Comparing Explanation Methods for Traditional Machine Learning Models Part 1: An Overview of Current Methods and Quantifying Their Disagreement

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ABSTRACT: With increasing interest in explaining machine learning (ML) models, the first part of this two-part study synthesizes recent research on methods for explaining global and local aspects of ML models. This study distinguishes explainability from interpretability, local from global explainability, and feature importance versus feature relevance. We demonstrate and visualize different explanation methods, how to interpret them, and provide a complete Python package (scikit-explain) to allow future researchers to explore these products. We also highlight the frequent disagreement between explanation methods for feature rankings and feature effects and provide practical advice for dealing with these disagreements. We used ML models developed for severe weather prediction and sub-freezing road surface temperature prediction to generalize the behavior of the different explanation methods. For feature rankings, there is substantially more agreement on the set of top features (e.g., on average, two methods agree on 6 of the top 10 features) than on specific rankings (on average, two methods only agree on the ranks of 2-3 features in the set of top 10 features). On the other hand, two feature effect curves from different methods are in high agreement as long as the phase space is well sampled. Finally, a lesser-known method, tree interpreter, was found comparable to SHAP for feature effects, and with the widespread use of random forests in geosciences and computational ease of tree interpreter, we recommend it be explored in future research.

SIGNIFICANCE STATEMENT: The primary goal of this paper is to make the atmospheric science community aware of recently developed explainability methods for traditional ML models and demonstrate their use in a software package developed by the authors (scikit-explain; Flora and Handler\textsuperscript{2022}). Another important goal is to highlight that these methods tend to disagree with each other, which can affect the trust in these products. Like forecast verification metrics that describe different aspects of forecast quality, some disagreement is to be expected as explainability methods are designed for different tasks. Finally, we offer some practical advice on explaining the behavior of ML models when different explanation methods disagree with each other. We hope that this will motivate future work to explore the quality of explainability methods. For example, in Part II of this study, we find that knowing the relative faithfulness of feature ranking methods can objectively improve explainability.

1. Introduction

Machine learning algorithms (ML) are increasingly common in severe weather applications (e.g., Gagne et al. \textsuperscript{2017}, Lagerquist et al. \textsuperscript{2017}, Cintineo et al. \textsuperscript{2020}). Many methods have been developed to better understand black box models, and in response, substantial research has emerged on topics such as interpretable ML and explainable artificial intelligence (XAI) (e.g., van Lent et al. \textsuperscript{2004}, Kim et al. \textsuperscript{2016}, Adadi and Berrada \textsuperscript{2018}, Rudin \textsuperscript{2018}, Gilpin et al. \textsuperscript{2018}, Miller \textsuperscript{2019}, Linardatos et al. \textsuperscript{2020}).

\begin{itemize}
\item \textbf{a. Interpretability vs. Explainability}
\end{itemize}

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Table 1. A non-exhaustive list of definitions of interpretability and explainability provided in the literature. Many studies not included here do not define the terms and use them interchangeably. These are partial quotes from each source, but for readability, quotation marks are omitted.

| Source                | Interpretability                                                                 | Explainability                                                                 |
|-----------------------|----------------------------------------------------------------------------------|-------------------------------------------------------------------------------|
| Kim et al. (2016)     | [...] a method is interpretable if a user can correctly and efficiently predict the method’s results. | N/A (no distinction made)                                                    |
| Doshi-Velez and Kim (2017) | [...] the ability to explain or to present [the model] in understandable terms to a human. | explaining the model after it is trained with post-hoc methods               |
| Adadi and Berrada (2018) | [...] interpretable systems are explainable if their operations can be understood by human[s]. | N/A (no explicit definition provided, but the terms are not treated interchangeably) |
| Rudin (2018)          | An interpretable machine learning model is constrained in model form so that it is either useful to someone, or obeys structural knowledge of the domain such as [...] the physical constraints that come from domain knowledge. | [...] where a second (post-hoc) model is created to explain the black box model |
| Gilpin et al. (2018)  | [...] describe the internals of a system in a way which is understandable to humans | N/A (no distinction made)                                                    |
| Murdoch et al. (2019) | [...] the use of machine-learning models for the extraction of relevant knowledge about domain relationships contained in data the degree to which a human can understand the cause of a decision. | N/A (no distinction is made)                                                 |
| Miller (2019)         | [ability] to identify cause-and-effect relationships within the system’s inputs and outputs. | Explainability, [...] is associated with the internal logic and mechanics that are inside a machine learning system. |
| Linardatos et al. (2020) | Adopts the definitions from Miller (2019) and Kim et al. (2016) | N/A (no distinction is made; instead distinguishes interpretability/explainability from explanation where explanation refers to explaining individual predictions). |
| Molnar (2020)         | An interpretable ML model obeys a domain-specific set of constraints to allow it to be more easily understood by humans. These constraints can differ dramatically depending on the domain. | Explaining a black box model with a simpler model                           |
| Rudin et al. (2021)   | describes the possibility to comprehend the ML model and to present the underlying basis for decision-making in a way that is understandable to humans. | the collection of features of the interpretable domain, that have contributed for a given example to produce a decision |
| Wikipedia             |                                                                                   |                                                                                     |

[Molnar et al. 2020; Rudin et al. 2021]. Given the nascency of these topics, the definitions of explainability and interpretability are inconsistent throughout the literature, and many articles treat them interchangeably (Table 1). In this paper, we define these terms as follows:

- **Interpretability** is the degree to which an entire model and its components are capable of being understood without additional methods; and

- **Explainability** is the degree to which any partially interpretable or uninterpretable model (i.e., black boxes) can be approximately understood through post hoc methods (e.g., verification, visualizations of important features or learned relationships).

This distinction between interpretability and explainability is needed, since some in the ML and statistics community favor producing interpretable models (i.e., restricting model complexity beforehand to impose interpretability; Rudin 2018 [Rudin et al. 2021]), while the general trend in the ML community is to continue developing partially interpretable and black box models and implementing post hoc methods to explain them. Lipton (2016) defines a fully interpretable model as one that has *simulatability* (the entire model can be considered at once), *decomposability* (each component of the model is human-understandable) and *algorithmic transparency* (one can understand how the model was trained). A partially interpretable model may only meet one of these criteria. Explainability can be further subdivided into *model-specific explainability* (where the components of the model can be used for the explanation) and *model-agnostic explainability* (where no components of the model itself are used and no assumption is made about the model structure).

