANOVA	✓	✓		✓			✗	spline smoothing	1993
Adaboost	✓				✓		✗	stump ensembles	1997
SS-ANOVA	✓	✓		✓	✓		✗	spline smoothing	2002
SUPANOVA	✓	✓		✓			coefficient-wise	SVM	2002
LBP	✓	✓		✓	✓		coefficient-wise	RKHS	2004
COSSO	✓			✓	✓		1D (Sobolev)	RKHS	2006
SpAM	✓			✓	✓		1D (functional)	kernel smoothing	2008
HDAM	✓			✓	✓		1D (sparse-smooth)	RKHS	2009
GAM	✓			✓	✓		✗	tree ensembles	2012
GA^{2}M	✓	✓		✓	✓		2D, stagewise	tree ensembles	2013
EBM	✓	✓		✓	✓		2D, stagewise	tree ensembles	2015
SALSA	✓	✓	✓	✓			order selection	kernel machines	2016
SpAM2	✓	✓		✓			2D, interaction selection	discretized	2016
NIT	✓	✓	✓	✓	✓		HO, online (neural-based)	neural	2018
BagNet	*✓				✓		✗	neural	2019
SSAM	✓	✓		✓			coefficient-wise	kernel machines	2020
GAMI-Net	✓	✓		✓	✓		2D, stagewise	neural	2021
NAM	✓			✓	✓		✗	neural	2021
NODE-GAM	✓	✓		✓	✓		2D, online (tree-based)	differentiable trees	2022
SNAM	✓			✓	✓		1D, online (group norm)	neural	2022
HONAM	✓	✓	✓	✓	✓		FM-style	neural bases	2022
ScalPol-AM	✓	✓	✓	✓	✓		FM-style	polynomials	2022
NBM	✓			✓	✓		✗	neural bases	2022
SIAN	✓	✓	✓	✓	✓		HO, interaction selection	neural	2022
G-SLAMMIN	✓	✓		✓	✓		2D, online (indicators)	differentiable trees	2023
AHOFM	✓	✓	✓	✓			FM-style	spline bases	2024
ORSF	✓			✓	✓		✗	stump ensembles	2025
TPNN	✓	✓	✓	✓	✓		FM-style	neural bases	2025
FM	✓	✓		✓	✓		FM-style	factorization machine	2010
HIFM	✓	✓		✓	✓		FM-style	linear factorization	2014
HOFM	✓	✓	✓	✓	✓		FM-style	factorization machine	2016
OptFeature	✓	✓	✓	✓	✓		GAM- and FM-style	factorization machine	2023
GAM-LSS	✓					✓	✗	parametrized distribution	2005
gamboostLSS	✓					✓	✗	parametrized distribution	2012
GAM-GP	✓					✓	✗	gaussian process	2013
KANOVA GP	✓	✓	✓			✓	kernel cross terms	gaussian process	2016
OAK	✓	✓				✓	✗	gaussian process	2022
NAM-LSS	✓					✓	✗	parametrized distribution	2024

This work would pick up later with a modernization in OAK (Lu et al., 2022) which combined modern sparse GP approaches with the additive GP assumption; Luo et al. (2022) would develop a similar extension around the same time. Max-Mod (López-Lopera et al., 2022) would also revisit the additive GP assumption, also providing support for monotonicity constraints.

Other approaches to GAM uncertainty would lean more heavily on Bayesian ideology, with SKIM-FA (Agrawal and Broderick, 2023) extending their linear kernel interaction trick (Agrawal et al., 2019) which applies an additive assumption directly on the kernel alongside hierarchical Bayesian modeling. NAM-LSS (Frederik Thielmann et al., 2024) would extend NAM approaches to the location, scale, and shape modeling of GAM-LSS. LA-NAM (Bouchiat et al., 2024) learned an independent Bayesian NN for each of the additive components of the NAM.

4.3.2 Factorization Machines

Another important model class which is closely related to the additive model (as well as being another type of commonly studied interaction selection mechanism) is the Factorization Machine (FM) (Rendle, 2010). This approach extends existing Matrix Factorization (MF) (Bell et al., 2008) approaches which are used under cases of extreme sparsity like in the Netflix problem of matching users to movies (Bennett and Lanning, 2007; Bell et al., 2010). In the original FM, first a multilinear assumption and a GAM-2 assumption are made resulting in the Equation 71. The parameters are the $w_\emptyset \in \mathbb{R}$ scalar, the $\vec{w} \in \mathbb{R}^d$ vector, and the $W \in \mathbb{R}^{d \times d}$ matrix. For large d, there may be insufficient data to adequately fit the quadratic $\mathcal{O}(d^2)$ number of coefficients in W. Accordingly, it is fit using a low-rank approximation $W \approx VV^T$ for some $V \in \mathbb{R}^{d \times r}$. This results in the FM equation in Equation 72 after the appropriate adjustments for symmetrizing W and removing the quadratic terms x_i^2.

$$f^{\text{bilinear}}(x) = w_\emptyset + \sum_{i=1}^{d} w_i x_i + \sum_{i=1}^{d} \sum_{j=1}^{d} W_{i,j} x_i x_j \tag{71}$$

$$f^{\text{FM}}(x) = w_\emptyset + \sum_{i=1}^{d} w_i x_i + \sum_{i=1}^{d-1} \sum_{j=i+1}^{d} \langle \vec{v}_i, \vec{v}_j \rangle x_i x_j \tag{72}$$

where $\vec{v_i} \in \mathbb{R}^r$ for each $i \in [d]$ represent the rows of V.

Later work like FHIM (Purushotham et al., 2014) add additional sparsity on the vectors $\vec{w}$ and $\vec{v}_i$ to compensate for high-dimensional data. They additional suggest the possibility of generalizing to higher-order feature interactions. In 2016, HOFM (Blondel et al., 2016) actually explores the higher-order factorization machine, decomposing the higher-degree tensors like $W^{(3)} \in \mathbb{R}^{d \times d \times d}$ using the CP decomposition (Chang, 1970; Harshman, 1970) of these tensors $W^{(3)}_{i,j,k} \approx \sum_{r=1}^{r_3} \vec{v}^{(3)}_{i,r} \cdot \vec{v}^{(3)}_{j,r} \cdot \vec{v}^{(3)}_{k,r}$ as seen in Equation 74.

$$f^{\text{multilinear}}(x) = w_\emptyset + W^{(1)} \odot \vec{x} + W^{(2)} \odot (\vec{x} \otimes \vec{x}) + \cdots + W^{(k)} \odot \vec{x}^{\otimes k} \tag{73}$$

$$f^{\text{HOFM}}(x) = w_\emptyset + \sum_{i=1}^{d} w_i x_i + \sum_{i=1}^{d-1} \sum_{j=i+1}^{d} \langle \vec{v}_i^{(2)}, \vec{v}_j^{(2)} \rangle \cdot x_i x_j + \\ \cdots + \sum_{i_1 < \cdots < i_k} \langle \vec{v}_{i_1}^{(k)}, \ldots, \vec{v}_{i_k}^{(k)} \rangle \cdot x_{i_1} \ldots x_{i_k} \tag{74}$$

where we abuse the Hadamard product notation ($\odot$) to also mean collapsing to a scalar and the notation $\langle \vec{v}_1, \ldots, \vec{v}_k \rangle$ is the extended dot product agreeing with the above low-rank CP formula. Note again that the multilinear assumption is notationally tedious to write, either requiring that we write the explicit sum over strictly increasing indices or requiring the awkward condition that each $W^{(k)}$ tensor only has nonzero entries for completely asymmetric entries. Accordingly, we write Equation 73 as the easier to write polynomial in tensor products with the understanding that these weight tensors may need to be further restricted as appropriate.

