Hands-On Tutorial Outline: Responsible Use Guidelines for Explainable Machine Learning

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INTRODUCTION & AGENDA

Explainable machine learning (ML) enables human learning from ML, human appeal of incorrect ML decisions, regulatory compliance, and security audits of ML models.[1,2,3] Explainable ML (i.e., e*x*plainable *a*rtificial *i*ntelligence or XAI) has been implemented in numerous open source and commercial packages and explainable ML is also an important, mandatory, or embedded aspect of commercial predictive modeling in industries like financial services.[4,5,6] However, like many technologies, explainable ML can be misused and abused, particularly as a faulty safeguard for harmful black-boxes, e.g., *fairwashing*, and for other malevolent purposes like stealing models or sensitive training data [1], [32], [35], [37]. To promote best-practice discussions for this already in-flight technology, this tutorial presents the following:

Agenda

- Definitions and examples. **(Section 1; 20 mins.)**
- Responsible use guidelines and corollaries:
  - Use explanations to enable understanding directly (and trust as a side-effect). **(Section 2.1; 40 mins.)**
  - Learn how explainable ML is used for nefarious purposes. **(Section 2.2; 30 mins.)**
  - Augment surrogate models with direct explanations. **(Section 2.3; 30 mins.)**
  - Use fully transparent ML mechanisms for high-stakes applications. **(Section 2.4; 50 mins.)**
- Conclusion: a holistic approach to ML. **(Section 3; 10 mins.)**

Total time: 180 mins.

[1]This outline and associated software do not contain, nor should they be construed to be considered, legal advice or requirements for regulatory compliance.

[2]In the U.S., interpretable models, explainable ML, and 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 (ECOA), the Fair Credit Reporting Act (FCRA), the Fair Housing Act, Federal Reserve SR 11-7, and the European Union (EU) Greater Data Privacy Regulation (GDPR) Article 22 [41].

[3]For various security applications, see: https://www.oreilly.com/ideas/proposals-for-model-vulnerability-and-security.

[4]Like H2O-3, XGBoost, and various other Python and R packages. See: https://github.com/jphall663/awesome-machine-learning-interpretability for a longer, curated list of relevant open source software packages.

[5]For instance Datarobot, H2O Driverless AI, SAS Visual Data Mining and Machine Learning, Zest AutoML, and likely several others.

[6]See: "Deep Insights into Explainability and Interpretability of Machine Learning Algorithms and Applications to Risk Management," Jie Chen, Wells Fargo Corporate Model Risk, https://ww2.amstat.org/meetings/jsm/2019/onlineprogram/AbstractDetails.cfm?abstractid=303053.

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https://fatconference.org/2020/callfortutorials.html.

1 DEFINITIONS & EXAMPLES

Explainable ML practitioners have seemingly not yet adopted a clear taxonomy of concepts or a precise vocabulary, though many authors have grappled with a variety of concepts related to interpretability and explanations, e.g., Gilpin et al. [14], Guidotti et al. [17], Lipton [26], Molnar [29], Murdoch et al. [30], and Weller [40]. To decrease ambiguity, this section provides working definitions or examples of *interpretable*, *explanation*, *explainable ML*, *interpretable models*, *model debugging techniques*, *bias*, and *fairness techniques*.

Interpretable: "the ability to explain or to present in understandable terms to a human." (Doshi-Velez and Kim [9])

Explanation: "a collection of visual and/or interactive artifacts that provide a user with sufficient description of a model's behavior to accurately perform tasks like evaluating, trusting, predicting, or improving a model." (Singh[7])

Explainable ML: analysis and techniques, typically post-hoc, employed to understand trained model mechanisms or predictions. Examples of common explainable ML techniques include:

- Local and global variable importance, e.g., Shapley and derivative-based variable attribution [3] [23], [28], [33], [36].
- Local and global model-agnostic surrogate models, e.g., surrogate decision trees and local interpretable model-agnostic explanations (LIME) [6], [7], [8], [20], [31], [39].
- Local and global visualizations of model predictions, e.g., accumulated local effect (ALE) plots, 1- and 2-dimensional partial dependence (PD) plots, and individual conditional expectation (ICE) plots [5], [13], [15].