An illustration of interpretability and explainability is provided in Figure 1. Fully interpretable models do not require post hoc explainability methods to improve understanding, while uninterpretable models have the most to gain from additional explanation methods. For example,
low-dimensional linear regression is fully interpretable and a shallow decision tree is partially interpretable. In contrast, a deep neural network (DNN) or a dense random forest is uninterpretable but, through external explanation methods, can be approximately understood. Explanation methods must be approximate, as they would otherwise be as incomprehensible as the black-box model itself. We do not view this as a limitation of explanation methods, as suggested by other studies (e.g., Rudin 2018; Rudin et al. 2021), since abstracting a complex model is required for human understanding. For example, it is common in the weather community to replace the full Navier-Stokes equation with conceptual models that are more understandable. However, the degree of explainability is controlled by the complexity of the model (Molnar et al. 2019). As the number of features increases or their interactions become more complex, the explanations for the behavior of the ML model become less compact and possibly less accurate. At the moment, it is unclear how much improvement in our understanding of high-dimensional, highly nonlinear models current and future explanation methods will offer (Fig. 1).

b. Explainability Methods and their Disagreements

The atmospheric science community is beginning to adopt explainability methods (e.g., Lakshmanan et al. 2015; Minokhin et al. 2017; Herman and Schumacher 2018; Rasop and Lerch 2018; McGovern et al. 2019; Jorgensen et al. 2020; Lagerquist et al. 2020; Gagne II et al. 2019; Handler et al. 2020; Hamidi et al. 2020; Mecikalski et al. 2021; Loken et al. 2022; Shield and Houston 2022). Given the increasing interest in model explainability, in this first part of a two-part study, we synthesize recent research on multiple explainability methods using ML models developed for severe weather prediction (Flora et al. 2021) and sub-freezing road surface temperature prediction (Handler et al. 2020). By highlighting multiple explainability methods, our goal is to also demonstrate the degree to which explanations of model behavior can disagree with each other. Only recently have studies begun to document the sometimes substantial disagreement between explainability methods (e.g., McGovern et al. 2019; Molnar et al. 2020; Krishna et al. 2022; Covert et al. 2020). McGovern et al. (2019) is a seminal text for introducing multiple traditional ML and deep learning explainability methods to the atmospheric science community, but the analysis of disagreement among methods was largely subjective. Krishna et al. (2022) is one of the first studies to quantify the disagreement of different explainability outputs, but their study was limited to local attribution methods and it is difficult to determine how their results translate to highly complex datasets commonly found in atmospheric sciences.

Although previous studies have highlighted explanation disagreement (e.g., McGovern et al. 2019; Krishna et al. 2022), a thorough and objective exploration of explanation disagreement for a variety of explainability methods and in the context of meteorological data is warranted. We adopt methods similar to those of Krishna et al. (2022) to measure the global feature ranking agreement and introduce similar metrics to measure the agreement of estimated feature effects. In Flora et al. (2022) (hereafter Part II), we perform experiments similar to those in Covert et al. (2020) to measure the validity of feature ranking methods. By interrogating and measuring the disagreement between explainability methods, we hope to motivate further research on explanation methods that evaluate properties such as those introduced in Agarwal et al. (2022) (e.g., faithfulness, stability, and fairness).

Our contributions include highlighting the distinction between interpretability and explainability (discussed above), summarizing the various explainability methods and their key ideas (Section 4), suggestions for interpreting the different explainability output, and providing practical advice for explaining ML models when explanations seemingly disagree with each other. Lastly, we introduce a complete Python package (scikit-explain; Flora and Handler 2022) that computes and visualizes all the explainability methods demonstrated here (and more not shown).

The structure of this paper is as follows. Sections 2 and 3 describe the severe weather and road surface datasets and the ML models used, respectively. Section 4 covers the global and local explanation methods explored in this study. We present the results in Section 5 and in Section 6, we provide some practical advice for explaining ML models, particularly when the explanations from different methods disagree. Finally, the conclusions and limitations of the study are discussed in Section 7.

2. Data

a. Description of the Severe Weather Dataset

The severe weather data set is derived from the output of the 2017-2019 Warn-on-Forecast System (WoFS), which is an experimental 3-km ensemble that produces rapidly updating forecast guidance at 0-6-h lead times. Additional details of the WoFS are found in Wheatley et al. (2015), Jones et al. (2016), and Jones et al. (2020). The ML dataset contains features derived from intrastorm and environmental variables extracted from within 30-min ensemble storm tracks (Flora et al. 2019; 2021) with additional features that describe the morphological attributes of the tracks themselves (e.g., minor and major axis length; see Table 1 from Flora et al. 2021). Environmental features are spatial averages (within a track) of the ensemble mean and standard deviation fields valid at the beginning of the 30-min forecast period. Intrastorm features include both the
spatial average values of ensemble mean and standard deviation fields (similar to environmental features) from time-composited fields and the ensemble mean and standard deviation of spatial 90th percentile values of each ensemble member within a storm track (meant to capture storm intensity). The same ML features are used for each severe weather hazard prediction model, but the target variable is whether the ensemble storm track is matched to a tornado, severe hail, or severe wind report, respectively. Although the same features are used for all hazards, the dates from which the features were computed varied to help ensure similarity between the training and testing datasets (Flora et al. 2021).

b. Description of the Road Surface Dataset

The road surface dataset from Handler et al. (2020) spans two cool seasons: 1 October 2016 – 31 March 2017 and 1 October 2017 – 31 March 2018. Thirty features were used for training, including near-surface variables from the High Resolution Rapid Refresh (HRRR) model as well as derived features (Handler et al. 2020 Table 1). The variables were informed by previous research that identified variables important for modulating surface road temperatures (e.g., Crevier and Delage 2001). Hourly road surface temperature observations from the Road Weather Information System (RWIS) sites were used as the target variable for training. Each example was labeled below or above freezing based on the temperature reported by the RWIS site. The RWIS sites used are shown in Fig. 1a of Handler et al. (2020).

3. Machine Learning Algorithms

For this study, we used classification random forests and logistic regression models available in the Python scikit-learn package (Pedregosa et al. 2011). Consistent with Handler et al. (2020) and Flora et al. (2021), the random forest is applied to the road surface dataset to predict whether a road will freeze while logistic regression is applied to the WoFS dataset to predict whether a storm track will be associated with a severe hail, severe wind, or tornado report, respectively.
a. Logistic Regression with Elastic Nets

A logistic regression model is a linear regression model designed for classification tasks. Given a binary outcome variable \( y \) (1 or 0), we can estimate the probability that \( y \) belongs to a particular class (e.g., \( P(y = 1|X) \)) as:

\[
P(y = 1|X) = \frac{1}{1 + \exp(-\beta_0 - \sum_{i=1}^N \beta_i x_i)}
\]

where \( \beta_i \) are the learned weights, \( x_i \) are the features and \( \beta_0 \) is the bias term. Although logistic regression is based on a linear model, the predicted probability is not linearly related to the input features. In fact, unless the features are binary, binary classification is inherently non-linear due to the non-linear transformation of continuous features into binary target variables (\( \mathbb{R}^{m \times n} \rightarrow \{0, 1\}^m \) where \( m \) and \( n \) are the number of examples and features, respectively). Given that the summation in eqn. 1 is an exponent, there is a multiplicative interaction between all \( N \) features. Therefore, the logistic regression model has questionable interpretability in probability space, especially as the number of features increases. In this study, we treat logistic regression as partially interpretable and explain it using both its coefficients and external explanation methods. Regularizations, both L1 and L2, are used for training. L1 regularization acts as a feature selection method by zeroing coefficients for bad features while L2 regularization encourages smaller weights and thereby discourages the model for heavily favoring features.