Around this time, two works claiming to be Sparse Factorization Machines (SFMs), Xu et al. (2016) and Pan et al. (2016), add additional sparsity to the bilinear factorization machine to better deal with the high-dimensional setting. Pan et al. (2016) follows a similar approach to Purushotham et al. (2014), focusing on entry-wise sparsity of the parameters. They replace the sparse Gaussian approach from Purushotham et al. (2014) with a Laplacian distribution and make the many necessary adjustments in methodology. Xu et al. (2016) instead aims for sparsity on the individual feature pairs, regularizing the rows of the V_1 and V_2 matrices of $f^{\text{SFM}}(x) = x^T V_1 V_2^T x$ with the $\| \cdot \|_{2,1}$ norm on V_1 and V_2. This norm encourages groupwise sparsity on each row of the decomposition matrix, allowing unnecessary features to be easily dropped out of the FM interaction representation.

It is additionally worth noting how closely related the factorization machine approach is to several higher-order extensions of GAMs. HONAM (Kim et al., 2022), ScalPol-AM (Dubey et al., 2022), and AHOFM (Ruegamer, 2024) all rediscover the same mechanism of using a nonlinear basis functions combined with the FM approach to multilinear basis coefficients for extending GAMs to higher-order interactions. It is interesting how this bridges one of the key distinguishing factors between the two research directions, sparse and high-dimensional discrete features vs. low-dimensional continuous features. Given this context, the assumptions of bilinearity and multilinearity are not actually a restriction for high-dimensional one-hot categorical features, unlike the GAM case. Beyond this, there is also a key difference in mindset: factorization machines are making the simplifying assumption of low-dimensional structure because it achieves the best performance on the challenging high-dimensional task; whereas, modern additive models are making this simplifying assumption because it provides clearer insight into the data.

Accordingly, many follow-up works to FM and HOFM are only focused on achieving the best performance through interactions, no matter the benefits or detriments to interpretability. We include a few of these works regardless for completeness. Meta-graph FMG (Zhao et al., 2017) appends additional knowledge graph features before applying a regularized FM structure. IAFM (Hong et al., 2019) modifies the FM with a courser field-level field aspect as well as an attention mechanism, and this work also consider neural network extensions for learning higher-order interactions. AutoInt (Song et al., 2019) focuses specifically on an interacting attention structure to implicitly learn higher-order factorization machine structure.

AutoFIS (Liu et al., 2020a) uses a higher-order interaction structure of HOFM alongside the neural network tricks of batch normalization and gating. GILDER 2020 (Tsang et al., 2020a) first runs a neural interaction detection procedure before retraining on an expanded set of cross features. TI and CS regularized FMs (Atarashi et al., 2021) introduce alternate sparse regularization approaches to better enable groupwise sparsity and interaction selection. AutoAIS (Wei et al., 2021) uses a meta architecture search across deep architectures for the embedding and interaction structure. AdaFS (Lin et al., 2022) uses a small MLP alongside mixed soft and hard selection to implicitly discover all higher-order interactions.

A major departure from this push towards neural factorization machines is the work on hybrid-grained interaction selection (Lyu et al., 2023). In this work, they make a clear distinction between the coarse-grained, field-level interactions (being modeled by an additive model) and the fine-grained, value-level interactions (being modeled by a factorization machine), providing a much clearer unification of how GAMs and FMs are part of the same hierarchical picture. In this language, the interaction selection of additive models discussed throughout the survey corresponds to selection at the coarse-grained level, whereas interaction selection in the sense of factorization machines occurs at the fine-grained level. In their work, they combine both levels of interaction selection into a model they call OptFeature. Overall, this coarse-grained/ fine-grained perspective allows for a better understanding of the key difference between GAM and FM interactions.

4.4 Feature Interaction Selection

Now that we have gone over the many types of feature interaction detection in Section 3.1 as well as modern higher-order additive models in Section 4.3, we pick back up the story of Section 4.2 on sparse feature selection and sparse interaction selection. In particular, we dedicate this section to clarifying the many different types of *feature interaction selection*, that is, the problem of choosing a sparse subset of the candidate interactions.

The first extensions from feature selection to interaction selection from Section 4.2 were only referring to interactions in the sense of the pairwise interactions between features. Another problem existing early on was the problem of degree selection, although as discussed in the historical details on additive modeling, this was in practice a choice between a degree one or a degree two model. Another popular version of interaction selection is in the sense of factorization machines which use matrix factorizations to represent interaction terms. The more general higher-order interaction selection is what we will tend to refer to as feature interaction selection, operating at the coarse-grained level of the additive model.

4.4.1 Pairwise Interaction Selection

First attempts at interaction selection were selection amongst singles and pairs of features $\mathcal{I} \subseteq \mathcal{I}^{\leq 2} := \{S : S \subseteq [d], |S| \leq 2\}$. This was originally done for the selection of linear and bilinear coefficients in a simple bilinear model as in Equation 75. This was done by early works like efficient heredity (Yuan et al., 2007, 2009), CAP (Zhao et al., 2009), SHIM (Choi et al., 2010), and hierarchical lasso (Bien et al., 2013).

$$f(x) = \beta_\emptyset + \sum_{i \in \mathcal{I}_1} \beta_i x_i + \sum_{(i,j) \in \mathcal{I}_2} \beta_{ij} x_i x_j \tag{75}$$

This setting later continued to be expanded on with even further guarantees in ultra-high-dimensional settings using the iFOR algorithm (Hao and Zhang, 2014) and the SIRI algorithm (Kong et al., 2017).

4.4.2 Interaction Order Selection

Another important special case is degree selection or order selection. This selects the highest order or the highest degree of the GAM model. That is, choosing the optimal k amongst $k = 1, 2, \ldots, d$ so that the GAM-k model will be the best performing.

$$f_{\leq k}(x) = \sum_{|S| \leq k} f_S(x_S) \tag{76}$$

Historically speaking, it was quite popular for people to automatically do this by selecting between a model of degree 1 or 2 (which were best performing choices in those times). Works would later codify the statistical intuition that additive models break the curse of dimensionality by providing the nonparametric convergence rates for these models (Stone, 1985; Andrews and Whang, 1990; Chen, 1991b). Later theory of this type came from work in the areas of series estimators and sieve methods (Newey, 1997; Chen, 2007) which focus on giving statistically valid but sufficiently flexible nonparametric estimators.

4.4.3 Fine-Grained Interaction Selection

Another important type of interaction selection is the selection of 'fine-grained' interactions either through the use of a factorization machine (Rendle, 2010; Blondel et al., 2016) or matrix factorization (Bell et al., 2008). This applies to problems where the individual variables dimensions x_i may themselves be high-dimensional (usually discrete variables with many possibilities like user ID). Recall that an FM will model an interaction between i and j on onehot features $x_i \in \mathbb{R}^{d_i}$ and $x_j \in \mathbb{R}^{d_j}$ via $V_i \in \mathbb{R}^{r \times d_i}$ and $V_j \in \mathbb{R}^{r \times d_j}$:

$$f^{\text{FM}}(x_i, x_j) = (V_i^T V_j) \cdot (x_i \otimes x_j) \tag{77}$$

which is different from fitting an arbitrary nonparametric function on the onehot features:

$$f(x_i, x_j) = W \cdot (x_i \otimes x_j) \tag{78}$$

Although linearized matrix factorizations are the only method which is widely used for fine-grained feature interaction selection, it can be imagined that other nonlinear techniques for this problem could also be developed. The importance of handling both the fine-grained interaction selection as described in this section and the coarse-grained interaction selection as described in the next section has also been explored before in a hybrid approach called OptFeature (Lyu et al., 2023). Generally speaking, there is no interpretability in this type of interaction selection because there is no goal to understand the learned low-rank structure.

