Guidelines for Responsible Use of Explainable Machine Learning

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Contents

What is explainable machine learning (ML)?

"A collection of visual and/or interactive artifacts that provide a user with sufficient description of the model behavior to accurately perform tasks like evaluation, trusting, predicting, or improving the model."

— Sameer Singh, *UCI*

Variously defined along with aliases or similar concepts:

- "Towards a Rigorous Science of Interpretable Machine Learning" (Doshi-Velez and Kim [8])
- "Explaining Explanations" (Gilpin et al. [13])
- "A Survey Of Methods For Explaining Black Box Models" (Guidotti et al. [16])
- "The Mythos of Model Interpretability" (Lipton [23])
- *Interpretable Machine Learning* (Molnar [26])
- "Interpretable Machine Learning: Definitions, Methods, and Applications" (Murdoch et al. [27])
- "Challenges for Transparency" (Weller [39]).

What is explainable ML?

What do ***I*** mean by explainable ML?

Mostly post-hoc techniques used to enhance ***understanding*** of trained model mechansims and predictions, e.g. ...

- **Direct measures of global and local feature importance**:
  - Gradient-based feature attribution (Ancona et al. [2])
  - Shapley values (Lundberg and Lee [25])
- **Global and local surrogate models**:
  - Decision tree variants (Bastani, Pu, and Solar-Lezama [6], Craven and Shavlik [7])
  - Anchors (Ribeiro, Singh, and Guestrin [28])
  - Local interpretable model-agnostic explanations (LIME) (Ribeiro, Singh, and Guestrin [29])
- **Global and local visualizations of trained model predictions**:
  - Accumulated local effect (ALE) (Apley [4])
  - Partial dependence (Friedman, Hastie, and Tibshirani [11])
  - Individual conditional expectation (ICE) (Goldstein et al. [14])

Why explainable ML?

Responsible Use of Explainable ML can enable:

- Human learning from machine learning
- Human appeal of automated decisions
- Regulatory compliance
- White-hat/red-team hacking

Misuse and Abuse of Explainable ML can enable:

- Model and data stealing (Tramèr et al. [36], Shokri et al. [34], Shokri, Strobel, and Zick [33])
- False justification for harmful black-boxes, e.g. "fairwashing" (Aïvodji et al. [1], Rudin [30])

Proposed Guidelines for Responsible Use

Explainable ML is already in-use: numerous open source[†] and commercial packages[‡] are available today.

Best-practices are needed to prevent misuse and abuse. So, four basic guidelines are proposed here:

- Use explainable ML to enhance understanding.
- Learn how explainable ML is used for nefarious purposes.
- Augment surrogate models with direct explanations.
- Use highly transparent mechanisms for high stakes applications.

[†] See: https://github.com/jphall663/awesome-machine-learning-interpretability

[‡] For instance Datarobot, H2O Driverless AI, SAS Visual Data Mining and Machine Learning, Zest AutoML

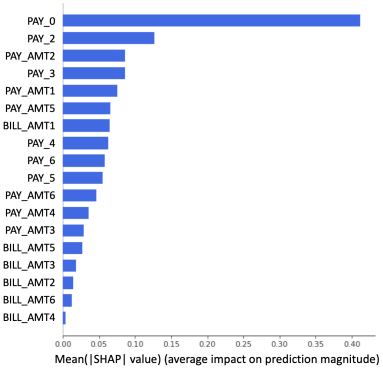
Use Explainable ML to Enhance Understanding.

Explanations enhance understanding directly, and increase trust as a side-effect.

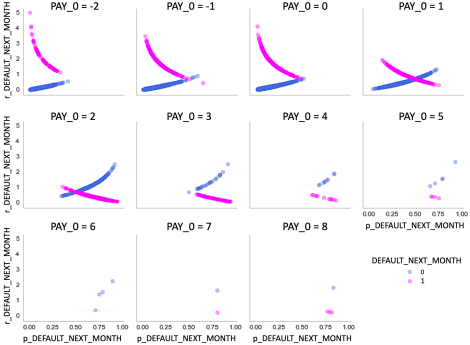
Models can be understood and not trusted, and trusted but not understood.

