Guidelines for Responsible Use of Explainable Machine Learning:
A 90-Minute Hands-On Tutorial

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INTRODUCTION

Explainable machine learning (ML) enables human learning from ML, human appeal of automated model decisions, regulatory compliance, and white-hat hacking and security audits of ML models.[1,2] Explainable ML (i.e. *explainable artificial intelligence* 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, 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], [33], [35].

AGENDA

In an effort to begin establishing best practices for this already in-service technology and also to promote nuanced discussion, this tutorial presents:

- Definitions, examples, and qualifications related to explainable ML. **(Section 1; 10 mins.)**
- Responsible use guidelines and corollaries:
  - Use explanations to enable understanding directly, and trust as a side-effect. **(Section 2.1; 20 mins.)**
  - Learn how explainable ML is used for nefarious purposes. **(Section 2.2; 15 mins.)**
  - Augment surrogate models with direct explanations. **(Section 2.3; 15 mins.)**
  - Use fully transparent ML mechanisms for high-stakes applications. **(Section 2.4; 25 mins.)**
- Conclusion **(Section 3; 5 mins.)**

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[1]In the U.S., interpretable models. post-hoc 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 [39].

[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.

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1 DEFINITIONS AND EXAMPLES

While explainable ML practitioners have seemingly not yet adopted a clear taxonomy of concepts or a precise vocabulary, many authors have grappled with a variety of general concepts related to interpretability and explanations. Some of these efforts include: "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]), and "Challenges for Transparency" (Weller [38]). To avoid ambiguity, this section addresses the terms and phrases *interpretable*, *explanation*, *explainable ML*, *white-box* or *interpretable models*, *model debugging*, *fairness*, and *human-centered ML*.

1.1 Interpretable and Explanation

From the review and survey corpus, this text selects for an internal definition of *interpretable*, "the ability to explain or to present in understandable terms to a human," from "Towards a Rigorous Science of Interpretable Machine Learning" (Doshi-Velez and Kim [7]). From "Explaining Explanations: An Approach to Evaluating Interpretability of Machine Learning" (Gilpin et al. [13]), "when you can no longer keep asking why," will serve as an internal working definition of a viable *explanation*. These two thoughtful characterizations link explanation to some ML process being interpretable and also provide an abstract objective for any given explanatory task.

1.2 Explainable ML and Interpretable or White-box Models

Herein *explainable ML* means mostly post-hoc analysis and techniques used to understand trained model mechanisms or predictions. Examples of common explainable ML techniques include:

- Local and global feature importance methods, in particular Shapley values [21], [26], [32], [34].
- Local and global model-agnostic surrogate models, such as surrogate decision trees and Local Interpretable Model-agnostic Explanations (LIME) [4], [5], [6], [20], [30], [37].
- Local and global visualizations of model predictions such as accumulated local effect (ALE) plots, 1- and 2-dimensional partial dependence plots, and individual conditional expectation (ICE) plots [3], [11], [14].

Although difficult to quantify, credible research efforts into scientific measures of interpretability are underway [10], [28]. Furthermore, the ability to measure degrees of interpretability implies it's not a binary, on-off quantity.[6] Here unconstrained, traditional

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[6]For instance, see Figure 3 in "Quantifying Interpretability of Arbitrary Machine Learning Models Through Functional Decomposition" (Molnar et al. [28]).

black-box ML models, such as multilayer perceptron (MLP) neural networks and GBMs, are said to be directly uninterpretable, potentially unsafe for use on humans, but not necessarily completely unexplainable. In this text *interpretable* or *white-box models* will include linear models, decision trees, constrained or Bayesian variants of traditional black-box ML models, or novel types of models designed to be directly interpretable. Additional examples of sophisticated and interpretable modeling techniques include explainable neural networks (XNNs), explainable boosting machines (EBMs), monotonically constrained gradient boosting machines (GBMs), scalable Bayesian rule lists, or super-sparse linear integer models (SLIMs), [36], [37], [40].[7,8,9]