4.4.4 Feature Interaction Selection (Higher-Order)

Finally, we discuss feature interaction selection in its full generality as a problem of selecting from all possible higher-order interactions, choosing an entire collection $\mathcal{I} \subseteq \mathcal{P}([d])$ from all

2^d possible feature subsets (Sugiyama and Borgwardt, 2019; Enouen and Liu, 2022).

$$f_{\mathcal{I}}(x) = \sum_{S \in \mathcal{I}} f_S(x_S) \tag{79}$$

Compared with the other versions of interaction selection, this higher-order feature interaction selection results in a doubly-exponential combinatorial problem, choosing from an extremely rich but numerous set of candidate $\mathcal{I}$ collections. This has forced practical implementations to lean heavily on the assumption of interaction heredity to be able to efficiently search the vast combinatorial space.

Unlike high-dimensional statistics, which is mainly applied to specific domains like biostatistics (where $d \gg n$ often holds), feature interaction selection is more widely applicable across machine learning tasks (since $2^d \gg n$ more commonly holds), especially in the ever-increasing presence of high-dimensional data. It is this property which we will refer to as medium-dimensional statistics or *medium dimensionality*. Even for relatively small dimensions such as $d = 20$ or $d = 30$, one will quickly face statistical limitations due to the sample size, n, being much smaller than $2^d = 1.0\text{e}6$ or $2^d = 1.1\text{e}9$.

4.5 Modern Topics

Given the long history and many varieties of additive models we discussed throughout this section, we now close with a focus on some of the topics which have attracted attention in modern GAM research. Of course additive models are first and foremost a predictive tool and thus any improvement on the set of methods available for quickly training accurate GAM models is always of continued interest. In this subsection we instead go into greater detail on the more nuanced research questions about generalized additive models, especially with respect to their position as an interpretable machine learning model.

Of great importance are questions relating to how interpretable and how robust the insights learned by additive models are. Furthermore, questions about how to incorporate domain knowledge, fine-grained structure, geometric symmetries, and other problem-specific structure into the assumptions of the GAM model remain important in domains of application. Questions about the underlying correlation structure of the input variables drive many of these other questions. Finally, extensions which combine additive principles with other principles like the logical pillar and the concept pillar look like promising directions for maintaining interpretability while achieving good performance.

4.5.1 Interpretability of GAMs

A major question in the usage of GAMs is 'How interpretable are GAMs, really?' Although an individual GAM is fundamentally interpretable because we can inspect its shape function, this ignores extraneous considerations to how we interpret those shape functions. Questions like **robustness** (would we get the same shape functions with slightly different data or models?), **sparsity** (are there few enough shape functions to reasonably look at all of them?), **correlations** (are certain variables and shape functions carrying redundant information about the target?), and **causality** (when can we interpret the shape functions as saying something causal about the relationship?) are critical for contextualizing the interpretability of GAM models.

Robustness The robustness of the GAM-provided explanation of the data is directly dependent on the robustness of the GAM model itself. Chang et al. (2021) explores in detail how even using different nonparametric methods to fit the shape functions can lead to significantly different results. This is further shown to have direct implications for algorithm fairness through varying importance and polarity of sensitive attributes. Enouen and Liu (2025) has shown how even a fixed model class can have very wide variance under mildly different fitting procedures. Schulte and Rügamer (2025) shows that boosted additive models follow an implicitly regularized gradient descent path, mainly leading to a shrinkage of the estimated effect compared to traditional spline-based approaches.

Sparse Explanations Another key point in interpreting shape functions is the requirement of actually looking at all shape function plots. Although manageable but tedious for 10-100 shape functions, this problem can become out of hand for too many shape functions (especially when utilizing interactions). COGAM (Abdul et al., 2020) proposes to repurposes sparse additive models specifically for this purpose of easier interpretation, further simplifying to linear coefficients in the cases where shape functions are close to linear. Of course, requiring increasingly sparse GAM models to allow for interpretability is in conflict with the goal of predictive accuracy, and thus must be balanced for the targeted application. Zhong et al. (2023) takes the alternate approach of finding the 'Rashomon set' of sparse additive models, meaning the collection of nearly-optimal-performing sparse models. Although this catches many alternate feature subsets which are deemed important by sparse additive models, this can accordingly raise the cognitive load significantly. Moreover, these sparse effects may only represent conflations between equally predictive features.

Correlated Effects There is a major weakness in GAM interpretations when applied to distributions with heavily correlated features. When considering a dataset which has two copies of the same feature, the GAM model can divide the shape function between the two copies in completely arbitrary ways. The robust solution would give half of the weight to each feature whereas a sparse solution would give all of the weight to only one. This issue is generally referred to as concurvity in GAMs (Ramsay et al., 2003; Siems et al., 2023; Zhang et al., 2025b). This fundamental conflict between robustness and sparsity in the correlated setting poses many practical challenges for using GAM models. This is only further complicated by the common misinterpretation that GAM shape functions are indicative of causal relationships.

Causal Interpretations There is a well-known bias to interpret shape function plots as describing the causal influence which a feature has on the target, rather than the predictive influence which the feature has on the target (Caruana, 2017). This is often natural in many tasks where the outcome does causally depend on the input features; however, it can easily lead to misinterpretations of the GAM model. For instance, it could be the case that most of the shape function is truly causal; however, a portion of the shape function actually is because of a second feature which is correlated with the first. This has led to no shortage of misinterpretations and there are no obvious solutions in sight, leaving this as another open topic of modern GAM research.

4.5.2 Correlations and Dependencies

The correlations amongst the input variables pose a *fundamental challenge* to the study of additive models.

> I went into researching additive models thinking that interactions would be the hard part, but I came out knowing that correlations... they are from the devil.
>
> Rich Caruana

Applying linear regression to linearly related features has long been known to lead to unstable results with uninterpretable coefficients, a problem called colinearity. As already mentioned, in the extreme case of duplicated features, coefficients are no longer well-defined and require implicit or explicit regularization from the learning algorithm to even be unique. Although common practice when constructing features may be to drop the redundant copy or when fitting models to use ridge regression (Hoerl and Kennard, 1970b,a), entire books are dedicated to identifying and resolving the problems induced in linear regression for predefined features (Belsley et al., 2005). Further approaches trying to improve the stability or interpretability of linear regression in these settings continue to the current day (Wold et al., 1984; Kejian, 1993; Haufe et al., 2014; Pazzani and Bay, 2020).

Given that there has yet to be a completely satisfactory resolution in the simple case of linear regression, it is no surprise that this remains an active topic in the research of additive models. In the space of GAMs, the issue of colinearity is replaced by the issue of *concurvity*, due to the fact that each of the shape function curves may be nonlinearly influenced by not only the linear correlations between two underlying features, but the higher-order dependencies between the two features. Although the term concurvity usually refers to the case of 1D GAMs, the issue is widespread for both higher-order dependencies and for higher-order interactions.