Explanations alone are neither necessary nor sufficient for trust.

Understanding Without Trust



g_{mono} monotonically-constrained probability of default (PD) classifier trained on the UCI credit card dataset over-emphasizes the most important feature, a customer's most recent repayment status, PAY_0 [21].



g_{mono} also struggles to predict default for favorable statuses, $-2 \leq \texttt{PAY\_0} < 2$, and often cannot predict on-time payment when recent payments are late, $\texttt{PAY\_0} \geq 2$.

Trust Without Understanding

Years before reliable explanation techniques were widely acknowledged and available, black-box predictive models, such as autoencoder and MLP neural networks, were used for fraud detection in the financial services industry [15]. When these models performed well, they were trusted.[§] However, they were not explainable or well-understood by contemporary standards.

[§]For example: https://www.sas.com/en_ph/customers/hsbc.html, https://www.kdnuggets.com/2011/03/sas-patent-fraud-detection.html.

Learn How Explainable ML is Used for Nefarious Purposes

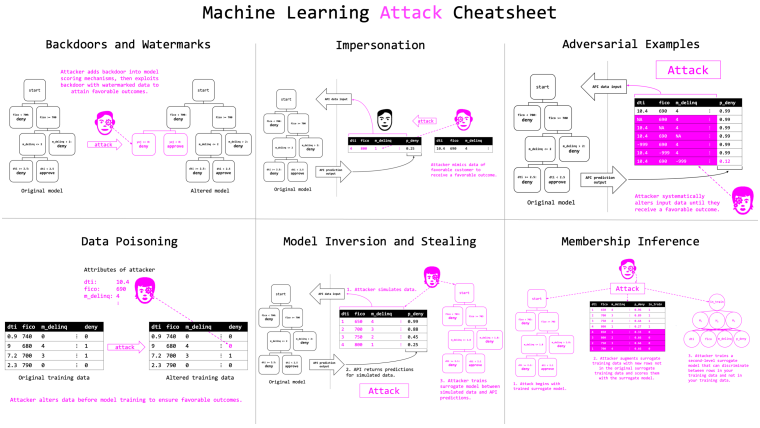
When unintentionally misused, explainable ML can act as a faulty-safeguard for a potentially harmful black-box.

When intentionally abused, explainable ML can be used for:

- Hacking of data, models, or other intellectual property.
- *Fairwashing*, to mask the sociological biases of a discriminatory black-box.

ML Hacking

Many ML hacks use, or are exacerbated by, explainable ML techniques.[¶]



[¶] See https://github.com/jphall663/secure_ML_ideas for full size image and more information.

White-hat Attacks

The flip-side of the dark side is community oversight of black-boxes.

Recent high profile analyses of commercial black-boxes, Propublica and COMPAS and Gendershades and Rekognition, can be viewed as white-hat attacks (model stealing, adversarial examples) on proprietary black-boxes.‖

‖This presentation makes no claim on the quality of the analysis in Angwin et al. (2016), which has been criticized, but is simply stating that such cracking is possible [3], [10].

Explanation ***is Not*** a Front Line Fairness Tool

Use fairness tools, e.g. ...

- Disparate impact testing (Feldman et al. [9])
- Reweighing (Kamiran and Calders [18])
- Reject option based classification (Kamiran, Karim, and Zhang [19])
- Adversarial de-biasing (Zhang, Lemoine, and Mitchell [41])
- aequitas, AIF360, Themis, themis-ml

... for fairness tasks: bias testing, bias remediation, and to establish trust.

Explanations can be used to understand and augment such results.

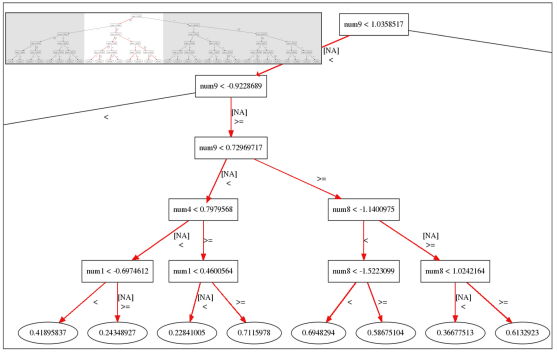
Surrogate Models

Models of models, or surrogate models, can be helpful explanatory or modeling tools, but they are usually approximate, low-fidelity explainers.