1.3 Model Debugging and Fairness

Herein *model debugging* refers to testing ML models to increase trust in model mechanisms and predictions. Examples of model debugging techniques include variants of sensitivity (i.e. "what-if?") analysis, residual analysis, assertions, and units test used to verify the accuracy or security of ML models.[10] Model debugging should also include remediating any discovered errors or vulnerabilities. Here *fairness* techniques refer to disparate impact analysis, model selection by minimization of disparate impact, and remediation techniques such as disparate impact removal preprocessing or equalized odds post-processing [8], [19].[11]

1.4 Human-Centered ML

Finally, this text does not seek to redefine *human-centered ML* which has a notable presence in the human computer interaction (HCI) literature and is often associated with interactive software for enabling greater human control and understanding of ML processes [12]. This text simply seeks to draw attention to mostly newer, but certainly some pre-existing or established, ML techniques that may further the goals of human-centered ML. This text also acknowledges the importance of informed user interaction and user interface design and implementation in the adoption of any proposed guidelines.

2 GUIDELINES

Four guidelines are presented and discussed in Sections 2.1 – 2.4 to assist practitioners in avoiding any unintentional misuse or in identifying any intentional abuse of explainable ML techniques. The guidelines are:

(1) Use explanations to enable understanding, not trust.
(2) Learn how explainable ML is used for nefarious purposes.
(3) Augment surrogate models with direct explanations.
(4) Use fully transparent ML mechanisms for systems that affect humans.

Important corollaries to the guidelines are also highlighted and simple, reproducible software examples accompany the guidelines to avoid hypothetical reasoning whenever possible.

2.1 Guideline: Use Explanations to Enable Understanding, not Trust.

While they are likely necessary for trust in many cases, explanations are certainly not sufficient for trust in all cases. Explanation, as a general concept, is related more directly to understanding and transparency than to trust.[12] Simply put, one can understand and explain a model without trusting it. One can also trust a model and not be able to understand or explain it. Consider the following example scenarios.

- **Explanation and understanding without trust**: In Figure 1, global Shapley explanations and residual analysis identify a pathology in an unconstrained GBM model, g_{GBM}, trained on the UCI credit card dataset [22].[13] g_{GBM} over emphasizes the input feature PAY_0, or a customer's most recent repayment status. Due to over-emphasis of PAY_0, g_{GBM} is often unable to predict on-time payment if recent payments are delayed (PAY_0 > 1), causing large negative residuals. g_{GBM} is also often unable to predict default if recent payments are made on-time (PAY_0 $\leq$ 1), causing large positive residuals. In this example scenario, g_{GBM} is explainable, but not trustworthy.
- **Trust without explanation and 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.[14] However, they were not explainable or well-understood by contemporary standards.

If trust in models is your goal, then explanations alone are not sufficient. However, as discussed in Sections 2.4 and 3 and illustrated in Figure 4, in an ideal scenario, explanation techniques would be used with a wide variety of other methods to increase accuracy, fairness, interpretability, privacy, security, and trust in ML models.

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

When used disingenuously, explainable ML methods can provide cover for misused or intentionally abusive black-boxes [1]. Explainable ML methods can also enable hacking or stealing of models through public prediction APIs or other endpoints [35]. Moreover, explainable ML methods are likely to be used for other nefarious purposes in the future and may be used for unknown destructive purposes now. Responsible practitioners need to understand the malevolent side of this technology to better detect and correct misuse and abuse. Given that explainable ML techniques have already

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[7]As implemented in the Microsoft 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 other similar techniques, say those mentioned here: https://users.cs.duke.edu/~cynthia/papers.html.

[10]And other similar techniques, say those mentioned here: https://debug-ml-iclr2019.github.io/.

[11]And other similar techniques, say those mentioned here: http://www.fatml.org/resources/relevant-scholarship.

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

[13]Code to replicate Figure 1 is available here: https://github.com/jphall663/responsible_xai.