Moreover, the issue of concurvity is directly problematic for the goals of robust, sparse, and causal explanations. The robustness of the fitted shape functions can be ruined by redundant information in the features but the sparsity of the fitted shape functions contradicts a robust fit that aggregates multiple noisy sources of the same information. The ability to causally interpret shape function plots is further befuddled by the dependencies which interlock several different shape functions as illustrating a single joint phenomenon. Although the lack of universal solution in the simple linear regression case should pose as a warning of its difficulty, the importance of this issue for interpreting GAMs is hard to overstate and only made more important by the modern success of deep learning on high-dimensional and correlated raw features.

Correlation-Adapted GAMs Many works have made progress on improving the robustness of GAMs under these more realistic settings. Lengerich et al. (2020) provides an algorithm for purifying higher-order shape functions, allowing for a unique interpretation of equivalent GAM models. Sun et al. (2022) directly solve for purified GAMs on discrete features by the usage of a 'pure coding' function. Zhong et al. (2023) looks at taking the entire family of well-performing sparse additive models, called the Rashomon set (Xin et al., 2022). This allows for considering an explanation as a set of sparse explanations, where the large set of models allows for robustness, the sparsity of the individual models prevents the

overall Rashomon set from becoming too uninterpretable. McTavish et al. (2024) asks the question of whether or not the missingness indicator should be grouped with its respective feature or be treated as its own feature, noting how missingness may itself be correlated with other features.

Siems et al. (2023) suggests minimizing the concurvity of GAMs by directly optimizing it in terms of minimizing the correlation coefficients.

$$\mathcal{L}^{\text{concurvity}}(f_1, \ldots, f_d) := \sum_{i<j} \Big|\mathbb{C}\text{orr}(f_i, f_j)\Big| = \sum_{i<j} \Big|\frac{\mathbb{C}\text{ov}(f_i, f_j)}{\sqrt{\mathbb{V}\text{ar}(f_i)}\sqrt{\mathbb{V}\text{ar}(f_j)}}\Big| \tag{80}$$

Enouen and Liu (2025) suggests directly regularizing according to masking the shape functions under the Shapley kernel distribution, $m(S)$ from Equation 11.

$$\underset{f_\emptyset, f_1, \ldots, f_d}{\text{argmin}} \left\{ \sum_{S \subseteq [d]} m(|S|) \cdot \mathbb{E}_X \left[\left(f(X) - f_\emptyset - \sum_{i \in S} f_i(X_i) \right)^2 \right] \right\} \tag{81}$$

Clark et al. (2025) suggests that in scenarios where the target Y generates the features X, it is preferable to only have shape functions which are directly correlated with Y. They follow the intuition of the PatternQLR method (Haufe et al., 2014) to linearly adjust shape functions to be maximally predictive of Y.

$$\begin{aligned} f_i^{\text{Pattern}} &= b_i f_i + d_i \qquad\qquad f_{i,j}^{\text{Pattern}} = b_{i,j} f_{i,j} + d_{i,j} \\ \text{where} \quad b_S, d_S &= \underset{b,d \in \mathbb{R}}{\text{argmin}} \Big\{ \mathcal{L}\text{oss}(Y; b \cdot f(X) + d) \Big\} \end{aligned} \tag{82}$$

Ironically enough, the additive model has also surprisingly proved to be a great tool for better understanding the correlation structures of the data. It does this by distinguishing specifically what is *not* a feature interaction. By considering the spectrum across all additive models, we can begin to identify which features are redundantly predictive and which features are synergistically predictive of the target. For more information, see the Amari decomposition described in the next section or see the works of König et al. (2025) and Enouen and Liu (2025) on purifying interactions with additive models.

4.5.3 Generalized Functional ANOVA

The beauty with which functional ANOVA uses the decomposition of variance formula in Equation 49 to break apart the function locally and globally at the same time has inspired multiple attempts to save the functional ANOVA approach in the case of dependent variables. Although there is no possibility of saving the variance decomposition formula, there are still many generalized functional ANOVA approaches which still maintain several other of the nice properties held by functional ANOVA in the dependence case.

Sobol'-Hoeffding ANOVA The original functional ANOVA, now called the Sobol-Hoeffding ANOVA (Hoeffding, 1948; Sobol', 1990), was designed for usage in sensitivity analysis, where researchers were free to make the assumption of independent input variables. It is worth mentioning that it is not always clear whether to say Sobol-Hoeffding refers to the marginal ANOVA decomposition or the conditional ANOVA decomposition because of this assumption; however, we will equate it with the conditional ANOVA as we feel is fairly common

throughout the literature. This then means that we have the baseline ANOVA, the marginal ANOVA, and the conditional ANOVA equaling the Sobol-Hoeffding ANOVA. We will then discuss two more functional ANOVAs: the Stone-Hooker ANOVA and what we will call herein the Amari ANOVA.

$$f(x) = \sum_{S \subseteq [d]} f_S^{\text{Sobol}}(x_S) \quad \text{where} \quad f_S^{\text{Sobol}}(x_S) := \sum_{T \subseteq S} (-1)^{|S|-|T|} [\mathcal{M}_T \circ f](x_S) \tag{83}$$

Stone-Hooker ANOVA Hooker (Hooker, 2004), in his study on additive structure in blackbox functions, had already discovered Sobol's functional ANOVA decomposition. He was also aware of the key limitations in using this decomposition in the case of dependent variables, so later based on the work of Stone (Stone, 1994) for orthogonalizing tensor product bases, he would develop a functional ANOVA decomposition for arbitrary functions and provide novel estimation approaches (Hooker, 2007).

$$f(x) = \sum_{S \subseteq [d]} f_S^{\text{Hooker}}(x_S) \quad \text{s.t.} \quad [\mathcal{M}_{S-s} \circ f_S^{\text{Hooker}}](x_{S-s}) = 0 \quad \forall x_{S-s} \ \forall s \in S \ \forall S \tag{84}$$

The Stone-Hooker decomposition was a large step towards understanding functional ANOVA decompositions in the case of dependent input variables, by satisfying the maximally achievable amount of hierarchical orthogonalities.

Mara and Tarantola (2012) had also identified issues with applying the typical Sobol indices in the case of dependent input variables. Recall that the Sobol variances (the typical indices) and the Sobol covariances are defined as:

$$V_S^{\text{Sobol}} := \mathbb{V}\text{ar}\left[f_S^{\text{Sobol}}\right] = \mathbb{E}_{X_S}\left[f_S^{\text{Sobol}}(X_S)^2\right] \tag{85}$$

$$C_S^{\text{Sobol}} := \mathbb{C}\text{ov}\left[f_S^{\text{Sobol}}, f\right] = \mathbb{E}_X\left[f_S^{\text{Sobol}}(X_S) \cdot f(X)\right] \tag{86}$$

Chastaing et al. (2012) revisits the Stone-Hooker decomposition and suggests to consider the Hooker covariances as a new Sobol index, where the Hooker variances and Hooker covariances are defined in the obvious way. They would reintroduce the matrix form of the projection equations for the small two-dimensional case and later follow ups would continue exploring this direction (Chastaing and Gratiet, 2015; Chastaing et al., 2015).

$$V_S^{\text{Hooker}} := \mathbb{V}\text{ar}\left[f_S^{\text{Hooker}}\right] = \mathbb{E}_{X_S}\left[f_S^{\text{Hooker}}(X_S)^2\right] \tag{87}$$

$$C_S^{\text{Hooker}} := \mathbb{C}\text{ov}\left[f_S^{\text{Hooker}}, f\right] = \mathbb{E}_X\left[f_S^{\text{Hooker}}(X_S) \cdot f(X)\right] \tag{88}$$

