A Survey of Model Interpretation Tools with Practical Recommendations

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Abstract

This paper analyzes several debugging and explanatory approaches beyond the error measures and assessment plots typically used to interpret machine learning models. The approaches: decision tree surrogate models, individual conditional expectation (ICE) plots, local interpretable model-agnostic explanations (LIME), partial dependence plots, Shapley explanations vary in terms of scope (i.e. global vs. local), fidelity (i.e. the exactness of generated explanations), and suitable application domains. Along with descriptions of the techniques, findings regarding explanation trustworthiness and practical guidance for usage are also presented.

1. Introduction

While understanding and trusting models and their results is a hallmark of good (data) science, model interpretability is a legal mandate in the regulated verticals of many major industries. Moreover, scientists, physicians, researchers, analysts, and humans in general have the need to understand and trust models and modeling results that affect their work and their lives. Today many organizations and individuals are embracing machine learning but what happens when people need to explain these impactful, complex technologies to one-another or when these technologies inevitably make mistakes?

- **What is interpretation?** The ability to explain or to present in understandable terms to a human. (Doshi-Velez & Kim, 2017)
- **What is a good interpretation?** "When you can no longer keep asking why." (Gilpin et al., 2018)
- **Why should you care?**
  - Understanding of an impactful and quickly expanding set of technologies.
  - Addressing accidental or intentional discrimination.
  - Preventing malicious hacking and adversarial attacks.
  - Enabling regulatory compliance and increased financial margins.

- **Spaces**.
  - The input features come from a set $\mathcal{X}$ contained in a P-dimensional input space (i.e. $\mathcal{X} \subset \mathbb{R}^P$).
  - The output responses come from a set $\mathcal{Y}$ contained in a C-dimensional output space (i.e. $\mathcal{Y} \subset \mathbb{R}^C$).

- **Dataset**. A dataset $\mathbf{D}$ consists of N tuples of observations: $[(\mathbf{x}^{(0)}, \mathbf{y}^{(0)}), (\mathbf{x}^{(1)}, \mathbf{y}^{(1)}), \ldots, (\mathbf{x}^{(N-1)}, \mathbf{y}^{(N-1)})], \mathbf{x}^{(i)} \in \mathcal{X}, \mathbf{y}^{(i)} \in \mathcal{Y}$.
  - The input data $\mathbf{X}$ is composed of the set of row vectors $\mathbf{x}^{(i)}$.
    * let $\mathcal{P}$ be the set of features $\{X_0, X_1, \ldots, X_{P-1}\}$, where $X_j = \left[x_j^{(0)}, x_j^{(1)}, \ldots, x_j^{(N-1)}\right]^T$.
    * then each i-th observation denoted as $\mathbf{x}^{(i)} = \left[x_0^{(i)}, x_1^{(i)}, \ldots, x_{P-1}^{(i)}\right]$ is an instance of $\mathcal{P}$.

2. Surrogate DT

- Given a learned function g and set of predictions $g(\mathbf{X})$, a surrogate DT can be trained: $\mathbf{X}, g(\mathbf{X}) \xrightarrow{\mathcal{A}_{\text{surrogate}}} h_{\text{tree}}$.
- h_{tree} displays a low-fidelity, high-interpretability flow chart of g's decision making process, and important features and interactions in g.

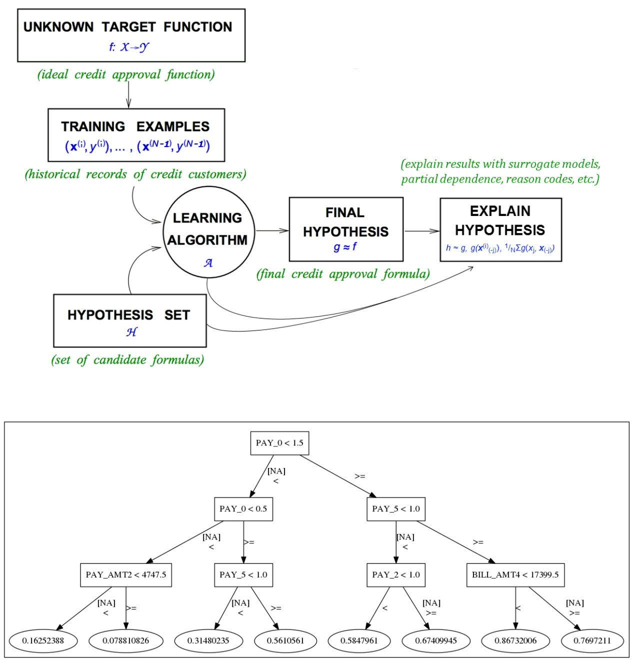

Figure 1. h_{tree} for Taiwanese credit card data (Lichman, 2013), and for machine-learned GBM response function g.

