Abstract
We recommend using a model-centric, Boolean Satisfiability (SAT) formalism to obtain useful explanations of trained model behavior, different and complementary to what can be gleaned from LIME and SHAP, popular data-centric explanation tools in Artificial Intelligence (AI). We compare and contrast these methods, and show that data-centric methods may yield brittle explanations of limited practical utility. The model-centric framework, however, can offer actionable insights into risks of using AI models in practice. For critical applications of AI, split-second decision making is best informed by robust explanations that are invariant to properties of data, the capability offered by model-centric frameworks.

Introduction
Artificial Intelligence (AI)-driven decision making is increasingly used to support human decisions. In practice, the adoption of intelligent systems hinges on the ability of users to understand why a prediction was generated and how to ensure a desired output. Trust and transparency in AI is essential in high-stakes application domains, including healthcare, counter-terrorism, management of nuclear facilities, etc., where wrong decisions may bear grave consequences. Lack of trust in AI systems is often due to lack of their understanding or interpretability (Reig et al. 2018), especially when safety is at risk (Morales et al. 2019).

Common explanatory tools, including Local Interpretable Model-Agnostic Explanations (LIME) (Ribeiro, Singh, and Guestrin 2016) and Shapley Additive Explanations (SHAP) (Lundberg and Lee 2017), are data-centric. They assess contributions of individual attribute values to predictive performance of the models. Insights gleaned from such analyses are primarily of confirmatory value; a clinician can confirm that the model pays attention to similar features that she would consider in analyzing her current patient. However, these tools can be brittle, hide biases, and do not provide useful diagnostic information about safety of the models.

We define brittleness of a model by its inability to adapt or generalize to conditions outside of a narrow set of assumptions. Britteness of a model could be lethal in safety-critical domains since an anomalous data point could be classified incorrectly. Further decreasing trust in the models. Alternatively, the explanations given by these models are of feature importance and do not inform the user what would be needed to change the outcome of the model, also dissuading people from using them. We define feature importance in the rest of the paper as the measure of an individual contribution of the corresponding feature for a the classification performance of the model (Saarela and Jauhiainen 2021).

Conversely, formal methods can be used to mathematically prove desired reliability properties of the models, eliminating human biases and statistical errors from the process (Gisolfi et al. 2021b).

We extend these methods to provide minimal-distance counterfactuals that find minimal changes to attribute values needed to cause the model to change its prediction. This analysis can expose limitations of models and data used to train them, enabling development of provably robust AI-driven decision support systems.

Related Work
Model interpretability is currently used to bridge the lack of trust in models in machine learning. It can be approached by model: intrinsic or post-hoc, by scope: local or global, or by method: model-specific or model-agnostic. They have the common goal to present concise and intelligible information to a human user that empowers them to determine whether or not the system is behaving in a safe manner. LIME and SHAP are among the most popular explainable methods. Both are post-hoc, local and model-agnostic. Nevertheless they come with a variety of drawbacks. Some of the disadvantages of these methods are that they require a human to perform a verification task to certify if the model behaves as expected, nonetheless, the process is error prone. Moreover, post-hoc explanation techniques might be unstable and unreliable (Lipton 2018). Ghorbani et al. show that some explanation techniques can be highly sensitive to small perturbations in the input even though the underlying classifier’s predictions remain unchanged (Ghorbani, Abid, and Zou 2019).

The LIME method interprets individual model predictions based on linear assumptions and locally approximating the model around a given prediction but the correct definition of the neighborhood is unknown (Ribeiro, Singh, and Guestrin 2016). LIME requires of human input to determine
the correct kernel setting based on whether the explanations are coherent; however, this process is susceptible to mistakes (Molnar 2019). Alvarez-Melis and Jaakkola showed that the explanations were very unstable given that for two very close points they varied greatly in a simulated setting and were often inconsistent with each other (Alvarez-Melis and Jaakkola 2018).

The SHAP method is derived from Shapley values in game theory, where they describe the contribution of each team player in a collaborative environment. In machine learning, it works by assigning each feature an importance value for a particular prediction (Lundberg and Lee 2017). One of the distinguishing factors of SHAP is that the prediction is fairly distributed among features. However, some disadvantages according to Molnar (Molnar 2019) are that users prefer selective explanations since an overwhelming number of features could create confusion among users. Since Shapley values return a value per feature, no conclusion can be made regarding a change in prediction for changes in the input. Similarly to many permutation-based interpretation methods, the Shapley value method can’t classify unrealistic data instances when features are correlated. This works however if features are independent since when a feature is missing it is then marginalized. This is achieved by sampling values from the feature’s marginal distribution.