[14]For example: https://www.sas.com/en_ph/customers/hsbc.html, https://www.kdnuggets.com/2011/03/sas-patent-fraud-detection.html.
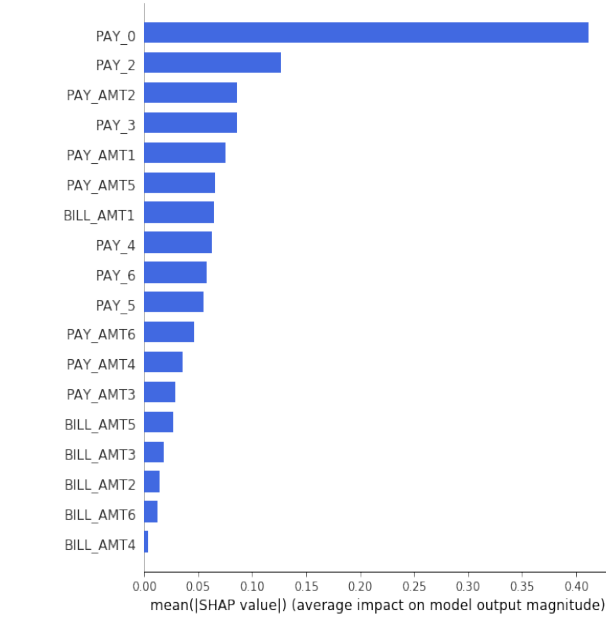
(a) Consistent global Shapley feature importance values for g_{GBM}.
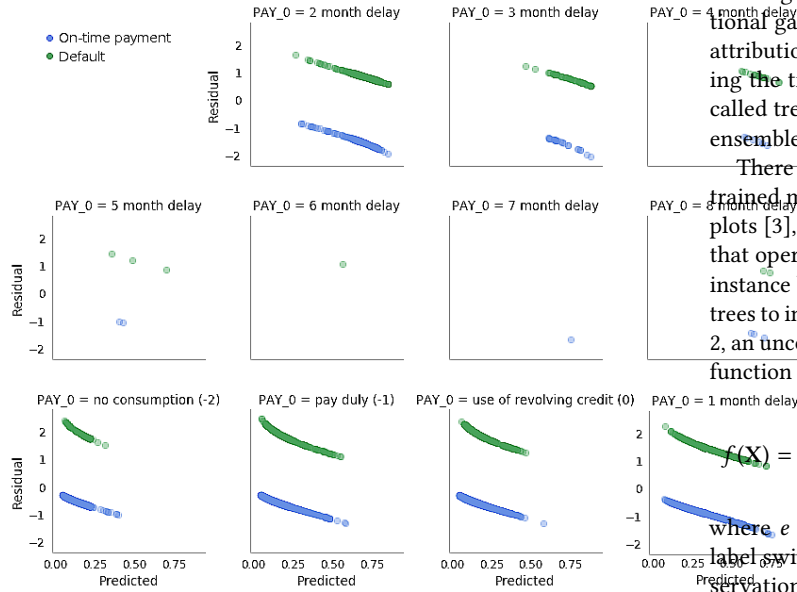
(b) g_{GBM} deviance residuals and predictions by PAY_0.

Figure 1: An unconstrained GBM probability of default model, g_{GBM}, generally over-emphasizes 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 $\leq$ 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.

been released in popular open source and commercial software, it seems there is a need for agreed-upon best practices and education on responsible use.

2.2.1 Guideline Corollary: Explainable ML Can be Used to Crack Nefarious Black-boxes. Used as white-hat hacking tools, explainable ML methods can draw attention to potential fairness or accuracy problems in proprietary black-boxes. See Angwin et al. [2] for evidence that cracking of commercial black-box models for oversight purposes is possible.[15] Such investigations would likely only be improved by advances in explanatory and fairness tools.