b. Random Forest

An increasingly popular ML algorithm is the random forest (Breiman 2001). A classification random forest is made up of multiple decision trees, each partitioning the feature space into subregions of increasing "purity" (homogeneity of the target variable). To improve the predictive accuracy of the random forest, each tree is trained on a bootstrapped resampled version of the data, and for each split only a small random subset of features is considered. For each tree, the prediction is the proportion of positive class examples (number of positive class examples divided by the total number of examples in the leaf node). The final prediction of the forest is the ensemble average of the separate tree predictions. The random forest in this study is treated as uninterpretable and we explain it using model-specific and model-agnostic explainability methods.

4. Explainability Methods

In line with Lipton (2016), Molnar (2020) identifies five scopes of ML explainability, which can be summarized into three main categories:

- **Algorithmic Transparency**: How does the algorithm create the model?
- **Global Explainability**: How does the trained model as a whole make predictions? How do parts of the model affect the predictions?
- **Local Explainability**: Why did the model make a certain prediction for a single example? Why did the model make specific predictions for a group of examples?

Model explainability typically refers to global or local explainability, whereas algorithmic transparency does not refer to a specific model or prediction. Both global and local explainability methods can be summarized as measuring and visualizing:

- **Feature importance**: the ranking of features or sets of features by how much they contribute to a model’s predictions or performance (e.g., Breiman 2001; Greenwell et al. 2018; Lundberg and Lee 2017);
- **Feature effects**: the expected functional relationship between a feature (or set of features) and a ML model’s prediction (e.g., Friedman 2001; Greenwell et al. 2018; Lundberg and Lee 2017); and
- **Feature interactions**: how a given feature’s effect is dependent on other features and the strength of that effect (e.g., Friedman and Popescu 2008; Greenwell et al. 2018; Molnar et al. 2019; Oh 2019; Kuhn and Johnson 2019).

Global approaches attempt to decompose the model into parts that can be understood individually (Murdoch et al. 2019; Molnar et al. 2020). Local approaches explain individual predictions. These methods can include, but are not limited to, decomposing a prediction into the contribution of each feature (e.g., Ribeiro et al. 2016; Lundberg and Lee 2017) or developing counterfactual explanations to form what-if scenarios (Molnar et al. 2020). It is important to employ multiple explanation methods, as no one method is "one-size-fits-all" (Molnar et al. 2021). A brief summary of the key ideas for each of the explainability methods discussed in the following sections can be found in Figure 2. Furthermore, inspired by Covert et al. (2020), Table 2 provides a summary of the properties of the different explainability methods used in this study.

a. Global Explainability Methods

1) **Feature Importance vs. Relevance**

Ranking features within a dataset or based on their contribution to the model is a crucial component of model interpretability and explainability. In the literature, feature ranking methods tend to fall into one of three categories:
### Explainability Methods

#### Key Ideas

**Backward and Forward SP PI**
- **Measures:** feature importance by permuting (backward)/unpermuting (forward) features one at a time
- **Pros:** quick to compute; parallelizable; model-agnostic
- **Cons:** highly sensitive to correlated features and does not account for multivariate relationships between features.

**Gini Impurity**
- **Measures:** feature importance within a decision tree or forest based on impurity score
- **Pros:** computed at training time
- **Cons:** highly sensitive to correlated features and assigns higher importance to features with higher variance; model-specific

**Shapley Additive Global Importance (SAGE)**
- **Measures:** feature importance based on using a modified and approximate version of Shapley theory
- **Pros:** model-agnostic; fast; computationally quicker than computing SHAP
- **Cons:** SAGE Python package is limited to cross-entropy and MSE; new method (sensitivities are relatively unexplored); longer compute times than SP PI; assumes features are independent.

**Backward and Forward MP PI & Grouped/Grouped Only PI**
- **Measures:** feature importance by permuting /unpermuting multiple features at a time
- **Pros:** parallelizable; model-agnostic; manually defined groups are highly understandable; for mutually exclusive groups grouped importance is quick to compute; MP PI includes feature co-dependencies when computing importance.
- **Cons:** MP PI is greedy and does not consider all combinations of features; MP PI is computationally expensive; automatically defining feature groups is difficult.

**Partial Dependence (PD) and Accumulated Local Effects (ALE)**
- **Measures:** global model sensitivity to a feature across the full range of its values.
- **Pros:** quick to compute; parallelizable; model-agnostic; both can be used for functional decomposition; both can be computed for higher-order interactions
- **Cons:** PD is sensitive to correlated features; ALE can be noisy or biased when sample size is low

**SHapley Additive Explanations (SHAP)**
- **Measures:** feature attributions using an approximate version of Shapley values
- **Pros:** model-agnostic; only method that assigns attributions fairly and satisfies certain desirable properties (e.g., additivity, missingness, etc); exact Shapley values for tree models (ignore decision paths with missing features)
- **Cons:** slow compute time for a large set of examples or features; documentation on the various methods in the SHAP Python package is lacking.

**Local Interpretable Model-agnostic Explanations (LIME)**
- **Measures:** feature attributions using the coefficients of a local linear model
- **Pros:** model-agnostic; fast compute time
- **Cons:** attributions do not add to the model's prediction; sensitive to the accuracy of the local model approximation

**Tree Interpreter**
- **Measures:** feature attributions using the path of a decision tree or forest
- **Pros:** quick to compute; attributes add to the model prediction
- **Cons:** model-specific; can assign lower attributions to features higher in the tree; new method (sensitivities are relatively unexplored)

### Visualizations

**Feature Attribution**
- **Positive Attribution Value**
- **Negative Attribution Value**

**Single Example**
- **Multiple Examples**

**Global Explainability**

**Local Explainability**

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**Fig. 2.** Explainability methods covered in this study, their key ideas and typical visualizations. SP and MP are short for single-pass and multi-pass, respectively. PI is short for permutation importance.