An explanation can be viewed from a constraint satisfaction problem perspective; can a model satisfy all constraints, and if not, why not? Satisfiability-based formal methods, i.e. SAT, SMT, MILP, provide these types of proofs for abstract mathematical representation of trained models. The explanations are instances of constraint satisfaction problems. Formal methods are on increasing interest in providing explanations for model behaviors (Karimi et al. 2020). Formal methods have also been used to assess the quality of explainable AI methods (Narodytska et al. 2019).

Providing explanations for model behavior under ideal conditions is still a significant challenge, however, one could argue that there is even higher imperative to provide explanations for model behavior under tough conditions. For instance, providing an explanation that illustrates a similarity between model predictions on two similar samples of data will not suffice when one of the data points in question is anomalous and no sufficiently similar neighbors exist. Explanations like the ones provided by LIME and SHAP are too brittle and thus should not be used for safety-critical applications.

**Methodology**

**Data and Models.** We use the publicly available Breast Cancer Wisconsin (Diagnostic) dataset (Dua and Graff 2017). It contains 30 numeric features which we standardized by removing the mean and scaling to unit variance. We explain Scikit-learn (Pedregosa et al. 2011) random forests, trained with a 50% train/test split. Our model consists of ten decision trees of the maximum depth of ten.

**Experiments.** We first created explanations for the same data point following the methods of LIME, SHAP and SAT, which are described in detail next. LIME (Ribeiro, Singh, and Guestrin 2016) provides local explanations of model predictions global by creating an approximation near the input. Feature importance can be inferred from this local linear approximation by looking at the feature weights. For our experiments, we mirrored the feature importance experiments of the LIME repository.

SHAP values (Lundberg and Lee 2017) provide the additive feature importance measure that adheres to local accuracy, missigness, and consistency.

$$\phi_f(x) = \sum_{z' \subseteq x'} |z'|!(M - |z'| - 1)!/M! \left[ E[f(z)|z_s] - f(z\setminus i) \right]$$

Where M is the number of simplified input features, |z’| is the number of non-zero entries in z’, and z’ \subseteq x’ represents all z’ vectors where the non-zero entries are a subset of the non-zero entries in x’, and S is the set of non-zero indexes in z’. The SHAP explanations were generated from code by Lundberg et al. (2018).

Our proposed framework uses the logical encoding strategy from (Gisolfi et al. 2021b), and extends those methods to find the minimal distance counterfactual explanation as detailed in Algorithm [1]. To find minimal distance counterfactual explanations, we start with a data points and a local neighborhood in which to search for another data point to which the model assigns a different predicted label. If such a point exists, a satisfying assignment detailing the model state for the two points is returned, otherwise, we increase the size of the local neighborhood and search again. This process continues until a counterfactual is found. The relevant differences between the two points which form the counterfactual can be revealed by finding all differences within the satisfying assignments. We only report encoded

![Figure 1: Decision Surface of a Decision Tree [left] and Random Forest [right]](image)

![Figure 2: Illustration of a minimal distance counterfactual.](image)
Figure 3: SHAP Explanation- Force Plot

Algorithm 1: Minimal distance counterfactual

1. $M \leftarrow$ trained random forest model
2. $x \leftarrow$ data point
3. $\delta \leftarrow$ initial local neighborhood
4. $\phi \leftarrow \text{Encode}(M, x, \delta)$ \cite{Gisolfi et al. 2021b}
5. while $\phi$ is UNSAT do
6. $\delta \leftarrow \delta + 1.01$
7. $\phi \leftarrow \text{Encode}(M, x, \delta)$
8. $x' \leftarrow$ counterexample from SAT assignment of $\phi$
9. return $x' - x$, the counterfactual

We studied the stochasticity of feature importance in the LIME \cite{Ribeiro, Singh, and Guestrin 2016} and SHAP \cite{Lundberg and Lee 2017} frameworks. Using those tools, we returned the $n$ most important features where $n = 1...30$. We iterated over all test data and recorded the $n$ most important features. We then evaluated the probability that each feature was one of the most influential variables in the test dataset when $n$ was set. We show feature importance attribution plots for LIME and SHAP where three features that were consistently picked as important for both are displayed in the bottom rows of Fig. 6 and the graphs for the rest of the features can be found in the Appendix figures 8 and 9. The horizontal axis in each of these plots shows the index of the feature in the importance ranking and the vertical axis shows the estimated probability of the feature attaining such rank. Generally, truly important features would have this probability raise quickly as a function of the rank index, and stay high. E.g., in the example shown in Fig. 6, feature mean concave points appears slightly more important than worst concave points and worst concavity.