2.3 Augment Surrogate Models with Direct Explanations.

Models of models, or surrogate models, can be helpful explanatory tools, but they are usually approximate, low-fidelity explainers. Aside from 1.) a global or local summary of a complex model provided by a surrogate model can be helpful sometimes and 2.) much work in explainable ML has been directed toward improving the fidelity and usefulness of surrogate models [4], [5], [6], [20], [37], *many explainable ML techniques have nothing to do with surrogate models!* One of the most exciting breakthroughs for supervised learning problems in explainable ML is the application of a coalitional game theory concept, Shapley values, to compute feature attributions which are consistent globally and accurate locally using the trained model itself [26], [34]. An extension of this idea, called tree SHAP, has already been implemented for popular tree ensemble methods [25].

There are many other explainable ML methods that operate on trained models directly such as partial dependence, ALE, and ICE plots [3], [11], [14]. Surrogate models and explanatory techniques that operate directly on trained models can also be combined, for instance by using partial dependence, ICE, and surrogate decision trees to investigate and confirm modeled interactions [18]. In Figure 2, an unconstrained GBM, g_{GBM}, models a known signal generating function f:

$$f(\mathbf{X}) = \begin{cases} 1 & \text{if } X_{\text{num1}} * X_{\text{num4}} + |X_{\text{num8}}| * X_{\text{num9}}^2 + e \geq 0.42 \\ 0 & \text{if } X_{\text{num1}} * X_{\text{num4}} + |X_{\text{num8}}| * X_{\text{num9}}^2 + e < 0.42 \end{cases}$$
(1)

where e signifies the injection of random noise in the form of label switching for roughly 15% of the training and validation observations.[16] g_{GBM} is then trained such that $g_{\text{GBM}}(\mathbf{X}) \approx f(\mathbf{X})$ in training and validation data. h_{tree}, displayed in Figure 2a, is extracted such that $h_{\text{tree}}(\mathbf{X}) \approx g_{\text{GBM}}(\mathbf{X}) \approx f(\mathbf{X})$ in validation data. Partial dependence and ICE plots are generated directly for g_{GBM} in the same validation data and overlaid in Figure 2b. The parent-child node relationship displayed between X_{num9} and X_{num8} for $\sim -0.923 < X_{\text{num9}} <\sim 1.04$ in 2a and the divergence of ICE and partial dependence curves in 2b for $\sim -1 < X_{\text{num9}} <\sim 1$ help confirm

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[15]This text makes no claim on the quality of the analysis in Angwin et al. (2016), which has been criticized [9]. This now infamous analysis is presented only as evidence that motivated activists can crack commercial black-boxes using surrogate models and other explanatory techniques.

[16]Code to replicate Figure 2 is available here: https://github.com/h2oai/mli-resources/tree/master/lime_shap_treeint_compare.
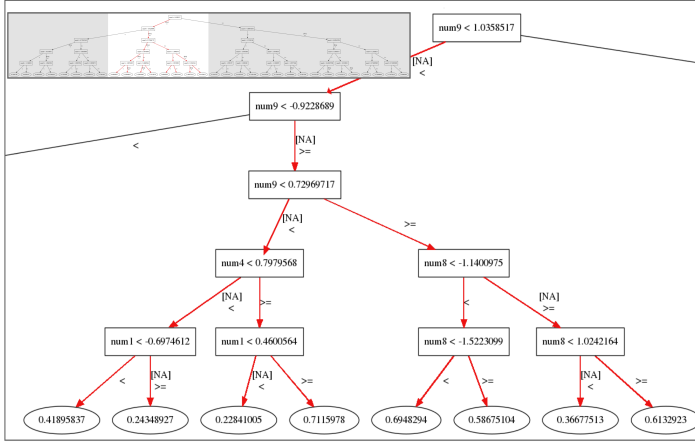
(a) Naïve h_{tree}, a surrogate model, forms an approximate overall flowchart for the explained model, g_{GBM}.
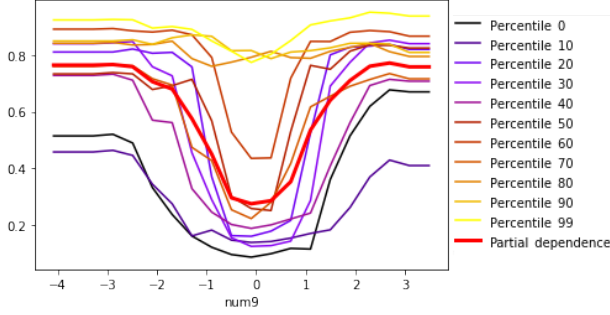
(b) Partial dependence and ICE curves generated *directly from the explained model, g_{GBM}*.