1. **Strength of univariate relationship with the target variable**
2. **Expected contribution to the magnitude of a model’s prediction**
3. Expected contribution to the model’s performance/accuracy

The first category does not involve the model itself and reflects characteristics of the data, such as correlations with the target variable or the Kullback-Leibler J measure (Lakshmanan et al. 2015). Regression coefficients, feature attribution methods (e.g., SHAP, tree interpreter, LIME; see Section 4b), and partial dependence/accumulated local effect variance (Greenwell et al. 2018) are examples of the second category, while different variations of permutation importance, Gini impurity importance (Breiman 2001; McGovern et al. 2019), Shapley Additive Global importance (SAGE; Covert et al. 2020) or sequential feature selection (McGovern et al. 2019) are examples of the third category.

In general, the first two categories can be defined as measures of feature relevance, while feature importance is formally defined with respect to model performance (van der Laan 2006; Covert et al. 2020). We can further separate the notion of feature importance into model-specific feature importance and model-agnostic feature importance. Model-specific importance quantifies how much a set of features contributes to the performance of a given model, while model-agnostic importance quantifies the hypothetical range in which any well-performing model may rely on a set of features for model performance (Fisher et al. 2018; Covert et al. 2020). For example, although sequential feature selection considers model performance, it does not do so with respect to the model trained on the original set of features, and situations can arise where, due to compensatory effects, one seemingly important variable is removed and the model adjusts using the remaining variables (Kuhn and Johnson 2019). Therefore, sequential feature selection is an approximation of model-agnostic feature importance, while variations on the permutation methods, which do not alter the original model, are forms of model-specific feature importance.

2) Permutation Importance Methods

Permutation importance is one of the most popular methods for assessing feature importance. It was first introduced in Breiman (2001), but was later expanded in Lakshmanan et al. (2015). Recent studies have referred to the methods in Breiman (2001) and Lakshmanan et al. (2015) as single-pass and multipass permutation importance methods, respectively (e.g., McGovern et al. 2019; Jergensen et al. 2020; Handler et al. 2020). The main goal of both methods is to measure the expected model accuracy when the values of a feature are permuted so that the feature becomes uninformative of the target variable, but the marginal distribution of the feature is maintained. If the expected model accuracy is relatively unchanged after the feature values are shuffled, then the feature is considered unimportant. The single-pass method permutes only one feature at a time. For the multipass method, the most important feature from the single-pass is left permuted, and then the remaining

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The idea of model-specific importance and model-agnostic importance is referred to as model-based predictive power and universal predictive power in Covert et al. 2020. Fisher et al. 2018 loosely refers to the notion of model-agnostic importance with the idea of model class reliance: the highest and lowest degree to which any well-performing model with a given class may rely on a predictor for prediction accuracy.
features are permuted one at a time to determine the second most important feature. The top 2 features are then left permuted to determine the third most important feature, and so on. Lakshmanan et al. (2015) developed this technique to emulate sequential backward selection (McGovern et al. 2019), except that instead of removing a feature and refitting the model, features are left permuted to effectively remove them from the model. Sequential forward selection can also be emulated by jointly permuting all features and then unpermuting them one at a time to determine the most important feature. The most important feature remains unpermuted, and each remaining feature is unpermuted again to determine the second most important feature (and so on). Similarly to the nomenclature for sequential feature selection, we can refer to the latter and former permutation methods as the backward and forward multipass permutation importance, respectively. In summary, backward methods measure how removing a feature (or set of features) reduces model performance, while forward methods measure how much the model performance relies solely on the unpermuted features.

A lauded advantage of the multipass method over the single-pass method is that by permuting more than one feature, it accounts for feature codependencies (Lakshmanan et al. 2015; Gregorutti et al. 2015). For example, multiple studies have found that when features are correlated, their single-pass permutation importance score can be reduced (Strobl et al. 2007, 2008; Gregorutti et al. 2015, 2017). Furthermore, when permuting more than one feature, the total importance is not equal to the sum of their individual importances, as it also depends on the codependencies between the features (Gregorutti et al. 2015). Thus, multipass permutation importance is usually interpreted as taking feature codependencies into account.

To summarize, the single-pass permutation importance measures the univariate contribution of features to the model performance, while the multipass permutation importance attempts to measure the multivariate contribution of features to the model performance. In the presence of codependent features, the predictive information is divided among them. For example, information about storm intensity is shared among variables like maximum updraft speed, composite reflectivity, and mid-level updraft helicity. A univariate measurement of importance would ignore those important codependencies and erroneously rank some features too low. For example, for the severe hail dataset, the low-level lapse rate and major axis length features may be ranked higher than the composite reflectivity and updraft features because the latter are correlated with each other (Fig. 3). One drawback of the multipass methods, however, is that, as more features are permuted, the importance score relies on more and higher-order dependencies and the latter are often poorly sampled.

For a high-dimensional dataset with a large number of colinear/correlated features, it is difficult to effectively determine how a feature uniquely contributes to a model. In this study, we demonstrate the concept of grouped permutation importance (Gregorutti et al. 2017; König et al. 2020; Au et al. 2021) where the goal is to highlight how a grouping of two or more features contributes to the performance of the model. Groupings can be determined automatically through feature clustering based on correlations, but for improved explainability, it is useful to manually select the feature groups (e.g., storm vs. environment features for severe weather; temperature vs. radiative features for road surface temperatures). Another key advantage of the grouped feature importance is the reduced computational time versus other permutation importance methods, assuming the number of groups \( \ll \) number of features. As with backward and forward permutation importance, we can conceptualize two forms of grouped feature importance:

- How does removing this group of features reduce model performance?
- How does the model perform when relying solely on this group of features?

For the first method, all features in the group have their samples jointly permuted such that the connection to the
target variable is lost, but the joint distribution between the features is preserved, whereas for the second method, all features not in the group are jointly permuted. Similarly to [Au et al. (2021)], we refer to these two methods as the Grouped and Grouped Only permutation importance, respectively.

According to Molnar (2020), favoring the training or testing dataset for feature importance remains an open question (see their section 5.5.2). Lakshmanan et al. (2015), however, argued for only using the training dataset. The goal of measuring feature importance is to quantify how the model relies on each feature and not how well the model generalizes to unseen data. If the ML model learned a pattern in the training dataset that is underrepresented in the independent dataset, then evaluating feature importance on the testing dataset can bias our understanding of how the model works. For example, the training dataset could have temperature ranges of $-15^\circ -10^\circ \text{C}$ while the testing dataset range is largely $-5^\circ -5^\circ \text{C}$. If the ML model heavily relied on temperatures $<-10^\circ \text{C}$ to predict freezing road surfaces, we would fail to determine that using the testing dataset. One could evaluate importance on both the training and testing to identify any discrepancies, but then you’d have to ascertain whether the difference is due to poor sampling or overfitting. Therefore, the feature importances and the various experiments in this study are evaluated using the training dataset.