Amari ANOVA Most recently, some approaches have completely embraced the connection with additive models and alternatively considered the optimized additive model of a certain degree as defining the functional ANOVA decomposition, rather than the historical use of the functional ANOVA as a proxy for selecting additive terms (König et al., 2025; Enouen and Liu, 2025). We will herein call this ANOVA approach the Amari decomposition in reference to his similar decomposition of a probability distribution using the Riemannian geometry of statistical manifolds (Amari, 2001).

$$\{f_S^{\text{Amari}}\}_{|S|=k} = \underset{\{g_S\}}{\text{argmin}} \left\{ \mathbb{E}_X \left[\left(f(X) - \sum_{|S|<k} f_S^{\text{Amari}}(X_S) - \sum_{|S|=k} g_S(X_S) \right)^2 \right] \right\} \quad \forall k \in \{0, 1, \ldots, d\} \tag{89}$$

König et al. (2025) uses this approach to be able to better decompose the full variance of a blackbox model, aiming to disentangle the variance which is coming from the synergies between two features and which is coming from the dependencies between two features. In order to do this, they directly fit a GAM model $f_j(x_j) + f_{-j}(x_{-j})$ to the data, bypassing non-uniqueness considerations with the variational formulation. Enouen and Liu (2025) additionally consider generalizing this variational approach to any possible higher-order additive model, providing the matrix-projection equations which characterize the solution to the variational problem (their Theorem 6).

4.5.4 Extensions Beyond Additive Models

Regional GAMs and Instance-wise Sparsity A large and important direction of extending additive models is the study of regionally additive models and localized sparse interactions. Regional additive models (Gkolemis et al., 2023), consider generalized additive models where certain interaction terms only exist within certain regions of the input space. This allows for much greater modeling flexibility while still having a semi-local GAM approximation to the model. This interpretable-by-design model type depends on their being relatively few regions, and generally trades between region complexity and interaction complexity. It is reminded that regionally additive models are a combination of the additive pillar with the concept pillar, recall Figure 3.

This approach can be seen as the interpretable-by-design dual concept to region-specific additive explanations like REPID (Herbinger et al., 2022) and GADGET (Herbinger et al., 2024) which focus on providing effect plots which are regionally interaction-free. Moreover, this is part of a larger trend to increase explanation flexibility through the use of instance-wise sparsity, which further relaxes from semi-local small regions to completely local individual data points. TabNet (Arik and Pfister, 2021) has local feature selection sparsity which may depend on all of the features (i.e. selecting the region), but the final prediction step will be dependent on those individual features (i.e. locally sparse model). Sum-of-Parts (You et al., 2025) provides an interaction attribution for natural images where the interaction sparsity pattern depends on the individual sample, again providing an explanation which is regionally an additive interaction explanation.

Tabular Foundation Models Although tabular data has been traditionally dominated by boosting methods from machine learning (Shwartz-Ziv and Armon, 2022; McElfresh et al., 2023; Borisov et al., 2024), a recent departure from this trend is the work of TabPFN (Hollmann et al., 2023). TabPFN uproots the usual deep learning pipeline by training a transformer to map directly from a dataset to a test prediction, which enables pretraining on a large corpus of synthetic tabular data. This raises questions about the future of machine learning and whether the traditional paradigms of fitting a single model to a single dataset are still relevant in the post-LLM, post-pretraining landscape of artificial intelligence. TabPFN points out that even the simple and ubiquitous tabular data is not immune

to having larger patterns across different datasets which are detectable by deep learning. GAMformer (Mueller et al., 2026) asks whether or not these globally learned patterns by a large-scale transformer can still be locally understood after fixing the training dataset. In particular, they train a TabPFN model which returns a 1D GAM model in terms of its predictions on new test samples.

Additional Hierarchies, Structures, and Geometries The incorporation of additional structure is also critical for GAM extensions attempting to perform well beyond the setting of tabular data with simple and interpretable features. Domains like natural language and computer vision, as well as data types like longitudinal data and graphical data require additional caution for additive modeling to be as useful as possible. Although basic modifications like grouping spatial coordinates, considering time as a distinguished feature, or grouping missingness indicators with features are often considered standard practice within their respective fields, there remain many research opportunities exploring the nuances of these and related choices, especially how they respect the correlation structures of each respective domain. For example, the hyperbolic structure of word hierarchies and image label categories (Nickel and Kiela, 2017; Khrulkov et al., 2020; Ermolov et al., 2022), the spatial structure of natural images (Burt and Adelson, 1987; LeCun et al., 1989), the autocorrelation structure of time series data (Whittle, 1951; Box et al., 1970), the connectivity structure of graphical data (Chung, 1997; Page et al., 1999; Perozzi et al., 2014; Kipf, 2016; Grover and Leskovec, 2016), or the fine-grained hierarchy structure of high-dimensional embeddings (Rendle, 2010; Lyu et al., 2023) are all of particular importance to their respective applications.

HCI Integration and Causal Insight As an interpretable method, it is also important to understand how GAMs are being interpreted and integrated into larger human-in-the-loop systems. Moreover, it is important to understand the heterogeneity of applications and their respective demands. This human-computer interaction (HCI) should always be considered as an extension of the GAM itself, and interpretability claims must be factored through the relevant application at hand (Bellotti and Edwards, 2001; Kaur et al., 2020).

Interpreting the claims of the GAM model causally is amongst the most abundant of mistakes made by practitioners and non-experts alike, begging for methods which can automatically understand the contextually relevant causal claims and/or process external causal assumptions into the overall pipeline. In many cases, understanding the interpretable insights of the GAM in a causal light may be critical for downstream actionability of the insights (Workshop on Actionable Interpretability @ ICML 2025). Although causality is infamous for its difficulty and nuance, many works are already beginning to make progress on utilizing causal assumptions to be incorporated into additive attribution (Biparva and Materassi, 2024; Gajewski et al., 2025).

5. Application Areas

After establishing the historical details of the major duality between Shapley additive explanations (§3) and generalized additive models (§4), we move on to discuss some of the key application areas of machine learning and deep learning. We will focus on the areas of vision (§5.1), language (§5.2), vision-language (§5.3), time series (§5.4), and graphs (§5.5).

As alluded to previously, many of these domains have the property that the raw input features are heavily correlated, resulting in challenges for additive interpretability and additive explainability as alluded to in previous sections. Nonetheless, we focus on how these domains use feature interactions and related methods, as well as discussing other traditional interpretability approaches which are popular in each domain.

5.1 Vision

Although a lot of the classical interpretability methods were developed with computer-vision applications in mind, nowadays, much like the other application domains in this section, one cannot make significant progress on CV interpretability without directly focusing on the topic. Although beginning with saliency and feature-based explanations, a significant amount of work now focuses on explaining *concepts* and understanding learned *representations*.

A substantial body of literature was born out of the concept-based reasoning style focused on handling the latent structures, part hierarchies, and compositional scenes of natural images. These are mostly born out of the research into prototypical parts by ProtoP-Net (Chen et al., 2019) and the concept labeling by CBM (Koh et al., 2020). Some important follow-ups include neural prototype tree (Nauta et al., 2021), Deformable ProtoPNet (Donnelly et al., 2022), PIP-Net (Nauta et al., 2023), ProtoConcepts (Ma et al., 2023), MCPNet (Wang et al., 2024a), and ProtoPairNet (Gurung et al., 2025), as well as concept embedding models (Zarlenga et al., 2022), posthoc CBMs (Yuksekgonul et al., 2023), probabilistic CBMs (Kim et al., 2023), label-free CBMs (Oikarinen et al., 2023), LaBo-CBM (Yang et al., 2023), and energy-based CBMs (Xu et al., 2024). As can be seen, a very heavy focus of modern CV interpretability is placed on these human-understandable concepts which are existing within the image.