Figure 2: h_{tree} displays known interactions in $f = X_{num1} * X_{num4} + |X_{num8}| * X_{num9}^2$ for $\sim -0.923 < X_{num9} <\sim 1.04$. 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 $\sim -1 < X_{num9} <\sim 1$. Explanations from a surrogate model have augmented and confirmed findings from a direct model visualization technique.

and understand how g_{GBM} learned the interaction between X_{num8} and X_{num9} in f. Like in Figure 1, combining different approaches provided additional, beneficial information about a complex ML model.

2.3.1   Guideline Corollary: Augment LIME with Direct Explanations.
LIME is important, imperfect (like every other ML technique), and one of many explainable ML tools. LIME, in it's most popular implementation, uses local linear surrogate models to explain regions of complex, machine-learned response functions [30]. Like other surrogate models, LIME can be combined with model-specific methods to yield deeper insights. Consider that tree SHAP can provide locally accurate and consistent point estimates for local feature importance as in 3b. LIME can then provide approximate information about modeled local linear trends around the same point. Table 1 contains LIME h_{GLM} coefficients for a local region of a

validation set sampled from the UCI credit card data defined by `PAY_0 > 1`, or customers with a fairly high risk of default due to late most recent payments.[17] h_{GLM} models the predictions of a simple interpretable decision tree model, g_{tree}, displayed in 3a. h_{GLM} coefficients show linear trends between features in the sampled set $X_{PAY\_0>1}$ and $g_{tree}(X_{PAY\_0>1})$. Because h_{GLM} is relatively well-fit (0.73 R^2) and has a logical intercept (0.77), 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. This additional information can be useful for model debugging and compliance purposes.

Table 1: Coefficients for a local linear interpretable model, h_{GLM}, with an intercept of 0.77 and an R^2 of 0.73. h_{GLM} is trained on a segment of the UCI credit card dataset containing higher-risk customers with late most recent repayment statuses, $X_{PAY\_0>1}$, and the predictions of a simple decision tree, $g_{tree}(X_{PAY\_0>1})$.

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 Systems That Affect Humans.

Explanation, along with white-box 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 like surrogate models, partial dependence plots, and global feature importance are already used to document, understand, and validate different types of models in the financial services industry [20], [37].[2, ??] Moreover, adverse action notices are mandated under the Equal Credit Opportunity Act (ECOA) and the Fair Credit Reporting Act (FCRA) for many credit lending, employment, and insurance decisions in the United States.[18] If ML is used for such decisions it must be explained in terms of adverse action notices.[19] Shapley values, and other local feature importance approaches, provide a convenient methodology to rank the direct contribution of input features to final model decisions and potentially generate customer-specific adverse action notices. In these application domains, interpretability is simply a

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[17]Code to replicate Table 1 is available here: https://github.com/jphall663/responsible_xai.
[18]See: https://consumercomplianceoutlook.org/2013/second-quarter/adverse-action-notice-requirements-under-ecoa-fcra/.
[19]This is apparently *already* happening: https://www.prnewswire.com/news-releases/new-patent-pending-technology-from-equifax-enables-configurable-ai-models-300701153.html.

legal necessity.

