Proposed Guidelines for Responsible Use of Explainable Machine Learning

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Contents

What is an Explanation in 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 [9])
- "Explaining Explanations" (Gilpin et al. [14])
- "A Survey Of Methods For Explaining Black Box Models" (Guidotti et al. [17])
- "The Mythos of Model Interpretability" (Lipton [24])
- *Interpretable Machine Learning* (Molnar [27])
- "Interpretable Machine Learning: Definitions, Methods, and Applications" (Murdoch et al. [29])
- "Challenges for Transparency" (Weller [42]).

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 [26], Shapley [34])
- **Global and local surrogate models**:
  - Decision tree variants (Bastani, Pu, and Solar-Lezama [6], Craven and Shavlik [8])
  - Anchors (Ribeiro, Singh, and Guestrin [31])
  - Local interpretable model-agnostic explanations (LIME) (Ribeiro, Singh, and Guestrin [32])
- **Global and local visualizations of trained model predictions**:
  - Accumulated local effects (ALE) (Apley [4])
  - Partial dependence (Friedman, Hastie, and Tibshirani [12])
  - Individual conditional expectation (ICE) (Goldstein et al. [15])

Why Explainable ML?

Responsible Use of Explainable ML can enable:

- Human learning from machine learning
- Human appeal of automated decisions
- Regulatory compliance[2]
- White-hat hacking and security audits of ML models

Even logistic regression is often "explained", or post-processed, for credit scoring, e.g. max. points lost method and adverse action notices.

[2] In the U.S., interpretable models, explanations, and the model documentation they enable may be required under the Civil Rights Acts of 1964 and 1991, the Americans with Disabilities Act, the Genetic Information Nondiscrimination Act, the Health Insurance Portability and Accountability Act, the Equal Credit Opportunity Act, the Fair Credit Reporting Act, the Fair Housing Act, Federal Reserve SR 11-7, and the European Union (EU) Greater Data Privacy Regulation (GDPR) Article 22 [43].

Why Propose Guidelines?

Misuse and Abuse of Explainable ML can enable:

- Model and data stealing (Tramèr et al. [39], Shokri et al. [37], Shokri, Strobel, and Zick [36])
- False justification for harmful black-boxes, e.g. "fairwashing" (Aïvodji et al. [1], Rudin [33])

Explainable ML is already in-use:

- Numerous open source[3] and commercial packages[4] are available today.
- At least gradient-based feature attribution, partial dependence, and surrogate models are used for model validation in financial services today.[5,6]

Regulatory guidance is not agreed upon yet.[7]

[3] Please contribute: https://github.com/jphall663/awesome-machine-learning-interpretability.

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

[5] See: https://ww2.amstat.org/meetings/jsm/2019/onlineprogram/AbstractDetails.cfm?abstractid=303053.

[6] See: Working paper: "SR 11-7, Validation and Machine Learning Models", Tony Yang, CFA, CPA, FRM. KPMG USA.

[7] See: https://www.americanbanker.com/news/regulators-must-issue-ai-guidance-or-fdic-will-mcwilliams.

Proposed Guidelines for Responsible Use

1. **Use explainable ML to enhance understanding.**
2. **Learn how explainable ML is used for nefarious purposes.**
3. **Augment surrogate models with direct explanations.**
4. **Use highly transparent mechanisms for high stakes applications (Rudin [33]).**

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Guideline 1: Use Explainable ML to Enhance Understanding

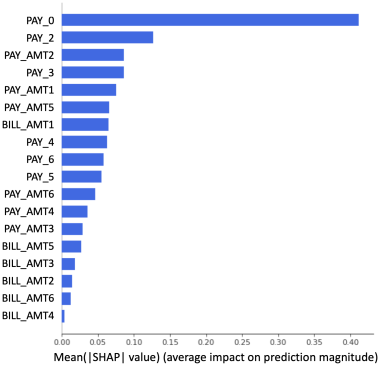
Explanations enhance understanding **directly**, and increase trust as a **side-effect**.

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

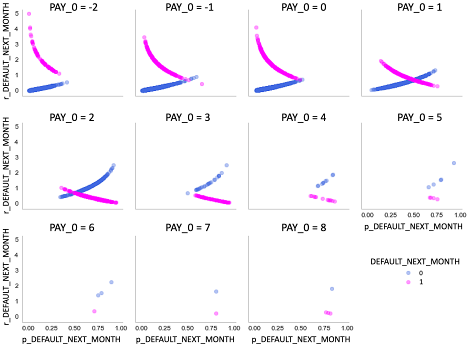
Explanations **alone** are neither necessary nor sufficient for trust.

Good explanations **enable human appeal** of model decisions.

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 [22].



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, PAY_0 ≥ 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 (Gopinathan et al. [16]). When these models performed well, they were trusted.[8] However, they were not explainable or well-understood by contemporary standards.