On the explainability side, there is the important Testing with Concept Activation Vectors (TCAV) (Kim et al., 2018) which finds the direction within a layer's latent feature space which is highly activating for concept-labeled set of images. There is also the concept whitening approach (Chen et al., 2020c) which attempts to orthogonalize an entire layer feature space to be better aligned with a set of labeled concepts.

Saliency remains a popular interest in computer vision research due to the variety of vision applications which need to understand 'where the network looks' as in image-based saliency. The majority of saliency work is coming from computer vision researchers not focusing on interpretability, who either use a quick and dirty application of GradCAM or attention, or use the word saliency in the vision sense, in a way different from feature-based explainability. Although, there is some continued research into gradient saliency (Li et al., 2025), there remains a continuously growing body of evidence which has largely put it out of fashion (Adebayo et al., 2018; Kokhlikyan et al., 2021; Binder et al., 2023; Hedström et al., 2023; Zhang et al., 2025a).

Some more recent approaches related to concept-based methods include CRAFT (Fel et al., 2023b) which provides attribution maps which operate at the level of concepts instead of exclusively the class labels. Lens (Fel et al., 2023a) continues with this approach demonstrating the larger methodological pattern of concept extraction followed by concept importance scoring. QPM (Norrenbrock et al., 2025b) instead uses a sparse feature selection

problem on ResNet features to ensure a small number of concepts are required for prediction and that moreover each class only requires few concepts. CHiQPM (Norrenbrock et al., 2025a) extends this approach through specifically reorganizing these learned features into a hierarchical decision-making process.

5.2 Language

Natural language was also a major focus of early interpretability works alongside computer vision. Compared with computer vision, however, the classical style of feature-based explanations has had a heightened staying power due to individual tokens having natural meaning, whereas individual pixels do not. In addition to these feature-based explanations, there are two explanation types which are specifically applied to natural language: *rationales* (sometimes, extractive rationales) and *natural language explanations* (sometimes, abstractive rationales). Rationales are word-based explanations with an emphasis on necessity and sufficiency, usually in the context of regularization towards human-extracted rationales (Arous et al., 2021). Natural language explanations are the more creative justifications which can be written in natural text to justify an answer, now exceedingly commonplace in the post-ChatGPT era (Kojima et al., 2022).

Beginning with the earlier approaches of LIME (Ribeiro et al., 2016) and SHAP (Shapley, 1953), we then had learning to explain (L2X) (Chen et al., 2018) which finds a subset of important words which align with the prediction and contextual decomposition (CD) (Murdoch et al., 2018) which designs an importance score specifically for LSTM architectures. Agglomerative Contextual Decomposition (ACD) (Singh et al., 2019) extends this to agglomerative hierarchies, HEDGE (Chen et al., 2020a) uses occlusion-based perturbation alongside a divisive hierarchy to create a hierarchical importance score which breaks as few interactions as possible, Sampling and Contextual Decomposition (SCD) (Jin et al., 2020) introduces hierarchical explanation and more natural sampling of word perturbations, and Sampling and OCclusion (SOC) (Jin et al., 2020) efficiently mixes occlusion-based perturbation with sampling-based perturbation.

Although tangential, it seems worth briefly noting that unlike other domains which explain classification using the color red for positive and blue for negative, the NLP explainability community often uses the opposite, with light blue for emotionally positive and red for emotionally negative (due to the popularity of the sentiment classification task).

A closely related approach to the feature-based scoring approaches is the approach of *rationales*. Generally, this can be interpreted as a binary importance score for each word which can either be important or unimportant, rather than giving a continuous score of importance strength (Zhang et al., 2016; Arous et al., 2021; Joshi et al., 2022; Gurrapu et al., 2023). This is often in the context of comparison against human-labeled rationales on the same inputs (Camburu et al., 2018; Arous et al., 2021) which can be incorporated into various training and regularization approaches to improve the predictions and performance (Jain et al., 2020; Chan et al., 2022; Joshi et al., 2022), although implicitly, these are commonly more closely related to sufficiency-based explanations (Carter et al., 2019a).

In more recent years, given the widespread success of language modeling, there has been a much greater push towards understanding generative interpretability as in the autoregressive sense of decoder-only transformers. Simultaneously, a major new approach to NLP

explainability occurred as LLMs began to generate plausible and coherent English which allowed them to directly generate their own explanations (Marasovic et al., 2022; Wiegreffe et al., 2022), but just like humans, this means there is no guarantee on the truthfulness of the provided explanation, called its *faithfulness*. Although using chain-of-thought prompting as the explanation (Kojima et al., 2022; Wei et al., 2022) at least has a causal impact on the final outputs, there are still no guarantees on faithfulness and this remains the major hindrance to using natural language explanations (Zhao et al., 2023; Lyu et al., 2024).

Given the widespread adoption of autoregressive language modeling for all natural language tasks, there has been a larger push to understand autoregressive language modeling directly. Next-token generation can be considered as a one-step classification problem which allows for all of the previously developed tools to be directly applied to this case. Unfortunately, applying these approaches directly is not without their drawbacks. In particular, the problem of next-token prediction has an output space which is as large as the vocabulary of the model, meaning tens or hundreds of thousands of possible tokens. This has led to the need for 'contrastive' approaches which explain the choice of word when contrasted against an alternative. Jacovi et al. (2021) studies classification tasks in the BIOS dataset for contrasting gender and occupation and the MultiNLI dataset for contrasting logical inferences. Yin and Neubig (2022) studies the language modeling task in the BLiMP dataset which provides grammatically contrastive pairs for twelve linguistic phenomena. Inseq (Sarti et al., 2023) applies existing explanation approaches to the entire sequence of generated words, providing an attribution matrix. TextGenSHAP (Enouen et al., 2024) introduces a Shapley-based framework for explaining the entire output sequence to determine which RAG documents were critical for question answering. CELL (Luss et al., 2025) uses contrastive explanations to determine which parts of the prompt were critical for the output response.

5.3 Vision-Language

Multimodal tasks involving both vision and language data, like visual question answering (VQA) (Antol et al., 2015; Johnson et al., 2017), have also been of great interest to deep learning. Early approaches to VQA used naturally interpretable compositional structures of a neurosymbolic approach to directly answer visual questions like neural module networks (Andreas et al., 2016b,a). Gradually, end-to-end systems overtook these early 'interpretable' types of approaches. In modern times, there is great interest especially in multimodal generation of text and image following the success of CLIP (Radford et al., 2021), with continued progress in the LLM era. Mechanistic interpretability remains one of the most prolific set of approaches for interpreting multimodal models including directly investigating neurons (Goh et al., 2021), directly investigating attention heads (Gandelsman et al., 2024), using a patch-based sparse autoencoder (Lim et al., 2025), and using a hierarchical sparse autoencoder (Zaigrajew et al., 2025). Nonetheless, concept-based approaches and interaction-based approaches have also seen some attention. SpLiCE uses linear concept embeddings for predefined concepts with natural language descriptions (Bhalla et al., 2024). FIxLIP uses a cross-modal extension of the Banzhaf interaction score to understand interactions between text tokens and image patches (Baniecki et al., 2025).