Aside from regulatory mandates, explanation enables logical appeal processes for automated 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? 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.[20]

Some may argue that, outside of regulated dealings, for a model with little or no impact on humans and that has been thoroughly and responsibly tested by knowledgeable practitioners, that explanation is *really* unnecessary. While that statement appears technically true, the counter argument in this case centers on human learning from ML models. Explanatory techniques allow practitioners to gain insights from complex models about nonlinear or faint phenomena and complex interactions – information that may sometimes be unlearnable by linear models. Also, why go through the weeks, months, or years of training and deploying a production ML system, and not take a small percentage of that time to learn about the model's findings?

2.4.1 Guideline Corollary: Use Interpretable Models Along with Explanation Techniques.
A few well-known publications have focused either on white-box modeling techniques (e.g. Ustun and Rudin [36], Yang et al. [40]) or on post-hoc explanations (e.g. Lundberg and Lee [26], Ribeiro et al. [30]), but the two can be used together in the context of a broader and more human-centered ML workflow as illustrated in Figure 4. Consider the seemingly useful example case of augmenting globally interpretable models with local post-hoc explanations. A practitioner could train a single decision tree, a globally interpretable model, then apply local explanations in the form of Shapley feature importance as illustrated in Figure 3.[21] This enables the practitioner to see accurate numeric feature contributions for each model prediction in addition to the entire directed graph of the decision tree. Even for interpretable models, such as linear models and decision trees, it has been shown that Shapley values present accuracy and consistency advantages over standard feature attribution methods [23], [25], [26]. Shapley values also enable the ranking of input features for each model decision, which is likely helpful for FCRA and ECOA compliance. Another twist on the idea of combining explainable ML methods and white-box models is described in "Surrogate Assisted Feature Extraction for Machine Learning (SAFE ML)" (Gosiewska et al. [16]). In the SAFE ML approach, features learned by more complex models are extracted and used in an explainable fashion to increase the accuracy of more interpretable models. Aren't either of these augmented processes more desirable than either a white-box model or post-hoc explanations alone?
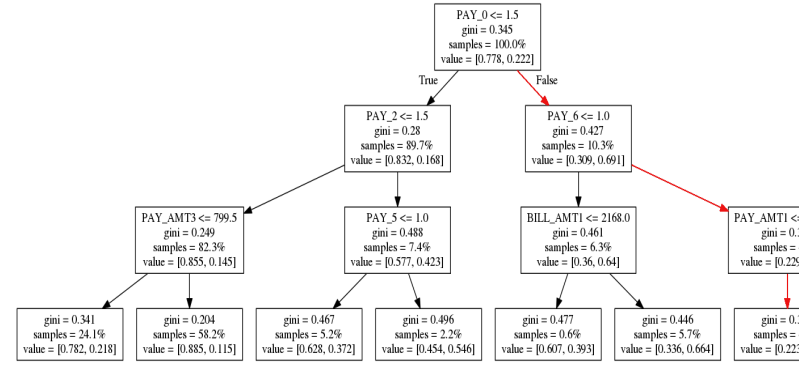
(a) Simple decision tree, g_{tree}, trained on the UCI credit card data to predict defau with validation AUC of 0.74. The decision policy for a high-risk individual is hig lighted in red.
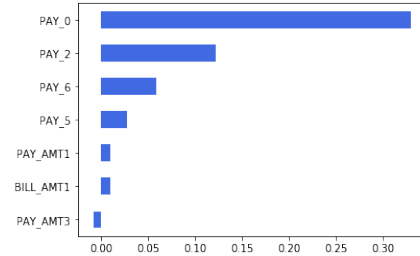
(b) Locally-accurate Shapley contributions for the highlighted individual's probability of default.

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 `PAY_2`, the individual's second most recent repayment status, which could be underestimated by examining the decision policy alone.