- Always use error measures to assess the trustworthiness of h_{tree}.
- Prescribed methods (Craven & Shavlik, 1996); (Bastani et al., 2017) for training h_{tree} do exist. In practice, straightforward cross-validation approaches are typically sufficient.
- Comparing cross-validated training error to traditional training error can give an indication of the stability of the single tree model, h_{tree}.
- (Hu et al., 2018) use local linear surrogate models, h_{GLM}, in h_{tree} leaf nodes to increase overall surrogate model fidelity while also retaining a high degree of interpretability.

3. PD and ICE

- Following (Friedman et al., 2001) a single feature $X_j \in \mathbf{X}$ and its complement set $X_{(-j)} \in \mathbf{X}$ (where $X_j \cup X_{(-j)} = \mathbf{X}$) is considered.
- $\text{PD}(X_j, g)$ for a given feature X_j is estimated as the average output of the learned function g when all the components of X_j are set to a constant $x \in \mathcal{X}$ and $X_{(-j)}$ is left untouched.
- $\text{ICE}(X_j, \mathbf{x}^{(i)}, g)$ for a given observation $\mathbf{x}^{(i)}$ and feature X_j is estimated as the output of the learned function g when $x_j^{(i)}$ is set to a constant $x \in \mathcal{X}$ and $\mathbf{x}^{(i)} \in X_{(-j)}$ are left untouched.
- PD and ICE curves are usually plotted over some set of interesting constants $x \in \mathcal{X}$.

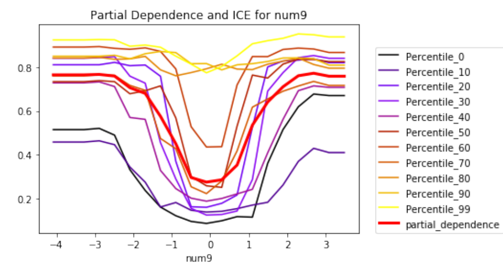

Figure 2. PD and ICE curves for $X_j = \text{num}_9$, for known signal generating function $f(\mathbf{X}) = \text{num}_1 * \text{num}_4 + |\text{num}_8| * \text{num}_9^2 + e$, and for machine-learned GBM response function g.

Overlaying PD and ICE curves is a succinct method for describing global and local prediction behavior and can be used to detect interactions. (Goldstein et al., 2015)

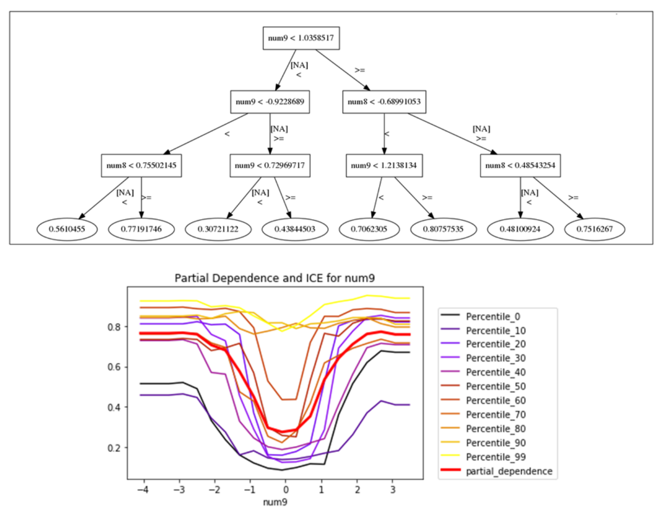

Figure 3. Surrogate DT, PD, and ICE curves for $X_j = \text{num}_9$, for known signal generating function $f(\mathbf{X}) = \text{num}_1 * \text{num}_4 + |\text{num}_8| * \text{num}_9^2 + e$, and for machine-learned GBM response function g.