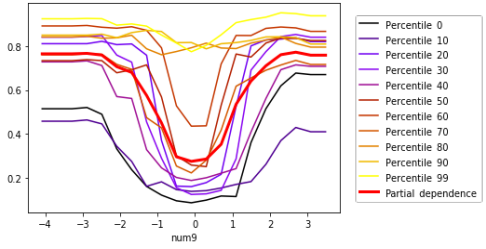
Much work in explainable ML has been directed toward improving the fidelity and usefulness of surrogate models (e.g., Bastani, Kim, and Bastani [5], Bastani, Pu, and Solar-Lezama [6], Craven and Shavlik [7], Hu et al. [17], Vaughan et al. [38])

Many explainable ML techniques have nothing to do with surrogate models!

Augment Surrogate Models with Direct Explanations



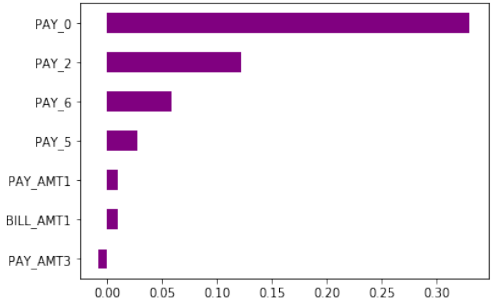
Naïve $h_{\textbf{tree}}$, *a surrogate model*, forms an approximate overall flowchart for the explained model, $g_{\textbf{GBM}}$.



Partial dependence and ICE curves generated *directly from the explained model*, $g_{\textbf{GBM}}$.

h_{tree} displays known interactions in $f = X_{\text{num1}} * X_{\text{num4}} + |X_{\text{num8}}| * X_{\text{num9}}^2$ for $\sim -0.923 < X_{\text{num9}} <\sim 1.04$. Modeling of the known interaction between X_{num9} and X_{num8} in f by g_{GBM} is confirmed by the divergence of partial dependence and ICE curves for $\sim -1 < X_{\text{num9}} <\sim 1$.

Augment LIME with Direct Explanations



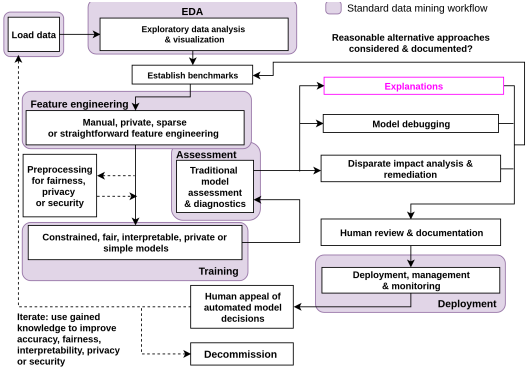
Locally-accurate Shapley contributions for a high risk individual's probability of default as predicted by a simple decision tree model, $g_{\mathbf{tree}}$. See slide 19 for a directed graph representation of $g_{\mathbf{tree}}$.

$h_{\mathbf{GLM}}$ Feature	$h_{\mathbf{GLM}}$ Coefficient
PAY_0 == 4	0.0009
PAY_2 == 3	0.0065
PAY_5 == 2	−0.0006
PAY_6 == 2	0.0036
BILL_AMT1	3.4339e−08
PAY_AMT1	4.8062e−07
PAY_AMT3	−5.867e−07

Coefficients for a local linear interpretable model, $h_{\mathbf{GLM}}$, with an intercept of 0.77 and an R^2 of 0.73., trained between the original inputs and predictions of $g_{\mathbf{tree}}$ for a segment of the UCI credit card dataset with late most recent repayment statuses, $\mathbf{X}_{PAY\_\mathbf{0>1}}$.

Because h_{GLM} is relatively well-fit and has a logical intercept, it can be used along with Shapley values to reason about the modeled average behavior for risky customers and to differentiate the behavior of any one specific risky customer from their peers under the model.