Interpretable models (i.e., *white-box* models): include linear models, decision trees, rule-based models, constrained or Bayesian variants of traditional black-box ML models, or novel interpretable-by-design models. Explainable neural networks (XNNs), explainable boosting machines (EBMs, GA2M), monotonic gradient boosting machines (GBMs), scalable Bayesian rule lists, or super-sparse linear integer models (SLIMs) are examples of newer interpretable models [38], [39], [42].[8,9,10]

Model debugging techniques: methods for testing ML models that increase trust in mechanisms and predictions. Debugging techniques include model assertions, security audits, variants of sensitivity (i.e., *what-if?*) analysis, variants of residual analysis and explanation, and unit tests to verify the accuracy or security of ML

[7]"Proposed Guidelines for Responsible Use of Explainable Machine Learning," Patrick Hall, H2O.ai, https://github.com/jphall663/kdd_2019.

[8]As implemented in the interpret library: https://github.com/microsoft/interpret.

[9]As implemented in XGBoost (https://xgboost.readthedocs.io/en/latest/tutorials/monotonic.html) or H2O-3 (https://github.com/h2oai/h2o-3/blob/master/h2o-py/demos/H2O_tutorial_gbm_monotonicity.ipynb).

[10]And similar methods, e.g., https://users.cs.duke.edu/~cynthia/papers.html.

models [2], [22].[11] Model debugging should also include remediating any discovered errors or vulnerabilities.

Bias: herein *bias* encompasses several forms of discrimination that may manifest in ML, including overt discrimination, disparate treatment, and disparate impact (DI), i.e., unintentional discrimination. DI may be caused by model misspecification, inaccurate or incomplete data, or data that has differing correlations or dependencies among groups of individuals, driving differences in rates of favorable model outcomes. A model is said to be biased if, (1) group membership is not independent of the likelihood of a favorable outcome, or, (2) under certain circumstances, membership in a *subset* of a group is not independent of the likelihood of a favorable outcome (i.e., *local bias*). Underlying discrimination that causes bias may or may not be illegal, depending on how it arises and applicable discrimination laws.

Fairness techniques: are used to diagnose and remediate bias in ML models. Diagnosis approaches include DI testing and other tests for bias [11]. Remediation methods tend to involve model selection by minimization of bias, preprocessing training data, e.g., reweighing (Kamiran and Calders [21]), training unbiased models, e.g., adversarial de-biasing (Zhang et al. [43]), or post-processing model predictions, e.g., by equalizing odds (Hardt et al. [19]).[12]

2 GUIDELINES

Four guidelines are presented in Sections 2.1 – 2.4 to assist practitioners in avoiding any unintentional misuse or in identifying any intentional abuse of explainable ML techniques. Important corollaries to the guidelines are also highlighted. Open and reproducible software examples accompany the guidelines at https://github.com/h2oai/xai_guidelines.

2.1 Guideline: Use Explanations to Enable Understanding Directly.

If trust in models is your goal, explanations alone are insufficient. Explanation, as a general idea, is related more directly to understanding and transparency than to trust.[13] Explanations enhance understanding directly (and trust as a side-effect when explanations are acceptable to human users). In short, ML can be understood and not trusted, and trusted but not understood.

- **Explanation & understanding without trust**: In Figure 1, global Shapley explanations and residual analysis identify a pathology in an unconstrained GBM model, g_{GBM}. In this example scenario, g_{GBM} is explainable, but not trustworthy.
- **Trust without explanation & understanding**: Years before reliable explanation methods were widely acknowledged and available, black-box models, such as artificial neural networks, were used for fraud detection in the financial services industry [16]. When these models performed well, they were trusted.[14] However, they were not explainable or well-understood by contemporary standards.

[11] And similar methods, e.g., https://debug-ml-iclr2019.github.io/.
[12] And similar methods, e.g., http://www.fatml.org/resources/relevant-scholarship.
[13] The Merriam-Webster definition of *explain*, accessed Sep. 8$^{\text{th}}$ 2019, does not mention *trust*: https://www.merriam-webster.com/dictionary/explain.
[14] See: https://www.sas.com/en_ph/customers/hsbc.html, https://www.kdnuggets.com/2011/03/sas-patent-fraud-detection.html.

2.2 Guideline: Learn How Explainable ML is Used for Nefarious Purposes.

When used disingenuously, explainable ML methods can enable:

- Misuse or intentional abuse of black-box ML [1], [32].
- Hacking or stealing of data and models through public prediction APIs or other endpoints [35], [37].

Explainable ML methods may be used for additional unknown destructive purposes today or in the future.