We use the normalized area under the performance diagram curve (NAUPDC; Flora et al. 2021; Miller et al. 2021) as our performance metric. The area under the performance diagram curve (AUPDC) is a summary of the performance diagram curve (Roebber 2009), which measures how well the model discriminates between correct predictions and false predictions while ignoring correct negatives. The normalization is to account for the sensitivity of AUPDC to the base rate (Boyd et al. 2012). To improve the ranking estimates, we recompute the rankfeatures with a higher cardinality (more unique values) to produce a curve. We then compute the “centered” partial dependence by subtracting the average partial dependence value so that the mean effect is zero:

$$PD_{centered}(x_j) = PD(x_j) - \frac{1}{V} \sum_{v=1}^{V} PD(x_{j,v})$$

where $V$ is the number of values for which $PD$ was computed for.

### 5) Accumulated Local Effects

Though the PD curves are easy to calculate and understand, they assume that the features are independent (correlated features can distort the PD curve; Molnar et al. 2021) and their marginal effect can hide heterogeneous effects (Molnar 2020). An alternative to PD is a recently developed method known as accumulated local effects (ALE; Apley and Zhu 2016). The ALE for the feature $x_j$ is:

$$ALE_j(x) = \int_{\min(z_j)}^{\max(z_j)} \left[ \frac{\partial f(X)}{\partial X_j} | X_j = z_j \right] dz_j - c$$

where $f$ is the ML model, $X$ is the set of all features, $z_j$ are the values of $x_j$, and $c$ is the integration constant. The standard deviation, so the relevance is theoretically based only on $|\beta_j|$. For random forests, we can use the impurity importance ([Breiman 2001] McGovern et al. 2019), which ranks the features according to how many examples they affect (e.g., whether they occur higher in the tree) and how effectively they split the data (i.e., increase the information gain). Unfortunately, this method is biased, as it will tend to rank features with a higher cardinality (more unique values) higher than other features and is sensitive to correlated features (Strobl et al. 2007, 2008).
constant $c$ is chosen as the mean of $ALE(x_j)$, so the mean effect is zero, similar to Eqn. [4].

For a given feature, ALE computes the expected change in prediction over a series of conditional distributions and then accumulates (integrates) them to return the feature effect. By computing the average change in prediction over a series of small windows, ALE isolates the effect of the feature from the effects of all other features and avoids the pitfall of partial dependence, which can suffer from unlikely or non-physical combinations of feature values. More details on the ALE calculation are provided in [Molnar 2020] and [Flora 2020].

Recently, Greenwell et al. (2018) introduced a simple method that ranks features based on the variance in their PD curve. In this study, we use the ALE curve instead of PD as we deal with multicollinear features. To measure the variance, we calculate the standard deviation of the first-order ALE for each feature. Whether using ALE or PD, the method assumes that the greater the variation in the curve, the more relevant the feature.

b. Local Explainability Methods

Though global explainability methods can provide a good overview of the model, the explanation of a single prediction can differ from the global explanation. A common technique to explain individual predictions (or some small subset thereof) is to approximate the final prediction $g(x)$ as the sum of individual contributions ($\phi_i$) from each feature:

$$ f(x) \approx g(x') = \phi_0 + \sum_{i=1}^{N} \phi_i x'_i $$

where $\phi_0$ is the bias (often the average prediction of model $f$), $N$ is the number of features and $x' \in \{0, 1\}^M$ (indicating whether a feature is contributing or not). Methods to determine these individual contributions are known as feature attribution methods. In the following sections, we briefly highlight three such methods. One goal of this paper is to determine whether local explainability methods can be scaled to provide global explanations. To capture global characteristics, we calculated the feature attributions values from 50,000 random samples extracted from each dataset. To assign a feature relevance score, we sum the absolute feature attribution values of each example per feature. To compute the feature effects, we compute the average feature attribution value per bin (using the same bins as for the ALE and PD curves).

1) Tree Interpreter

Tree interpreter is a feature attribution method for decision tree-based models [Saabas 2014, Loken et al. 2022]. For a classification decision tree with $M$ leaf nodes, the feature space is divided into $M$ regions. The prediction is then defined as follows:

$$ f(x) = \sum_{m=1}^{M} c_m I(x, R_m) $$

where $R_m$ is the $m$th region, $c_m$ is the proportion of positive examples in $R_m$ (from the training dataset), and $I$ is the indicator function (return 1 if $x \in R_m$, 0, otherwise). When producing a prediction from a decision tree, we can visualize the path the data take through the various branches until they reach a leaf node. For example, Figure 4 has a 2-feature domain split into 5 regions (Fig. 4a) based on the decision tree in Fig. 4b. To compute the feature attributions for the single data point (shown in red), we progressively parse the domain as we pass through the nodes of the decision tree. Initially, the data are not split and $k_0$ is the proportion of positive examples in the highlighted region.
from $k_0$ to $k_1$ is attributed to the feature $X_1$. With each additional split, there are additional feature attributions for $X_1$ or $X_2$. In terms of equation 6, $\phi_0 = k_0$ and $\phi_1 = \sum \Delta k^i$ where $\sum \Delta k^i$ is the sum of changes to $k$ associated with the $i$th feature. For a random forest, we can determine the contribution breakdown for each tree and then average the results together.

2) Local Interpretable Model-Agnostic Explanations

Linear regression models are highly interpretable models (see Fig. 1), and we can leverage their interpretability by using them as local surrogates for more complex models to explain individual predictions. The local interpretable model-agnostic explanation (LIME; Ribeiro et al. 2016) fits a weighted linear regression model on perturbed data in the neighborhood of the example to be explained. The input features in the local model are binary representations of themselves such that the coefficients are $\phi_i$ and follow equation 6. To determine the neighborhood, LIME uses an exponential smoothing kernel. One drawback of this method is the need to determine the properties of this kernel (e.g., its width). We use the default kernel width of 0.75 times the square root of the number of features, a sample size of 2500, and compute the coefficients for all features.

3) Shapely-based Methods

Shapley values (Shapley 1953), which are rooted in game theory, have become one of the most promising methods for explaining ML predictions, as they can be useful for both local and global explainability. The Shapley value for the feature $x_j$ is the weighted average difference in model prediction (its contribution) when $x_j$ is included and not included in a feature subset $S$ for all possible $S$. From a game theory perspective, when players are cooperating in a coalition, Shapley values are the fairest possible payouts to the players depending on their contribution to the total payout. In terms of ML, we can think of players as features and payouts as their contributions to the final prediction (the total payout). A more complete description of the Shapley values is provided in Molnar (2020).

One limitation of traditional Shapely values is that they treat features independently, ignoring correlated or multicollinear features. To address this, we can group the features into coalitions and compute an extension of the Shapley values known as Owen values (Owen 1977; López and Saboya 2009). To compute the Owen value for $x_j$, we compute the weighted average change in model prediction when $x_j$ is included and not included in all possible feature subsets, but such that the subsets exclude features from one grouping. We repeat the calculation with each feature grouping being excluded, and average those values. Another key benefit of the Owen values is that the number of feature subsets to evaluate is greatly reduced, especially for a smaller set of feature groupings. The Owen values are calculated using the Shapely Additive Explanation (SHAP) Python package Lundberg and Lee (2017) and we use feature correlations to determine the feature groups (using SHAP’s partition masker).

