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] 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.[3,4,5] 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], [31], [34], [36]. To begin a best-practices discussion for this already in-flight technology, this tutorial presents the following agenda:

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 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. Guidotti et al. [16], Lipton [25], Molnar [28], Murdoch et al. [29]), and Weller [39]. To decrease ambiguity, this section provides working definitions or examples of *interpretable*, *explanation*, *explainable ML*, *interpretable models*, *model debugging techniques*, 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 the model behavior to accurately perform tasks like evaluation, trusting, predicting, or improving the model.” (Singh[6])

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 feature importance, e.g. Shapley values and derivative-based feature attribution [3] [22], [27], [32], [35].
- Local and global model-agnostic surrogate models, e.g. surrogate decision trees and local interpretable model-agnostic explanations (LIME) [6], [7], [8], [19], [30], [38].
- Local and global visualizations of model predictions, e.g. accumulated local effect (ALE) plots, 1- and 2-dimensional partial dependence plots, and individual conditional expectation (ICE) plots [5], [13], [14].

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 GBMs, scalable Bayesian rule lists, or super-sparse linear integer models (SLIMs) are examples of newer interpretable models [37], [38], [41].[7,8,9]

Model debugging techniques refer to methods for testing ML models that increase trust in mechanisms and predictions. Examples of debugging techniques include model assertions, security audits, variants of sensitivity (i.e. *what-if?*) analysis, variants of residual analysis and explanations, and unit tests to verify the accuracy or security of ML models [2], [21].[10] Model debugging should also include remediating any discovered errors or vulnerabilities.

[1] 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 [40].

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

[3] 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.

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

[5] For instance, “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.

ACM FAT Call for Tutorials – UNDER REVIEW, Barcelona, 2020*
https://fatconference.org/2020/callfortutorials.html.

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

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

[8] 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).

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

[10] And similar methods, e.g. https://debug-ml-iclr2019.github.io/.

Fairness techniques are used to diagnose and remediate unwanted sociological bias in ML models. Diagnosis approaches include disparate impact testing and other tests for unwanted sociological bias [11]. Remediation methods tend to involve model selection by minimization of bias, preprocessing training data, e.g. reweighing (Kamiran and Calders [20]), training unbiased models, e.g. adversarial de-biasing (Zhang et al. [42]), or post-processing model predictions, e.g. by equalizing odds (Hardt et al. [18]).[11]

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.[12] 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 autoencoder and MLP neural networks, were used for fraud detection in the financial services industry [15]. When these models performed well, they were trusted.[13] However, they were not explainable or well-understood by contemporary standards.

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

When used disingenuously, explainable ML methods can enable:

- Misuse or intentionally abuse of black-box ML [1], [31].
- Hacking or stealing of data and models through public prediction APIs or other endpoints [34], [36].

Explainable ML methods may be used for additional unknown destructive purposes today, and are also likely to be used for other nefarious purposes in the future.

2.2.1 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.[14]

2.2.2 Corollary: Explainable ML is a Privacy Vulnerability. Recent research shows that providing explanations along with predictions eases attacks that can compromise sensitive training data [33].

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 partial dependence and ICE, highlight and confirm modeled interactions [17].

2.3.1 Corollary: Augment LIME with Direct Explanations. LIME can be combined with direct explanations to yield deeper insights. Table 1 contains LIME h_{GLM} coefficients that can be used along with the local Shapley feature 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.

Table 1: Coefficients for a local linear interpretable model, $h_{\mathbf{GLM}}$, with an intercept of 0.77 and an R^2 of 0.73. $h_{\mathbf{GLM}}$ is trained on a segment of the UCI credit card dataset containing higher-risk customers with late most recent repayment statuses, $\mathrm{X}_{PAY\_0>1}$, and the predictions of a simple decision tree, $g_{\mathbf{tree}}(\mathrm{X}_{\mathbf{PAY\_0}>1})$. Code to replicate Table 1 is available here: https://github.com/h2oai/xai_guidelines.

h_{GLM} Feature	h_{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

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

Many high-stakes applications are regulated. Explanation, with interpretable models, model debugging, disparate impact 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, understand, and validate different types of models in the financial services industry [19], [38].[2, 5,15]