2.4.2 Guideline Corollary: Use Explanations Along with Disparate Impact Analysis.
Like white-box models, fairness methods (e.g. Feldman et al. [8], Hardt et al. [19]) are often presented in different articles than post-hoc explanatory methods. However, in banks, using post-hoc explanatory tools such as partial dependence plots to comply with model documentation guidance often goes along with using disparate impact analysis to comply with fair lending regulations.[??,22,23]. To clarify, explanatory techniques should *not* replace disparate impact testing for bias detection purposes, but in general, explanations increase transparency and understanding of

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model mechanisms and predictions while disparate impact auditing and remediation increases trust that model predictions are as fair as possible. As in previous sections, trust and understanding are different but complimentary goals achieved by combining multiple approaches.

Table 2: Basic group disparity metrics across different marital statuses for monotonically constrained GBM model, g_{mono}, trained on the UCI credit card dataset.

|	Adverse Impact Disparity	Accuracy Disparity	TPR Disparity	TNR Disparity	FPR Disparity
married	1.00	1.00	1.00	1.00	1.00
single	0.89	1.03	0.99	1.03	0.85
divorced	1.01	0.93	0.81	0.96	1.25
other	0.26	1.12	0.62	1.17	0

Table 2 displays basic group disparity metrics for a monotonically constrained GBM model, g_{mono}, trained on the UCI credit card data.[24] In this example scenario, g_{mono} displays group parity according to the four-fifths rule with married as the reference level for single customers, but exposes potential disparate impact for divorced customers and customers with martial status of other (for which there is very little training data). Alternative models with less disparate impact or other remediation processes should be considered in such cases to increase trust ML systems.

3 CONCLUSION

ML systems are used today to make life-altering decisions about employment, bail, parole, and lending.[25] The scope of decisions delegated to ML systems seems likely only to expand in the future. Many researchers and practitioners are tackling disparate impact, inaccuracy, privacy violations, and security vulnerabilities with a number of brilliant, but perhaps siloed, approaches. By presenting some straightforward explainable ML guidelines, this short text 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 new and more human-centered type of ML potentially better-suited for use in business- and life-critical decision support than conventional methods.

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[24]Code to replicate Table 2 is available here: https://github.com/jphall663/responsible_xai.

[25]ICLR 2019 model debugging workshop CFP: https://debug-ml-iclr2019.github.io/.
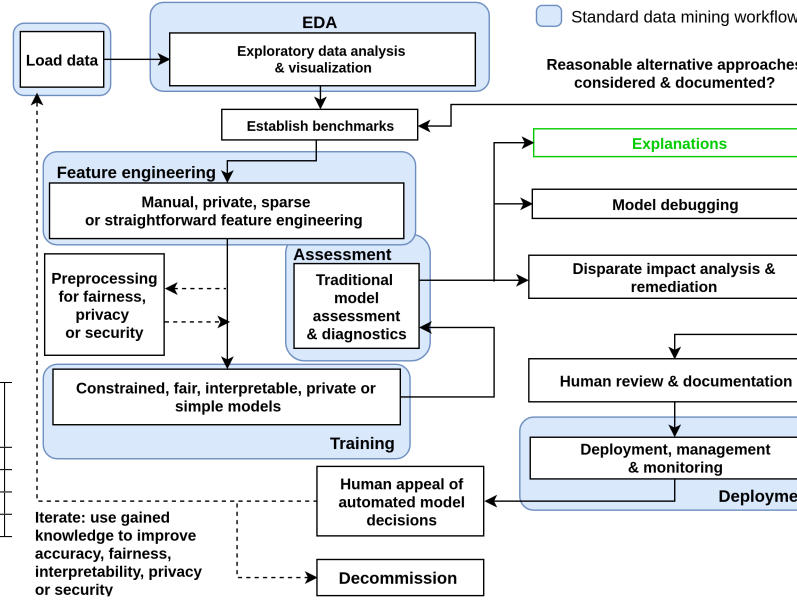
Figure 4: A diagram of a proposed human-centered ML workflow in which explanations (highlighted in green) are used along with interpretable or white-box models, disparate impact analysis and remediation techniques, and other review and appeal mechanisms to create a fair, accountable, and transparent ML system.

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