2.2.1 *Corollary: Use Explainable ML for red-team testing.*

Use explainable ML techniques to test ML systems for vulnerabilities to model stealing and inversion attacks and membership inference attacks.

2.2.2 *Corollary: Explainable ML Can be Used to Crack Nefarious Black-boxes.*

Used as white-hat hacking tools, explainable ML can draw attention to fairness or accuracy problems in proprietary black-boxes. See Angwin et al. [4] for evidence that cracking of commercial black-box models for oversight purposes is possible.[15]

2.2.3 *Corollary: Explainable ML is a Privacy Vulnerability.*

Recent research shows that providing explanations along with predictions eases attacks that can compromise sensitive training data [34].

2.3 Augment Surrogate Models with Direct Explanations.

Models of models, or surrogate models, can be helpful explanatory tools, but they are often approximate, low-fidelity explainers. Combine direct explanation methods with approximate global or local summaries provided by surrogate models to enhance both types of explanations. In Figure 2, a surrogate decision tree and direct explanations, in the form of PD and ICE, highlight and confirm modeled interactions [18].

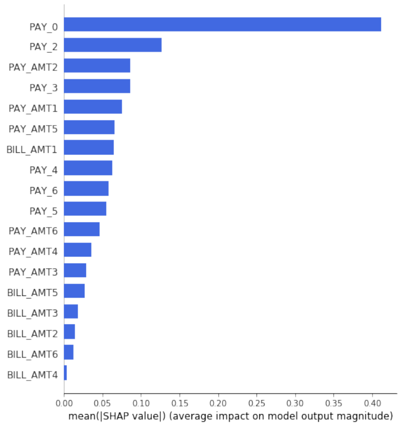
2.3.1 *Corollary: Augment LIME with Direct Explanations.*

LIME can be combined with direct explanations to yield deeper insights. The tutorial notebook available at https://github.com/h2oai/xai_guidelines/blob/master/dt_shap_lime.ipynb contains LIME coefficients that can be used along with the local Shapley variable contributions in Figure 3 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 for debugging and compliance purposes.

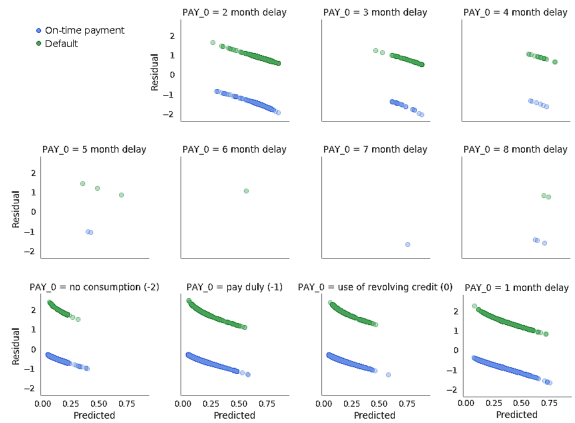
2.4 Use Fully Transparent ML Mechanisms for High-Stakes Applications.

Many high-stakes ML applications are regulated. Explanation, with interpretable models, model debugging, DI analysis, and the documentation they enable, are often required under numerous regulatory statutes in the U.S. and E.U., and explainable ML tools are already used to document, explain, and validate different types of

[15] This text makes no claim on the quality of the analysis in Angwin et al. (2016), which has been criticized [12]. This now infamous analysis is presented only as evidence that motivated activists can crack commercial black-boxes using surrogate models and other explanatory techniques. Moreover, such analyses would likely improve with established best-practices for explainable ML.

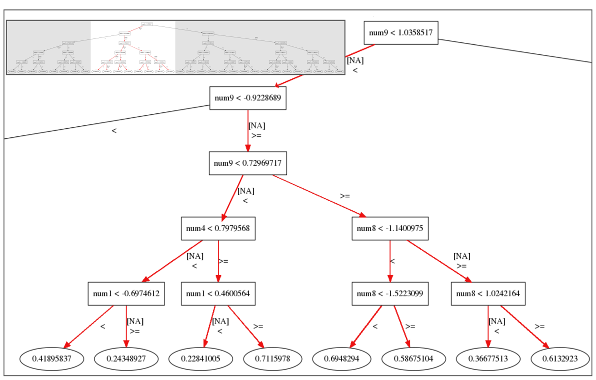


(a) Global Shapley variable importance for g_{GBM}.