5.4 Longitudinal and Time Series

Longitudinal and time series data form a domain with a long and seasoned history in statistics, being a key domain of interest for statistical modeling and stochastic analysis, and having innumerable applications throughout weather forecasting, signal processing, econometrics, financial forecasting, and general time series forecasting. Although longstanding statistical models like ETS, harmonic regression, and ARIMA still often perform on par or better than more recent machine learning and deep learning approaches (Hewamalage et al., 2023), progress continues to be made with scaling deep learning approaches (Nie et al., 2023) and developing time series foundation models (Hoo et al., 2024), leading to a growing need for interpretability in these domains. In addition to TS regression and TS classification, time series data also has other prediction tasks like time-to-event, anomaly detection, and exceedance forecasting.

A very well-studied model for the task of survival analysis is the Cox additive model (Cox, 1972), which uses a generalized additive model structure for the problem of survival analysis with a time-varying baseline hazard. Due to the re-interpretation of additive models as interpretable, several works have used Cox additive models with sparsity or interactions (Utkin et al., 2021; Jiang, 2022; Van Ness and Udell, 2025). On the explainability side, SurvSHAP (Krzyziński et al., 2023) extends the Shapley value to survival analysis settings. See Langbein et al. (2025) for a more comprehensive review of the work on survival analysis.

Works like NATM (Jo and Kim, 2023) and GATSM (Kim et al., 2024) take additive modeling into the tasks of TS regression and classification. TimeMIL (Chen et al., 2024) uses multiple instance learning for time series, claiming interpretability through the sparsity of important instances. TimeSHAP (Bento et al., 2021) extends the Shapley value to recurrent model prediction for time series. TIMEX++ (Liu et al., 2024) compresses input multivariate time series into informative embeddings to isolate the location of key information, while MILLET (Early et al., 2024) achieves a similar compression strategy through the use of multiple instance learning. FDTempExplainer (Yang et al., 2024) looks at distinguishing interactions and dependencies in time series models. OrderSHAP (Hill et al., 2025) uses the Sanchez-Bergantiños value designed to respect the temporal ordering of Shapley permutations.

5.5 Graphical and Natural Sciences

Graphical data is another key domain which has seen the adaptation of specialized deep learning techniques and specialized interpretability techniques. Data coming from networks like citation networks and social networks as well as from scientific data like molecular graphs and physical interaction diagrams obey specified graphical connections. Furthermore, deep learning with graph neural networks (GNNs) has shown incredible promise in leveraging the large amount of data obeying graph-like structural connections (Zhou et al., 2020).

GNAN (Bechler-Speicher et al., 2024) uses NAM's additive structure for graph neural networks. GNN Explainer (Ying et al., 2019) finds important subgraphs related to GNN predictions. GStarX (Zhang et al., 2022) uses the Hamiache-Navarro value to explain GNN predictions. SAME (Ye et al., 2023) uses a different extension of the Shapley value to provide graph-structure-aware explanations. MAGE (Bui et al., 2024) uses the Myerson-Taylor value to explain predictions. GNN-SHAP-IQ (Muschalik et al., 2025) uses interaction-based

Shapley explanations for GNNs, additionally providing exact SHAP explanations for shallow GNNs.

Geospatial approaches also commonly incorporate graphical data, for instance between networks of sensors like in traffic forecasting (Li et al., 2017) and weather forecasting (Ravuri et al., 2021). Traditional methods in kriging (Clark and Harper, 2000; Banerjee et al., 2025) have modern counterparts in additive kriging (Durrande et al., 2011) and additive geoadditive regression (Kneib et al., 2009; Schmid et al., 2011). Furthermore, the explanatory power of higher-order interactions has been recognized independent of the study of interpretable machine learning across many of the natural sciences, including physics (Battiston et al., 2021), dynamical systems (Boccaletti et al., 2023; Zhang et al., 2023), epidemiology (Wang et al., 2024d), ecology (Grilli et al., 2017), genetics (Riesselman et al., 2018; Kuzmin et al., 2018), and neuroscience (Panzeri et al., 2022; Varley et al., 2023).

6. Future Directions

Before closing, we touch on some directions of future research for the field of interpretability as a whole, especially those made more overt by the depth of connections within the additive interpretability pillar as discussed in this survey. In particular, we highlight: (i) further deepening our understanding of the three pillars and their fundamental properties; (ii) clarifying whether these interpretability varieties can be cohesively integrated or will remain permanently conflicting; and (iii) developing AI interpretability for other application settings beyond supervised learning.

6.1 Building up the Pillars

Improving Additivity Although the study of higher-order feature interactions seems to be comprehensive in building up the additive pillar to represent arbitrarily complex functions, there are still many remaining directions for better understanding the necessity of higher-order interactions in additive modeling beyond better developing our algebraic and geometric understanding of higher-order feature interactions. In particular, there are the key questions of how the robustness of an additive model remains in the presence of sparsity constraints and higher-order dependencies. Given that the interpretability of the additive model is partially dependent on both the sparsity of the additive model and the independence of the contributions, it is natural to further study what happens under these practical settings. Section 4.5 describes many such active research directions.

There are also natural extensions into generative modeling with energy-based modeling (Goodman, 1970; Koller and Friedman, 2009) and causal modeling (Bühlmann et al., 2014), which provide a pathway for better understanding the correlation structure and the causal insight into the additive model using a second additive model over the distribution. There are also regional additive models which combine the regional locality of concept-based modeling with the low-degree interactions of additive modeling (Gkolemis et al., 2023). These extensions beyond the main additive pillar are discussed further in Sections 6.2 and 6.3.

Connecting Circuits Although there is a vast literature on understanding the representability of functions in terms of circuits (Darwiche and Marquis, 2002; Vergari et al., 2021), there is a lack of integrating these known results into the explainability framing. In

particular, there are seemingly large opportunities for applying the existing circuit hierarchies into providing necessary and sufficient explanations for otherwise blackbox algorithms (Shih et al., 2018; Carter et al., 2019a; Darwiche and Hirth, 2020).

The duality between GAM and SHAP highlighted in the additive regime (Herren and Hahn, 2022; Bordt and von Luxburg, 2023; Enouen and Liu, 2025) is part of a larger program defining post-hoc explanations as good explanations only insofar as they are able to distinguish individual models within a class of interpretable models (Günther et al., 2025). Thus, it seems completely feasible to apply these principles to the cases of decision trees and decision circuits. Applying the wealth of knowledge in boolean circuits to the cases of explaining boolean functions seems like a natural and underexploited resource for putting sufficiency explanations and context-specific sufficiency explanations on more stable ground with respect to their ability to explain simpler classes of circuits. Furthermore, given the interest of mechanistic interpretability in circuit discovery, there are many opportunities for how to rigorously define this abstraction, see Section 6.2.

Once these inadequacies of sufficiency-style and abduction-style explanation approaches are also more thoroughly comprehended, it seems plausible to more fairly compare the strengths and weaknesses of the additive approach and the logical approach. It is assumed that neither approach would be strictly better in all cases. From this, further progress could be made on understanding the situations and applications in which each is able to better deliver on interpretability promises and match alongside human intuitions. Further still, an understanding of how these two approaches could combine to achieve a balance of the (behavioral) additive interactions and the (mechanical) logical interactions would greatly enhance the coverage of interpretability approaches for structured input features, discussed further in Sections 6.2 and 6.3.

Rigorizing Concepts The concept of concepts has been a huge success for the interpretability community, allowing for the adequate describing of a large variety of catch-all situations which obey our human intuition on why something is easily understood; however, the flexibility of concepts also makes them just as hard to specifically nail down. Although particular cases like k-NN models are clearly simple enough for data valuation approaches to explainability, how to extend notions of similarity beyond fixed-distance metrics to increasingly abstract notions of concepts in a systemized fashion remains missing from the current literature. There are no standardized general classes of models which obey the same straightforward dualities which seem to exist in additive interpretability and logical interpretability.