For all feature attributions, we would like the following axioms to be satisfied.

1. Local accuracy (additivity): The sum of the contributions of each feature plus the average prediction of the model must be equal to the final prediction for a given instance (Eqn. 6).

2. Consistency (monotonicity): If an ML model changes so that the marginal contribution of a feature increases or stays the same, the feature attribution must also increase or stay the same, respectively.

3. Missingness: Missing features (e.g., features that have been marginalized out) must have a contribution of zero to the model.

Of the three feature attribution methods discussed above, the Shapley/Owen values are the only method that satisfies all three of these properties (Shapley 1953; Young 1985 Lundberg et al. 2018, 2020). Using an approximate linear model, LIME cannot guarantee the principle of local accuracy, whereas the Tree interpreter satisfies the local accuracy principle but has consistency issues as features near the root can incorrectly be given less weight (Lundberg et al. 2020). Although the tree interpreter and LIME do not completely satisfy all three principles, in terms of run time (time to generate an explanation for a new sample), LIME and the tree interpreter are considerably faster (Lundberg et al. 2020), and therefore we consider them for this study.

Recently, Covert et al. (2020) used the concept of additive contributions and extended Shapley values to global explainability. The Shapely Additive Global importance (SAGE) method explains how each feature contributes to the expected model loss rather than to an individual prediction. SAGE is a global and model-agnostic extension of the LossSHAP method (Lundberg et al. 2020), which computes feature attributions for local loss, but only for tree-based models. One drawback for SAGE is that for missing features it relies on a marginal rather than conditional distribution approach, which is undesirable for datasets with correlated or dependent features. Covert et al. (2020) note that by using marginal distributions, though, it ensures that features not used by the model receive zero attribution. To compute the SAGE values, we are using the SAGE python package Covert and Algaba (2022) with default settings.
5. Results

a. Global Feature Rankings

Fig. 5 compares the feature rankings for the top 10 features of the WoFS tornado dataset. There is some consensus on the main features, but there are examples of significant disagreements. For example, the v-component of the 10-m wind is the top feature for both BSP and BMP (which is by default as the first step of multipass is the singlepass result), the ALE variance has major axis length as the top feature (cf. Fig. 5g), and the remaining methods have 0-2 km vertical vorticity as the top feature. Although there is disagreement between the feature ranking methods, each ranking is physically plausible. Thus, relying on a single explanation could lead to confirmation bias when assessing feature significance. Molnar et al. (2021) and Ghassemie et al. (2021) found that a third of their participants (out of 25) tended to favor an explanation if it better matched their intuition. In Part II, we explore the validity of the different ranking methods and find that the variance in the feature rankings decreases somewhat when excluding methods that poorly assign importance (e.g., assigning higher importance to features that weakly contribute to model performance).

To summarize the disagreement among the feature ranking methods, we use the top feature and feature rank agreement statistics from Krishna et al. (2022). The top feature agreement measures the fraction of common features between two top \( N \) feature rankings, while the feature rank agreement measures the fraction of top-\( N \) features with identical rankings. For this study, instead of requiring identical ranks for a given feature, we count situations where the rank of a feature is off by one between two rankings (e.g., feature \( x_i \) is ranked third in one ranking, but fourth in another). Requiring an exact rank match between two methods is likely to overestimate disagreement, especially when tiny differences can separate ranks (e.g., when the
number of similarly important features increases) and the explanation of model behavior is nearly identical.

Fig. 6 shows the top 10 feature and feature rank agreement, respectively, between each pair of feature ranking methods. In general, there is fairly high agreement on the top 10 features for the road surface datasets (Fig. 6i) whereas there is more modest agreement for the WoFS datasets (Fig. 6c-e).

To some extent, disagreement between the explainability methods is anticipated, as different explainability methods are designed for different tasks. This is a concept that is echoed in forecast verification, where different metrics are designed to measure different aspects of forecast quality (Murphy 1993). However, even when designed for a particular task, disagreements between explainability methods can arise due to the impact of correlated features (Gregorutti et al. 2017), bringing into question the validity of their feature rankings. For example, when there are correlations among informative features, their single-pass permutation importance can be reduced, and depending on the strength of the correlations, the features less correlated with the target variable may appear more important (Gregorutti et al. 2017). There is decent agreement on the top 10 features between the BSP and the logistic regression coefficients (Fig. 6a-d), which, when the features are independent, should provide identical feature rankings (Gregorutti et al. 2017). Similarly, there is high agreement between SHAP and the logistic regression coefficients (Fig. 6a-d), another pair of methods that should provide identical rankings given independent features. This is consistent with the fact that the logistic regression model uses L1 norm regularization and the SHAP values are based on Owen values, both of which mitigate the effects of the correlations between features. ALE and SAGE generally agree most with the forward-pass methods, which is consistent with the fact that forward methods largely ignore feature interactions (since they begin with all features permuted), and the ALE variance is determined by first-order effects and SAGE assumes feature independence. The local attributions (LIME, TI, and SHAP), tend to have higher agreement for all four datasets, but only have modest agreement with the feature importance methods. This result suggests that local attributions can scale as global feature relevance methods, but may not translate as global feature importance methods.

Explainability methods can disagree by design, but it is unclear whether the disagreement is inflated due to the inclusion of poorer performing methods (i.e., assigning higher importance to a feature that contributes weakly to model performance). It is possible that by evaluating a large set of feature ranking methods disagreement is likely to be higher. However, the disagreement among all the methods is similar to the average disagreement between the feature importance and feature relevance methods. This similarity suggests that the disagreement is not solely based on including several feature ranking methods or due to the explainability methods being designed for different tasks or including several methods, but is partly attributable to differing accuracy among the methods (explored in Part II).

In terms of rank agreement, there is more agreement on the rank for the severe wind and road surface datasets (Fig. 6i-h) than for the tornado and severe hail datasets (Fig. 6c-f). In Part II, we find that the severe wind and road surface datasets have weaker feature interactions than the tornado and severe hail datasets (see Section 6a of Part II), which means that the models rely more heavily on first-order effects. By relying more on first-order effects, the feature importance estimate is improved since the importance varies less across the feature space (i.e., more agreement between local and global explainability). As mentioned above, the logistic regression coefficients and the BSP methods should provide identical rankings if the correlations do not strongly impact the identification of the top 10 features. However, there was little rank agreement between the two methods (Fig. 6i-h) indicating a strong influence of correlated features. An outlier is the perfect agreement between SAGE and FSP for the WoFS datasets (Fig. 6g). Recall that FSP measures the importance of a feature when all other features are permuted, which breaks up any feature interactions or correlations. The similarity between SAGE and FSP suggests that SAGE may be ignoring feature interactions, but further research is required to test this hypothesis. Lastly, the TI method had the greatest rank agreement with Gini importance (GIN, 0.7), which can poorly assign rank when features are correlated (Strobl et al. 2007, 2008). We know that this limitation is by-product of how random forests are trained (Strobl et al. 2008), which is likely negatively impacting TI as a model-specific explainability method.