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

Guideline 2: Learn How Explainable ML is Used for Nefarious Purposes

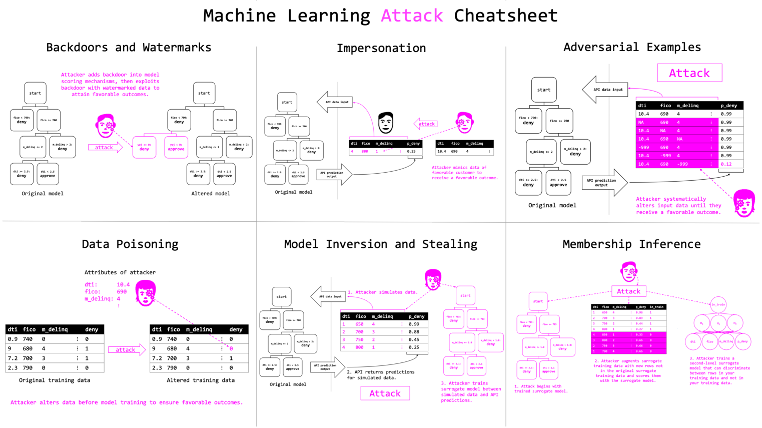
When unintentionally misused, explainable ML can act as a faulty safeguard for potentially harmful black-boxes.

When intentionally abused, explainable ML can be used for:

- Stealing 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.[9]



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

Corollary 2.1: White-hat Attacks Can Crack Potentially Harmful Black-boxes

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

Recent high profile analyses of commercial black-boxes, e.g. ...

- Propublica and COMPAS (Angwin et al. [3])[10]
- Gendershades and Rekognition (Buolamwini and Gebru [7], Raji and Buolamwini [30])

... **could** be characterized as white-hat attacks on proprietary black-boxes (respectively, model stealing and adversarial examples).

[10] 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], [11].

Corollary 2.2: Explanation ***is Not*** a Front Line Fairness Tool

Use fairness tools, e.g. ...

- Disparate impact testing (Feldman et al. [10])
- Reweighing (Kamiran and Calders [19])
- Reject option based classification (Kamiran, Karim, and Zhang [20])
- Adversarial de-biasing (Zhang, Lemoine, and Mitchell [45])
- 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.

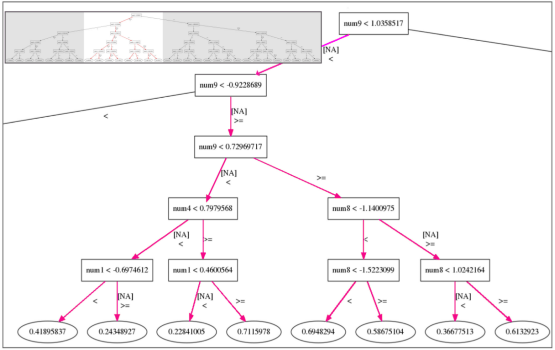
Surrogate Models

Models of models (i.e. surrogate models, compressed models, extracted models) can be helpful explanatory or modeling tools, but they can also be approximate, low-fidelity explainers.

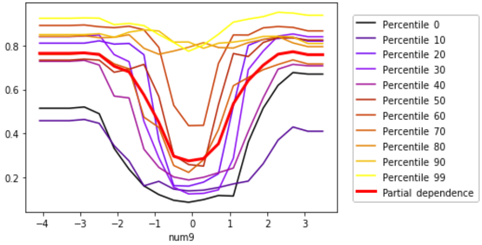
Much work in explainable ML has been directed toward improving the fidelity and usefulness of surrogate models (e.g., Bastani, Kim, and Bastani [5], Bastani, Pu, and Solar-Lezama [6], Craven and Shavlik [8], Hu et al. [18], Ribeiro, Singh, and Guestrin [31], Vaughan et al. [41])

(BUT many explainable ML techniques have nothing to do with surrogate models!)

Guideline 3: Augment Surrogate Models with Direct Explanations



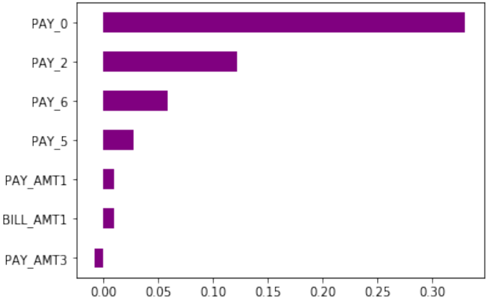
Naïve h_{tree}, *a surrogate model*, forms an approximate overall flowchart for the explained model, g_{GBM}.