We explored explanations generated by SAT. Firstly, we looked at the 17 points in the test data that were misclassified. Each explanation had a set of features that needed to be changed to flip the prediction. We iterated over all the explanations and recorded the percentage change over the range of values of each feature that would be required to modify the prediction, and visualized their distributions in kernel density estimation plots. Then we repeated the same procedure with all the correctly classified points. The top row of Fig. 6 shows these characteristics for the same three features previously mentioned, the rest can be found in the Appendix figure 7. Model-centric explanation suggests that fixing these 17 errors will require increasing the value of worst concavity by 5-10%. The other two features do not show such a consistent recipe for error correction, even though LIME suggests they are important.

Analysis

The LIME explanations as shown in Figure 4 demonstrate feature attributions [left] where the most influential is at the top and current values [right] for the breast cancer mass. Feature importance attenuates quickly down the list, and attributes at the bottom have little relevance in the explanation at hand. An interesting observation is that the most relevant features in this particular explanation wind up describing the opposite of the predicted class.

Fig. 5 shows an example model-centric explanation generated by our framework for one query. The current feature value for the suspected breast cancer mass is denoted in bold while the value it would need to be modified to is shown in italics. The left part of the graph shows the seven attribute changes required by the model to change its prediction, and the right part shows the percentage change of value of each feature needed to cause such change.
Figure 5: SAT Explanation - Counterfactual. Our explanation presents a set of the smallest changes necessary to change the model output. The bar graph shows the percent change that is required along each attribute to change the output of the model.

Figure 6: Aggregate summary of SAT counterfactual explanations [first] in addition to feature attribution for LIME [second] and SHAP [third].

Figure 5: SAT Explanation - Counterfactual. Our explanation presents a set of the smallest changes necessary to change the model output. The bar graph shows the percent change that is required along each attribute to change the output of the model. This result has multiple potentially useful consequences. One example is confirmatory analysis of a prediction made by an AI-driven tool used by a clinician to help her diagnose a patient. If only a small change of one of the features, reflecting, e.g., some laboratory test result, can flip the prediction, the doctor may consider repeating the test to ascertain its outcome, or order a more precise test. Similarly, when designing AI-based decision systems that operate on measurements collected with noisy sensors with known sensor noise models, the design engineer may use the proposed analysis to verify that the expected magnitude of sensor noise does not exceed the range of robustness revealed for the corresponding feature of the AI model.

To accomplish the second task type, we can leverage SAT score characteristics as shown in the top row of Fig. 6 focusing on the correctly classified test data. Features mean concave points and worst concave points are highly important according to LIME and SHAP, but their SAT score distribution characteristics show large probability masses in the range of very small percentage changes needed to invert the model prediction. The physician and the engineer from our examples should be very careful and, if possible, measure values of these features with very high accuracy. On the other hand, features that would need greater changes to modify their predictions such as worst concavity, leaves our engineer with some margin of error, because non-trivial changes of its value are required to impact the model prediction. The engineer can compare this margin with the characteristics of various sensors that can be used to measure the particular property of interest, and choose the least expensive sensor whose error model safely fits within the identified slack of robustness of the AI model.

Concentrated distributions show that the same magnitude change is present among a group of explanations for multiple data points. Some features may cause more fragility in the system than others because their percent change concentrates in the low range of values i.e. as observed in mean concave points, while for worst concavity a large change in the observations would be needed to break robustness thus the latter is more reliable. If the misclassified points have a percent change smaller than the rest of the points, it would mean that changing the features would most likely result in the improvement of the model. While this trend is prevalent in our dataset, a few counterexamples exist for which changing their values would most likely decrease the performance of the model.

Conclusion

Model-centric formal methods provide useful capabilities complementary to the existing explanatory analysis tools. They are based on mathematical logic and yield provable results that can be verified exactly, as opposite to the prevalent statistical methods that produce results with margins of confidence. We envision beneficial use of these methods at all stages of life of AI systems: from design to field application.

Limitations and Future Work

A limitation of the current work is that the implemented verification framework does not take into account the mutability of feature. Some features, such as age, cannot be changed, making the counterfactuals less actionable. This is a limitation of the implementation alone, and previous work has addressed this by making certain features protected (Gisolfi et al. 2021a). In future work we hope to further validate these
methods by applying them to a variety of datasets. Additionally, these methods should be validated with human studies, similar to those found in (Ribeiro, Singh, and Guestrin 2016).

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Appendix

Figure 7: Aggregate summary of SAT counterfactual explanations
Figure 8: Probability of feature importance in LIME when n features are chosen.
Figure 9: Probability of feature importance in SHAP when n features are chosen.