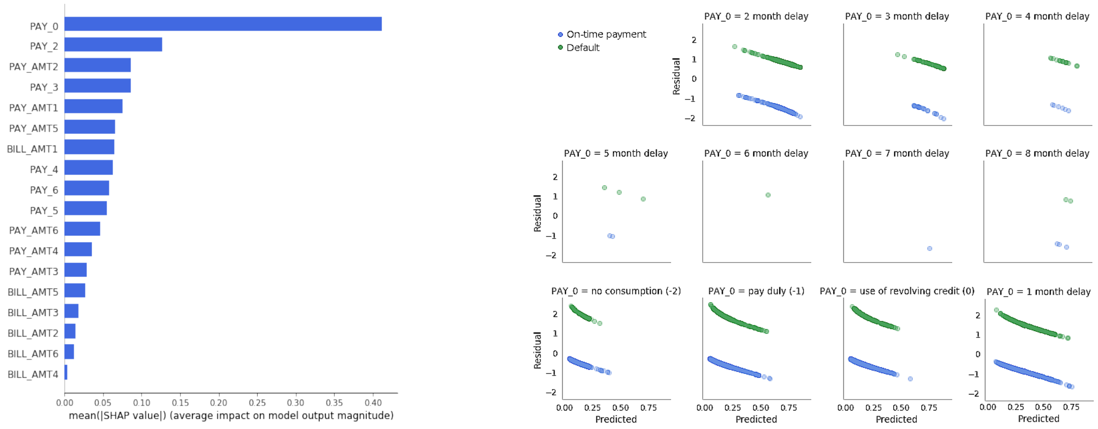
[11] And similar methods, e.g. http://www.fatml.org/resources/relevant-scholarship.

[12] The Merriam-Webster definition of *explain*, accessed May 8th 2019, does not mention *trust*: https://www.merriam-webster.com/dictionary/explain.

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

[14] 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 on improve with established best-practices for explainable ML.

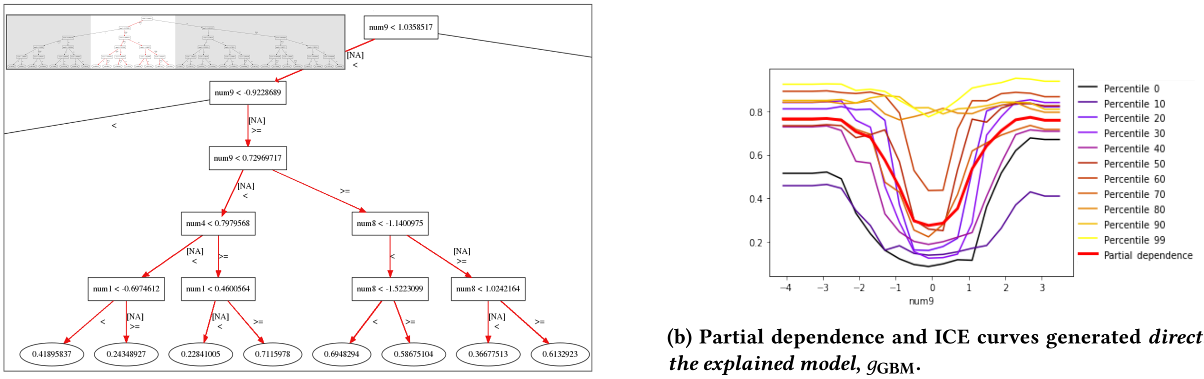
[15] This is *already* happening: https://www.prnewswire.com/news-releases/new-patent-pending-technology-from-equifax-enables-configurable-ai-models-300701153.html.



(a) Global Shapley feature 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[23], g_{GBM}, generally overemphasizes the importance of the input feature `PAY_0`, a customer's most recent repayment status. g_{GBM} produces 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.



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

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

Figure 2: 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 confirmed by the divergence of partial dependence and ICE curves for $\sim -1 < X_{\text{num9}} <\sim 1$. Explanations from a surrogate model have augmented and confirmed findings from a direct model visualization technique. Code to replicate Figure 2 is available here: https://github.com/h2oai/xai_guidelines.

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? [16]