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

h_{tree} displays known interactions in $f = X_{\text{num1}} * X_{\text{num4}} + |X_{\text{num8}}| * X^2_{\text{num9}}$ 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 also highlighted by the divergence of partial dependence and ICE curves for $\sim -1 < X_{\text{num9}} <\sim 1$.

Corollary 3.1: 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_{tree}. See slide 20 for a directed graph representation of g_{tree}.

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

Coefficients for a local linear interpretable model, h_{GLM}, with an intercept of 0.77 and an R^2 of 0.73, trained between the original inputs and predictions of g_{tree} for a segment of the UCI credit card dataset with late most recent repayment statuses, $\mathbf{X}_{PAY\_0>1}$.

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.

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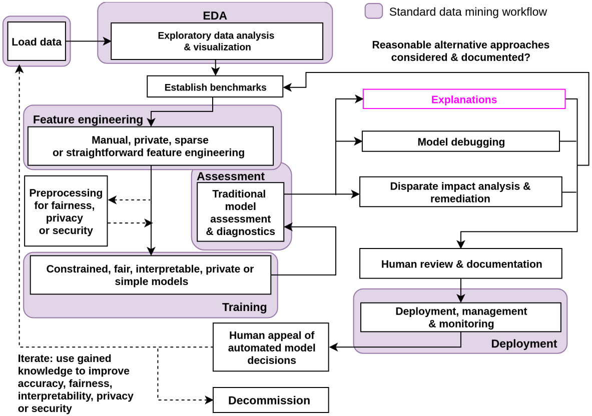
Guideline 4: Use Highly Transparent Mechanisms for High Stakes Applications



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

Corollary 4.1: Use Interpretable Models for High Stakes Applications (Rudin [33])

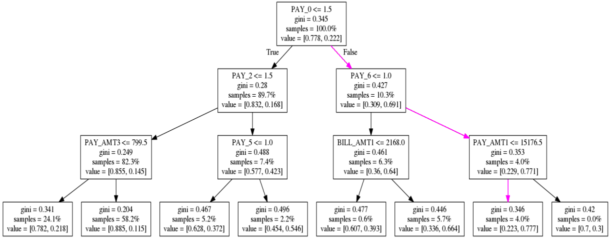
In addition to penalized GLM, decision trees, and conventional rule-based models, many other types of accurate and interpretable models are available today, e.g. ...

- Explainable boosting machine (EBM)
- Monotonic GBM in h2o or XGBoost
- RuleFit (Friedman, Popescu, et al. [13])
- Super-sparse linear integer model (SLIM) (Ustun and Rudin [40])
- Explainable neural network (XNN) (Vaughan et al. [41])
- Scalable Bayesian rule list (Yang, Rudin, and Seltzer [44])

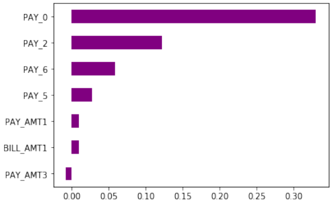
... use them for human-centered or other high stakes ML applications.[11]

[11] There are shades of interpretability in models. Interpretability is probably not a binary, on-off quality. For instance see Figure 3: https://arxiv.org/pdf/1904.03867.pdf [28].

Corollary 4.2: Explanations and Interpretable Models are Not Mutually Exclusive



Simple decision tree, $g_{\mathbf{tree}}$, trained on the UCI credit card data to predict default with validation AUC of 0.74. The decision policy for high risk individuals is highlighted in fuschia.



Locally accurate Shapley contributions for the highlighted individual's probability of default. See slide 17 for LIMEs for the high risk customers in $g_{\mathbf{tree}}$.

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.

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Interlude: An Ode to the Shapley Value

1. **In the beginning**: A Value for N-Person Games, 1953 [34]
2. **Nobel-worthy contributions**: *The Shapley value: Essays in honor of Lloyd S. Shapley*, 1988 [35]
3. **Shapley regression**: Analysis of Regression in Game Theory Approach, 2001 [23]
4. **First reference in ML?** Fair Attribution of Functional Contribution in Artificial and Biological Networks, 2004 [21]
5. **Into the ML research mainstream, i.e. JMLR**: An Efficient Explanation of Individual Classifications using Game Theory, 2010 [38]
6. **Into the real-world data mining workflow ... *finally***: Consistent Individualized Feature Attribution for Tree Ensembles, 2017[12] [25]
7. **Unification**: A Unified Approach to Interpreting Model Predictions, 2017[13] [26]

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[12] See h2o, LightGBM, or XGBoost for implementation.
[13] See shap for implementation.

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Corollary 4.3: 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 9 for global Shapley feature importance for g_{mono} and slide 14 for an important note about explanation and fairness techniques.

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

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

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[14] My world anyway ... and in alphabetical order by first name.

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https://www.github.com/jphall663/kdd_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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