Combining Surrogate DT models with PD and ICE curves is a convenient method for detecting, confirming, and understanding important interactions.

4. LIME

(Ribeiro et al., 2016) defines LIME for some observation $\mathbf{x} \in \mathcal{X}$:

$$\arg\max_{h \in \mathcal{H}} \mathcal{L}(g, h, \pi_{\mathbf{X}}) + \Omega(h) \tag{1}$$

Here g is the function to be explained, h is an interpretable surrogate model of g, often a linear model h_{GLM}, $\pi_{\mathbf{X}}$ is a weighting function over the domain of g, and $\Omega(h)$ limits the complexity of h.

Typically, h_{GLM} is constructed such that

$$\mathbf{X}^{(*)}, g(X^{(*)}) \xrightarrow{\mathcal{A}_{\text{surrogate}}} h_{\text{GLM}} \tag{2}$$

where $\mathbf{X}^{(*)}$ is a generated sample, $\pi_{\mathbf{X}}$ weighs $\mathbf{X}^{(*)}$ samples by their Euclidean similarity to $\mathbf{x}$, local feature importance is estimated using $\beta_j x_j$, and L_1 regularization is used to induce a simplified, sparse h_{GLM}.

- LIME is ideal for creating low-fidelity, highly interpretable explanations for non-DT models and for neural network models trained on unstructured data, e.g. deep learning.
- Always use regression fit measures to assess the trustworthiness of LIME explanations.
- LIME can be difficult to deploy, but there are highly deployable variants. (Hu et al., 2018); (Hall et al., 2017)
- Local feature importance values are offsets from a local intercept.
  - Note that the intercept in LIME can account for the most important local phenomena.
  - Generated LIME samples can contain large proportions of out-of-range data that can lead to unrealistic intercept values.
- To increase the fidelity of LIME explanations, try LIME on discretized input features and on manually constructed interactions.
- Use cross-validation to construct standard deviations or even confidence intervals for local feature importance values.
- LIME can fail, particularly in the presence of extreme nonlinearity or high-degree interactions.

5. Tree Shap

Shapley explanations are a class of additive, consistent local feature importance measures with long-standing theoretical support, (Lundberg & Lee, 2017). For some observation $\mathbf{x} \in \mathcal{X}$, Shapley explanations take the form:

$$\phi_0 + \sum_{j=0}^{j=\mathcal{P}-1} \phi_j \mathbf{x}'_j \tag{3}$$

Here $\mathbf{x}' \in \{0,1\}^{\mathcal{P}}$ is a binary representation of $\mathbf{x}$ where 0 indicates missingness. Each ϕ_j is the local feature importance value associated with x_j.

- Calculating Shapley values directly is typically infeasible, but they can be estimated in different ways.
- Tree Shap is a specific implementation of Shapley explanations that leverages DT structures to disaggregate the contribution of each x_j to $g(\mathbf{x})$ in a DT or DT-based ensemble model. (Lundberg et al., 2018)
- Tree Shap is ideal for high-fidelity explanations of DT-based models, perhaps even in regulated applications.
- Local feature importance values are offsets from a global intercept.
- LIME can be constrained to become Shapley explanations, i.e. kernel shap.
- A similar, popular method known as *treeinterpreter* appears untrustworthy when applied to GBM models.

6. Recommendations

- Monotonically constrained XGBoost, Surrogate DT, PD and ICE plots, and Tree Shap are a direct and open source way to create an interpretable nonlinear model.
- Global and local explanatory techniques are often necessary to explain a model.
- Use simpler low-fidelity or sparse explanations to understand more accurate and complex high-fidelity explanations.
- Seek consistent results across multiple explanatory techniques.
- Methods relying on generated data are sometimes unpalatable to users. They want to understand *their* data.

- Surrogate models can provide low-fidelity explanations for model mechanisms in original feature spaces if g is defined to include feature extraction or engineering.
- To increase adoption, production deployment of explanatory methods must be straightforward.

7. Software

Comparison of Explanatory Techniques on Simulated Data:
https://github.com/h2oai/mli-resources/tree/master/lime_shap_treeint_compare

In-depth Explanatory Technique Examples:
https://github.com/jphall663/interpretable_machine_learning_with_python

"Awesome" Machine Learning Interpretability Resource List:
https://github.com/jphall663/awesome-machine-learning-interpretability

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