As noted in Section 4.1.2 and given the disagreement between explanation methods, it becomes increasingly difficult to effectively distinguish how a feature uniquely contributes to model performance when it is colinear/correlated with other features. Thus, we demonstrate the concept of grouped permutation importance where the goal is to highlight how a grouping of two or more features contributes to the performance of the model. For the WoFS-based datasets, we separated the features into one of three groups: intrastorm, environmental, and storm morphology. For the road surface dataset, we created temperature- and radiation-based groups.

For the WoFS datasets, intrastorm features were the most important, especially for the Grouped Only results (Fig. 7), which is not surprising given that storm-scale information remains predictable at these lead times (Flora et al. 2018) and the intrastorm features are the most causally related to storm hazards. We do not conclude that environmental and storm morphological features are unimportant but rather...
that, by themselves, they are not nearly as predictive as the intrastorm features are by themselves. For example, the importance of the environmental features is much higher for the Grouped than Grouped Only, indicating that if they are missing the model performance suffers (Fig. 7b,c,d), but without the other features they contribute little to model skill (Fig. 7g,h). This result aligns with another ML study that leveraged the WoFS dataset where intrastorm predictors were found to be more important than environmental predictors (Clark and Loken 2022).

For the road surface dataset, it is not surprising that temperature-based features are more valuable to the ML model than radiation-based features. However, unlike the WoFS dataset, there is little difference between the Grouped and Grouped Only results, suggesting that the road surface model is strongly dependent on the temperature-based predictors, which largely agrees with the individual importances (see Fig. 4g in Part II). Note that the two groups in the road surface dataset do not mutually account for all features. If they had, then Grouped and Grouped Only results would be identical by default.

b. Global Feature Effects

To improve our understanding of the feature rankings and the ML models, we can estimate the feature effects. For this study, we compare feature effects estimated by PD, ALE, SHAP, LIME, and tree interpreter (TI). To aid in the interpretation of the feature effects, we compute the conditional event rate per feature [i.e., \( p(y = 1 | x_i) \)]. To compute the conditional event rate, we use a Bayesian histogram method (Python package bayeshist; Hafner 2022). This method assumes a beta distributed prior [\( p(y = 1) \approx \mathcal{B} (\alpha, \beta) \)] where \( \alpha \) and \( \beta \) are shape parameters and a similar distribution for the posterior [\( p(y = 1 | n^+_i, n^-_i) \approx \mathcal{B} (\alpha + n^+_i, \beta + n^-_i) \)] where \( n^+_i, n^-_i \) are the number of positive and negative samples in the ith bin, respectively. By binning feature \( x_i \)'s values, we can compute \( \mathcal{B} \) in a series of quantiles. To keep only significant bins, the method compares each pair of neighboring bins and combines the pair if they are likely from the same event rate sample.

The measured feature effects and the event rate curve are shown for the top three features of each dataset (Fig. 8). The top features were determined based on the median feature rankings based on all methods (this ranking can be seen in Fig. 4 in Part II). The general similarity between the feature effect curves and the conditional event rate suggests that the ML models are learning appropriate relationships. By comparing against the conditional event rate we can better determine whether the learned relationships match physical intuition, which can lead to improved trust in the model. For example, higher vertical vorticity corresponds to a higher probability of a tornado (Fig. 8a) and lower surface temperature (\( T_{s fc} \)) corresponds to a higher probability of a road surface freezing (Fig. 8j). One notable outlier is the 3-5 km maximum reflectivity...
Feature rankings based on the Grouped (top row) and Grouped Only (bottom row) methods for the original road surface (first column), tornado (second column), severe wind (third column), and severe hail (last column) datasets. Grouped importance assesses how removing a group of features (jointly permuting them) reduces model performance while Grouped Only assesses how the model performs when solely relying on a group of features (i.e., all other features are jointly permuted). For the severe weather datasets, color-coding same as Fig. 5. For the road surface dataset, temperature-based are shown in green and radiation-based are shown in blue.

(Fig. 8d) where the learned relationship is opposite to the event rate trend. Composite reflectivity (Fig. 8f), which is highly correlated with 3-5 km maximum reflectivity (not shown), has a better learned relationship to the prediction. We attribute these results to the fact that when two features are highly correlated, regression models can learn opposite effects for the two features with the feature that is the stronger predictor of the target variable having the "correct" effect. These results highlight the inherent difficulties of applying explainability methods to models with physically correlated data and motivate the use of dimensionality reduction approaches to reduce the impact of correlated features (see Part II).

In terms of the correspondence between methods, ALE and SHAP tend to agree well with each other and with the event rate, while PD seriously underpredicts some feature effects. PD can have difficulty estimating the mean effect due to its inability to distinguish between the effects of correlated features. The correspondence of LIME with other methods and the event rate varies by dataset and feature. For example, LIME is similar to the other curves for the road surface dataset (Fig. 8j-l), but has weaker correspondence for higher values of vertical vorticity, hail, and 80-m wind speed in the tornado dataset (Fig. 8a-c). While ALE is designed to measure the global feature effects, SHAP is a local explainability method; the similarity between SHAP and the event rate suggests that SHAP can scale well (i.e., summarizing local explanations leads to useful global explanations). ALE and SHAP have modest disagreements on some of the features (e.g., Fig. 8a, Fig. 8b, Fig. 8e). For example, for higher values of 0-2 km vertical vorticity ALE has a higher estimated effect than SHAP, which corresponds with the higher base rate for higher vorticity values suggesting that SHAP is underestimating the global feature effect. In general, the correspondence between the methods seems largely dependent on sample size, where smaller sample sizes are associated with larger feature effect disagreement.