Even simple definitions for concepts as any intermediate representation do not remain valid in the continuous setting without additional scaffolding like requiring smooth mappings into and out of concepts. Slightly more specific definitions which require concepts to be representations which are related to the classification or regression target in a 'simple' way bake this requirement into the definition of concepts themselves, but also do not necessarily provide a clear paths for how to define simple in a sufficiently general manner. In the case of fully discrete variables, simplicity of the intermediate representation can be achieved through compressibility and tools from information theory; however, no interpretability frameworks or measures of compressibility have yet been developed on top of these existing tools. Beyond this, there are the distinct approaches which use human-interpretable concepts

as the fixed benchmark versus those which use AI-interpretable concepts and try to restrict those notions as well as bridging between the two. Moreover, the concept pillar also seems to be the most naturally amenable to compositionality, begging the question of whether they are better conceptualized as not a pillar in their own right, but potentially the glue needed for compositionally enhancing interpretability at large, see Section 6.2.

Rigorizing the definition of concepts in a sufficiently general manner while also having a balanced restriction on their capacity which is able to provide simplicity guarantees and interpretable understanding would be a key development into research on concept-based interpretability approaches which seems to be missing from the literature insofar.

6.2 Compositionality

The general inability to combine the different pillars remains one of the most major limitations for vastly expanding the coverage of interpretability methods. It is clear in many contexts how the naive combinations of different interpretable reasoning styles leads to an approach which is uninterpretable in aggregate. Providing a greater understanding of the conditions under which different interpretability methods can be compositionally combined and remain interpretable would be a critical development in our understanding of interpretability approaches overall.

Although using concept-based interpretability as an intermediate layer to define concepts plays relatively nicely with the other two pillars (concept then logical giving interpretable neurosymbolic models and concept then additive giving certain concept bottleneck models), there are also other combinations of these approaches which fail to provide interpretability. Applying additivity after distance-based similarity results in the kernel machine. Similarly, applying concepts after circuits makes the discovered mechanisms worthless to the final interpretation. Additionally, neurosymbolic reasoning over defined concepts implicitly assumes that we have understood the concepts well enough that we don't conflate them with existing concepts coming from human understanding. Mixing additive and logical interpretability generally seems to fail in current approaches.

With this background, it becomes unclear whether these pillars are the only valid approaches to interpretability or if there are less common approaches to interpretability which are not covered by these three categories which might help to bridge these gaps. Furthermore, in many senses, the concept-based approaches feel the most amenable to being used for compositionality (with the hierarchical construction of features being the entire motivation of deep learning in the first place). Whether or not this earns concept-based approaches a special recognition in comparison to the other two pillars is yet to be seen in any especially rigorous way. It could equally be imagined that concept approaches do form a basic building block and it is higher-order compositionality which requires this 'glue' for combining different interpretability methods. Although many threads starting to apply compositionality have begun to appear in the interpretability literature, a full understanding of composability seems as of yet far off.

Although better theoretical understanding will probably continue to not come from the fields of post-hoc explanations and mechanistic interpretability explanations, these fields will probably continue to drive forward progress for the overall field. One of the key stated objectives of mechanistic interpretability is to find the underlying circuits and algorithms

being run by LLMs, even those operating on higher-level concepts. Accordingly, many empirical works have been pushing towards this blend of composing logical interpretability and concept interpretability, hoping to use their human intuition to directly search for these occurrences amongst the many, many weights of the neural network. Although the lack of standardization in the fields of logical interpretability and concept interpretability has likely prevented stable progress towards this goal, they have made significant empirical discoveries into the inner workings of convolutional neural networks and large language models which would still be completely unknown if interpretability researchers were to be collectively waiting for the tools of interpretability theory to catch up.

Advancing our understanding of the compositionality of interpretability methods is (a) key for making interpretability research useful beyond the garden of researchers who are interested in understanding these blackbox models only for the sake of understanding them.

6.3 Generative Interpretability

With the incredible progress in generative AI in recent years, the need and desire for interpretability of generative models has tremendously increased in recent years. The success of autoregressive LLMs is in large part what fueled the growth of the field of mechanistic interpretability. Although there is a huge variety of AI learning techniques beyond supervised learning, we focus on three particular cases which are of very heightened interest in the current research landscape: autoregressive self-supervised learning, classical unsupervised learning, and reinforcement learning.

The case of autoregressive self-supervised learning has obviously risen hugely in popularity since the advent of ChatGPT and commercialization of LLMs, giving it a heightened status as an important method of generative modeling. Beyond natural language generation, another key application using autoregressive generation is the domain of time series. Here, there are also many opportunities for interpretability, possibly making it a better test bed for interpretability theory for the autoregressive case. Although traditional models like Cox additive modeling provides an interpretable prediction of event likelihood, extending autoregressive time series models like ARMA to better understand their interpretability properties remains very open. How the autoregressive bias has been so successful for the generation of natural language also remains a mostly unsolved problem.

In the case of typical unsupervised learning, where new samples are generated completely from scratch, there are more existing connections with classical interpretability approaches. For the map depicted in Figure 3 of the three pillars defined in the discriminative setting, there is also the 'back of the map' which instead focuses on generative AI applications. Each of the interpretability pillars seem to have somewhat natural extensions in the context of generative modeling, with additive models replaced by generalized additive models like graphical models and other energy-based additive models (Goodman, 1970; Koller and Friedman, 2009; Enouen and Sugiyama, 2024), logical circuits replaced by probabilistic circuits (Choi et al., 2020; Vergari et al., 2021), and concept models replaced by concept-bottlenecked generative models (Ismail et al., 2023; Sun et al., 2024; Kulkarni et al., 2025). This area remains much more unsolved than the increasingly established areas of 'classical interpretability', leaving many more opportunities for understanding how to apply interpretability to increasingly capable AI systems.

The case of reinforcement learning is of very high significance for the future of AI research. It can be argued that the study of reinforcement learning is the only study of artificial intelligence, whereas other related topics are only studying machine learning. Under this view, it might not be too harsh to say that understanding RL in sufficient detail would be to understand parts of the nature of existence itself. As it stands for the interpretability literature in this field, there are several existing approaches applying interpretability to specific reinforcement learning problems; however, the field remains almost completely open in terms of setting up the scope for the problems and solutions of interest. This study has also grown in contemporary interest as some of the biggest successes of LLMs have come from their tuning through reinforcement learning (RLHF (Ouyang et al., 2022), DPO (Rafailov et al., 2024), RLVR (Lambert et al., 2025; Guo et al., 2025), GRPO (Shao et al., 2024)). Given the short-term and long-term impact of the field, making progress in understanding interpretability in the generative setting of reinforcement learning is of continued and growing importance, despite the dauntingly unconstrained and challengingly difficult nature of the problem.

7. Conclusion

Interpretability is an incredibly diverse field of study with an abundance of different styles and approaches. Nonetheless, feature interactions and additive models have shown themselves to be particularly descriptive of a wide variety of interpretability approaches existing in the current literature. Furthermore, their long history in statistics makes them well-studied objects with a deep foundation for supporting future extensions. In these ways, the study of feature interactions seems to have a high potential for unifying the discussion over the many topics in interpretability, or at least for providing a shared language to compare and contrast existing methods. It is hoped that this survey can serve as a sufficiently detailed resource for reference on these connections between the many directions of progress in the interpretability literature.

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