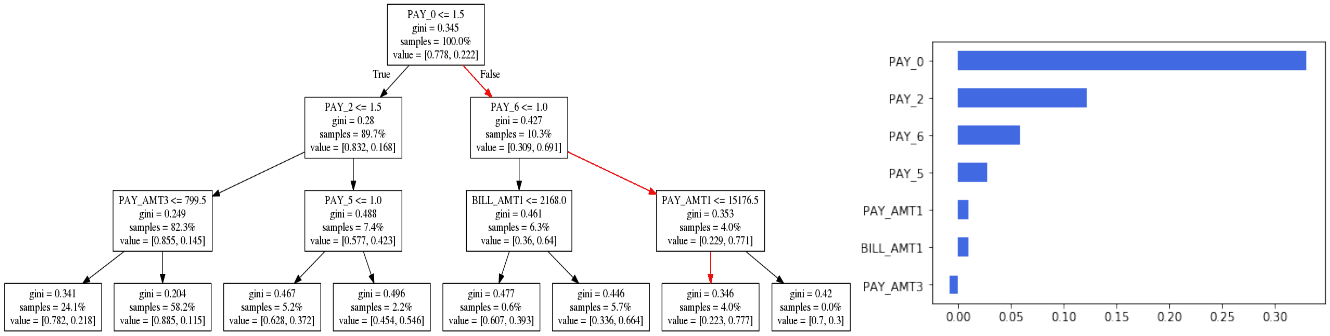
2.4.1 Corollary: Use Interpretable Models Along with Explanation Techniques. Interpretable models and explanations can be used together in a holistic ML workflow as illustrated in Figure 4. Figure 3 displays a globally interpretable model and accurate numeric feature contributions for a model prediction. Even for interpretable models, such as linear models and decision trees, Shapley values present accuracy and consistency advantages over standard feature attribution methods [24], [26], [27].

2.4.2 Corollary: Use Explanations Along with Bias Testing and Remediation. In banks, using post-hoc explanatory tools along with disparate impact analysis is necessary to comply with model documentation guidance and with fair lending regulations.[5,17,18]

[16] This too 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.

[17] See: https://www.aba.com/Compliance/Documents/FairLendingWhitePaper2017Apr.pdf.

[18] See: https://www.govinfo.gov/content/pkg/FR-1994-04-15/html/94-9214.htm.



(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. g_{tree} has a validation AUC of 0.74. 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.

2.4.3 Corollary: Explanation is Not a Frontline Fairness Tool. In many high-stakes and commercially viable applications 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 model predictions cannot be explained using common explainable ML techniques. Even when demographic attributes can be used in predictive models, it has been shown that explanations may not detect unwanted social bias [1]. Given these known drawbacks, it is recommended that fairness techniques are used to test for and remediate unwanted sociological bias, and explanations are used to augment and understand bias when appropriate.

2.4.4 Corollary: Use Bias Testing Along with Constrained Models. Because unconstrained ML models have the ability to treat similar individuals differently based on 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 unwanted sociological bias when using machine learning, and to ensure standard bias testing methods are most effective, pair bias testing techniques with constrained models.

3 CONCLUSION: A HOLISTIC ML APPROACH

ML is used today to make life-altering decisions about employment, bail, parole, and lending.[19] 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 decision support than conventional workflows.

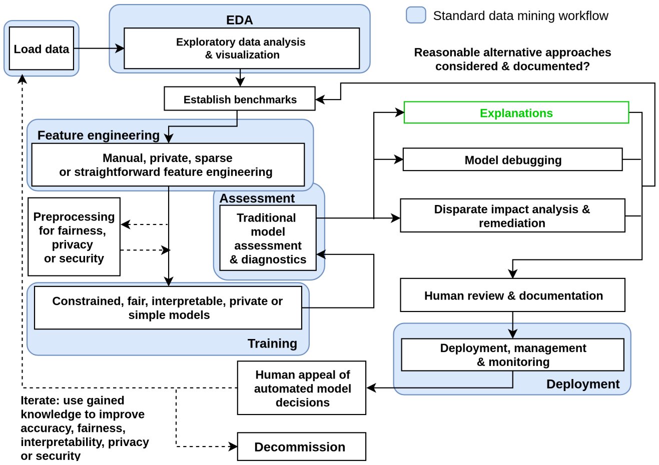

Load data
EDA
Exploratory data analysis & visualization
Standard data mining workflow
Reasonable alternative approaches considered & documented?
Establish benchmarks
Explanations
Feature engineering
Manual, private, sparse or straightforward feature engineering
Model debugging
Assessment
Preprocessing for fairness, privacy or security
Traditional model assessment & diagnostics
Disparate impact analysis & remediation
Constrained, fair, interpretable, private or simple models
Human review & documentation
Training
Deployment, management & monitoring
Human appeal of automated model decisions
Deployment
Iterate: use gained knowledge to improve accuracy, fairness, interpretability, privacy or security
Decommission

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.

SOFTWARE RESOURCES

This tutorial uses Jupyter notebooks and Python code stored in a public GitHub repository with an Apache 2.0 license https://github.com/h2oai/xai_guidelines. Notebooks will be deployed in H2O.ai's free educational cloud environment, Aquarium: http://aquarium.h2o.ai. Attendees will only need an email address (to receive a password after Aquarium registration) and to bring their laptop to access and execute the materials.

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

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