To summarize the disagreement between two methods, we calculated the root mean squared difference (RMSD) for all features and computed the variance-weighted average (variance in the feature effect curve). To show the differences in terms of agreement, Fig. 9 is based on 1–RMSD. Unlike the feature ranking agreement (Fig. 6), there is fairly strong agreement amongst the different methods on feature effects. This result aligns with our subjective impression of Fig. 8 that the curves correspond well with each other when the sample size is large enough. ALE, SHAP, LIME, and TI tend to agree more with each other, while PD has lower agreement with the other methods. However, PD is more consistent with other methods in the road surface datasets than in severe weather datasets (cf. Fig. 9d and Fig. 9a-c). The feature correlations in the severe weather datasets are stronger and more frequent than in the road surface dataset (correlation diagrams are shown in Figs. 1 and 2 of Part II), which possibly explains why PD is inconsistent with the other methods in the severe weather datasets.
6. Practical Advice on Model Explainability

We have demonstrated that ML explanation methods can substantially disagree in terms of feature rankings and feature effects. A significant source of disagreement is due to correlated features as distinguishing individual importance/relevance becomes an involved process. Despite these disagreements, our attempts to understand our ML models are not in vain; rather, we should approach this task with certain expectations. For example, for the datasets and models used in this study, the different feature ranking methods were in reasonable agreement on the top 10 features, but disagreed on exact rankings (Fig. 6). If we de-emphasize interpreting exact rank, then by using multiple ranking methods, we can increase our confidence about the top contributors to our model. One such approach is demonstrated in Part II where we compute the median feature ranking from all methods and display the IQR as a measure of ranking uncertainty. By incorporating uncertainty information, we can improve our confidence and trust in the output from the various explainability methods.

In most cases, the different feature effect methods had high agreement (Fig. 8 and Fig. 9). Disagreements were largely confined to poorly sampled regions where we should be especially cautious about interpreting any explanation method. Fig. 10 shows the method-average feature effect for composite reflectivity for the severe hail model. There is decent consistency amongst the methods for low and moderate composite reflectivity values, but effect uncertainty increases as the sample size decreases. The uncertainty does start to increase prior to diminishing samples for composite reflectivity, which is related to the limited sample sizes of the other features (not shown). We can still conclude that higher composite reflectivity values increase the likelihood of severe hail, but we must also acknowledge that the magnitude of this effect becomes uncertain at high reflectivity values.
7. Conclusions

Motivated by the increasing interest in explaining machine learning models, the first part of this two-part study synthesizes recent research on many explainability methods. This includes distinguishing explainability from interpretability (Fig. 1), local versus global explainability (cf. section 4a and section 4f), and feature importance versus feature relevance (section 4a.1). We demonstrate visualizations of the different explainability methods, how to interpret them, and provide a comprehensive Python package [Flora and Handler 2022] to enable other researchers to use these methods. Summaries of the key ideas for each method are provided in Fig. 2 and Table 2.

The growing number of ML model explainability tools can make it difficult to select the best method to explain a particular dataset or model. We know that no single method can describe all aspects of model explainability, but the degree to which explanations tend to disagree with each other and how much the validity of the different methods varies has not been thoroughly explored. We have therefore reviewed various explanation methods and analyzed the differences between for global feature rankings and global feature effects. To generalize the results, we applied the explainability methods to two very different meteoro-
logical datasets: a convection-allowing model dataset for severe weather prediction, and a nowcasting dataset for sub-freezing road surface prediction. We conclude the following:

- The feature ranking methods explored in this study tend to agree on the top features ($N=10$), but substantially disagree on specific ranks. Given the large number of correlated features in our data sets, this result suggests that correlations affect the ranking of top features without radically changing the top features set. This hypothesis is further supported by consistently high agreement between backward single-pass permutation importance and logistic regression coefficient-based rankings.

- The overall disagreement between all the feature ranking methods for the top features was similar to the average disagreement between the feature importance and feature relevance methods. This suggests that the disagreement is not solely attributable to the feature ranking methods being designed for different tasks.

- Grouped feature importance (Au et al. 2021) can mitigate issues associated with correlated features and may provide clearer interpretations than individual importances.

- The different feature effect estimations had high agreement though PD was least consistent with other methods. Method disagreements were largely due to small sample sizes.

- Like global feature rankings, the feature attribution methods had high agreement on the top features and less agreement on specific ranks. Although the tree interpreter has inconsistency issues (Lundberg et al. 2020), its similarity to SHAP and its much faster runtime suggest that it should be further explored in future studies.

- Tree interpreter (TI) is a relatively unexplored method, but it is being leveraged in the atmospheric science community (Loken et al., 2022). TI has inconsistency issues (Lundberg et al., 2020) and we found it ranked features similar to Gini importance, which has known issues with correlated features (McGovern et al., 2019). However, as a global feature effect method, TI had nearly perfect agreement with SHAP. Given these mixed results, we recommend it be explored further.

This study was one of the first to quantify differences in the various explanation methods, but there were limitations. First, a common criticism of interpretability and explainability is that there is no objective definition of these terms (Molnar et al., 2020). The fields related to improving ML model understanding — interpretable ML and explainable artificial intelligence — are rapidly developing and not yet mature, and so it is not surprising that the nomenclature is still evolving. In this paper, we have provided clear definitions of interpretability and explainability, as well as a brief summary of related terms. Although we did not provide quantitative definitions, we believe that such definitions are not required to quantify important aspects of explainability like ground-truth faithfulness, predicted faithfulness, stability and/or fairness (Agarwal et al., 2022). In recent research, benchmark datasets where the ground truth is known are being used to evaluate explanation methods for deep learning (Mamalakis et al., 2021), and in Part II and Covert et al. (2020), experiments are performed to measure the correspondence between feature importance scores and model performance. Second, a key component of model explainability, feature interactions (i.e., the impact on a feature’s effect due to the relationship with another feature), was not explored in this study. After establishing the important predictors and their first-order effects, it is useful to assess the existence and strength of the relationships between the predictors. For many real-world problems, we know that the effect of two or more predictors working together can contribute significantly to explaining a phenomenon and the performance of the ML model. Modeling feature interactions is touted as one strength of ML models, but limited work has been done to measure them. Friedman and Popescu (2008) have developed the most comprehensive set of metrics for evaluating feature interactions, including various statistics that describe how much second-order effects depart from the additive effect between two predictors. However, feature interaction explainability methods are often computationally intractable for more than two features and distinguishing the significance of second- or higher-order interactions from noise is prohibitively difficult. Lastly, we need to improve our understanding of how disagreements between explanation methods impact end user trust and the biases that may develop from a developer or end user selecting certain methods. For example, Krishna et al. (2022) found that in practice, practitioners often rely on heuristics when choosing explainability methods. In light of these limitations of extant research, we recommend that more concerted effort be devoted to improving our understanding of explainability methods, their strengths and limitations, and their applicability.
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Data availability statement. The experimental WoFS ensemble forecast data and road surface dataset used in this study are not currently available in a publicly accessible repository. However, the data and code used to generate the results here are available upon request from the authors. The explainability methods were computed and visualized using the scikit-explain python package (Flora and Handler 2022) developed by Dr. Montgomery Flora and Shawn Handler. The python scripts used to generate the figures in Part I and II are available at https://github.com/monte-flora/compare-explain-methods.

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