Use Highly Transparent Mechanisms for High Stakes Applications



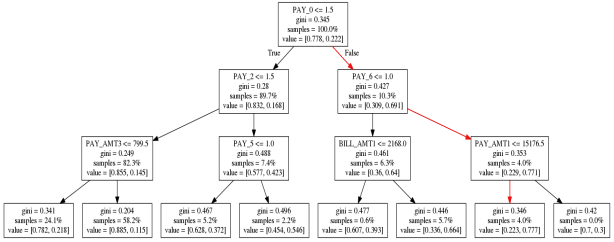
A diagram of a proposed low risk ML workflow in which explanations (highlighted in fuschia) are used along with interpretable or white-box models, disparate impact analysis and remediation techniques, and other review and appeal mechanisms to create a fair, accountable, and transparent ML system.

Interpretable Models

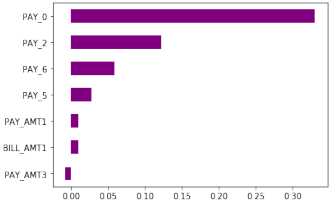
Many types of novel interpretable models are freely available today, e.g.

- Explainable boosting machine (EBM)
- Monotonic GBM in h2o or XGBoost
- RuleFit (Friedman, Popescu, et al. [12])
- Super-sparse linear integer model (SLIM) (Ustun and Rudin [37])
- Scalable Bayesian rule list (Yang, Rudin, and Seltzer [40])

Explanations and Interpretable Models are Not Mutually Exclusive



Simple decision tree, g_{tree}, trained on the UCI credit card data to predict default with validation AUC of 0.74. The decision policy for a high risk individual is highlighted in red.



Locally-accurate Shapley contributions for the highlighted individual's probability of default. See slide 16 for LIMEs for the high risk customers in g_{tree}.

The Shapley values are helpful because they highlight the local importance of features not on the decision path, which could be underestimated by examining the decision policy alone.

An Ode to the Shapley Value

1. **In the beginning**: A Value for N-Person Games, 1953
2. **Nobel-worthy contributions**: *The Shapley value: Essays in honor of Lloyd S. Shapley*, 1988
3. **Shapley regression**: Analysis of Regression in Game Theory Approach, 2001
4. **First reference in ML?** Fair Attribution of Functional Contribution in Artificial and Biological Networks, 2004
5. **Into the ML research mainstream, i.e. JMLR**: An Efficient Explanation of Individual Classifications using Game Theory, 2010
6. **Into the real-world data mining workflow ... *finally***: Consistent Individualized Feature Attribution for Tree Ensembles, 2017. **
7. **Unification**: A Unified Approach to Interpreting Model Predictions, 2017. ††

** See h2o, LightGBM, or XGBoost for implementation.
†† See shap for implementation.

Explanation and Fairness Techniques are Not Mutually Exclusive

	Adverse Impact Disparity	Accuracy Disparity	TPR Disparity	TNR Disparity	FPR Disparity	FNR Disparity
`single`	0.89	1.03	0.99	1.03	0.85	1.01
`divorced`	1.01	0.93	0.81	0.96	1.25	1.22
`other`	0.26	1.12	0.62	1.17	0	1.44

Basic group disparity metrics across different marital statuses for monotonically constrained GBM model, g_{mono}, trained on the UCI credit card dataset. See slide 8 for global Shapley feature importance for g_{mono} and slide 13 for an important note about explanation as fairness techniques.

Many fairness techniques are freely available today: aequitas, AIF360, Themis, themis-ml.

Traditional disparate impact testing tools are best-suited for constrained models because average group metrics cannot reliable identify local instances of discrimination that can occur when using complex, unconstrained models.

References

This presentation:
https://www.github.com/jphall663kdd_2019

Code examples for this presentation:
https://www.github.com/jphall663/interpretable_machine_learning_with_python
https://www.github.com/jphall663/responsible_xai

Associated texts:
https://arxiv.org/pdf/1810.02909.pdf
https://arxiv.org/pdf/1906.03533.pdf

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