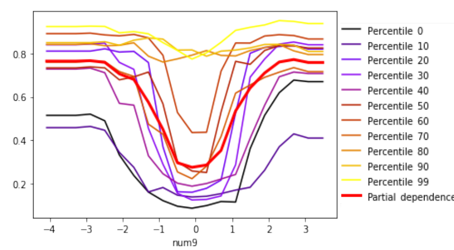


(b) g_{GBM} deviance residuals and predictions by `PAY_0`.

Figure 1: An unconstrained GBM probability of default model trained on the UCI credit card data [24], g_{GBM}, over-emphasizes the importance of the input variable `PAY_0`, a customer's most recent repayment status. g_{GBM} can produce large positive residuals when `PAY_0` indicates on-time payments (`PAY_0` ≤ 1) and large negative residuals when `PAY_0` indicates late payments (`PAY_0` > 1). Combining explanatory and debugging techniques shows that g_{GBM} is explainable, but probably not trustworthy. Code to replicate Figure 1 is available here: https://github.com/h2oai/xai_guidelines/blob/master/global_shap_resid.ipynb.



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



(b) PD and ICE curves generated *directly from the explained model*, g_{GBM}.

Figure 2: h_{tree} displays known interactions in the g_{GBM}-modeled function $f = X_{\text{num1}} * X_{\text{num4}} + |X_{\text{num8}}| * X^2_{\text{num9}}$ for $\sim -1 < X_{\text{num9}} <\sim 1$. Modeling of the known interactions in f by g_{GBM} is confirmed by the divergence of PD and ICE curves for $\sim -1 < X_{\text{num9}} <\sim 1$. Explanations from a surrogate model have augmented findings from a direct explanation technique. Code to replicate Figure 2 is available here: https://github.com/h2oai/xai_guidelines/blob/master/dt_surrogate_pd_ice.ipynb.

models in the financial services industry [20], [39].[2, 6,16]

Aside from regulatory concerns, explanation enables logical appeal processes for incorrect decisions made by ML models. Consider being negatively impacted by an erroneous black-box model decision, say for instance being mistakenly denied a loan or parole. How would you argue your case for appeal without knowing how model decisions were made? [17]

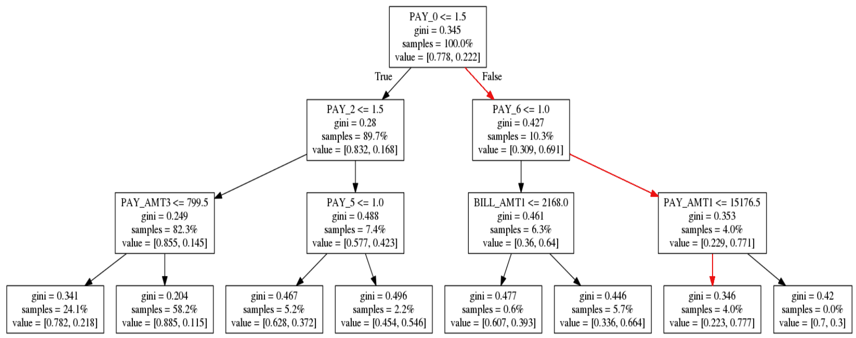
[16]For instance: https://www.prnewswire.com/news-releases/new-patent-pending-technology-from-equifax-enables-configurable-ai-models-300701153.html.

[17]This is happening *today*. According to the New York Times, a man named Glenn Rodríguez found himself in this unfortunate position in a penitentiary in Upstate New York in 2016: https://www.nytimes.com/2017/06/13/opinion/how-computers-are-harming-criminal-justice.html.

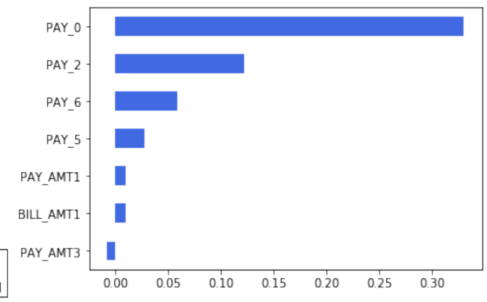
2.4.1 Corollary: Use Interpretable Models Along with Explanation Techniques. Figure 3 displays an interpretable model and Shapley numeric variable contributions for a single model prediction. Even for interpretable models, such as linear models and decision trees, Shapley values present accuracy and consistency advantages over standard variable attribution methods [25], [27], [28].

2.4.2 Corollary: Use Explanations Along with Bias Testing and Remediation. For example, in banks, using post-hoc explanatory tools along with DI analysis is often necessary to comply with model documentation guidance and with fair lending regulations.[18]

[18]See: https://www.ffiec.gov/pdf/fairlend.pdf, https://files.consumerfinance.gov/f/documents/201510_cfpb_ecoa-narrative-and-procedures.pdf.



(a) 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.



(b) Locally-accurate Shapley contributions for the highlighted individual's probability of default.

Figure 3: A simple decision tree, g_{tree}, is trained on the UCI credit card dataset to predict probability of default. The decision-policy for a high-risk customer is highlighted in 3a and the locally-accurate Shapley contributions for this same individual's predicted probability are displayed in 3b. The Shapley values are helpful because they highlight the local importance of features not on the decision path in this particular encoding of the unknown signal-generating function, i.e., g_{tree}, which could be underestimated by examining the decision policy alone. Code to replicate Figure 3 is available here: https://github.com/h2oai/xai_guidelines/blob/master/dt_shap_lime.ipynb.

2.4.3 Corollary: Explanation is Not a Frontline Fairness Tool. In high-stakes and commercially viable uses of explainable ML in credit lending, insurance, and employment in the U.S. that fall under FCRA, ECOA, or other applicable regulations, demographic attributes cannot be used in predictive models and thus their contribution to models cannot be assessed using accurate, direct explainable ML techniques. Even when demographic attributes can be used in models, it has been shown that explanations may not detect bias [1]. Given these drawbacks, it is recommended that fairness techniques are used to test for and remediate bias, and explanations are used to understand bias when appropriate.

2.4.4 Corollary: Use Bias Testing Along with Constrained Models. Because unconstrained ML models can treat similar individuals differently due to small differences in their data values, unconstrained models can cause local bias that is not detectable with standard bias testing methods that analyze group fairness [10]. To minimize local bias when using machine learning, and to ensure standard bias testing methods are most effective, pair bias testing with constrained models.

The tutorial notebook https://github.com/h2oai/xai_guidelines/blob/master/dia.ipynb addresses corollaries 2.4.2, 2.4.3, and 2.4.4.

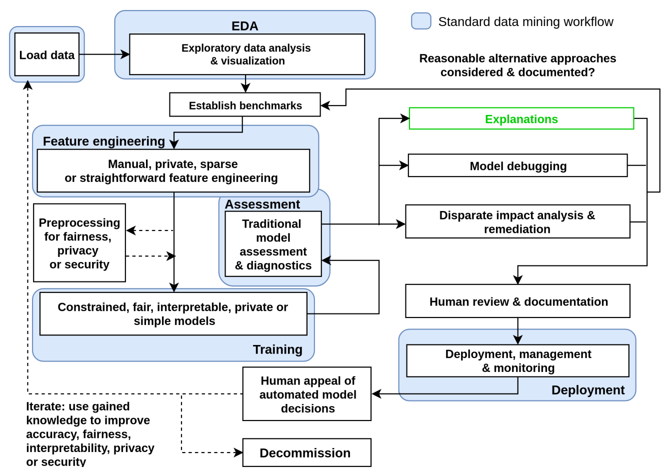


Figure 4: A diagram of a proposed holistic ML workflow in which explanations (highlighted in green) are used along with interpretable models, bias testing and remediation techniques, and other review and appeal mechanisms to create a fair, accountable, and transparent ML system.

3 CONCLUSION: A HOLISTIC ML APPROACH

ML is used today to make life-altering decisions about employment, bail, parole, and lending[19], and the scope of decisions delegated to ML systems seems likely only to expand in the future. By presenting explainable ML guidelines, this tutorial also gives examples of combining innovations from several sub-disciplines of ML research to train explainable, fair, and trustable predictive modeling systems. As proposed in Figure 4, using these techniques together can create a more holistic approach to ML, potentially better-suited for use in business- and life-critical decisions than conventional workflows.

[19]ICLR 2019 model debugging workshop CFP: https://debug-ml-iclr2019.github.io/.

SOFTWARE RESOURCES

This tutorial uses Jupyter notebooks and Python code with permissive licenses stored in a public GitHub repository: https://github.com/h2oai/xai_guidelines. Notebooks are deployed in H2O.ai's free educational cloud environment, Aquarium: http://aquarium.h2o.ai. Attendees only need an email address (to receive a password after Aquarium registration) and their laptops to run the materials.

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