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Responsible Machine Learning

with Interpretable Models, Post-hoc Explanation, and Disparate Impact Testing

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Abstract: This text outlines a viable approach for training and evaluating machine learning systems for high-stakes, human-centered, or regulated applications using common Python programming tools. The accuracy and intrinsic interpretability of two types of constrained models, monotonic gradient boosting machines (M-GBM) and explainable neural networks (XNN), a deep learning architecture well-suited for structured data, are assessed on simulated data with known feature importance and sociological bias characteristics and on realistic, publicly available lending data. For maximum transparency and the potential generation of personalized adverse action notices, the constrained models are analyzed using post-hoc explanation techniques including plots of partial dependence and individual conditional expectation (ICE) and global and local gradient-based or Shapley feature importance. The constrained model predictions are also tested for disparate impact and other types of sociological bias using straightforward group fairness measures. By combining innovations in interpretable models, post-hoc explanation, and bias testing with accessible software tools, this text aims to provide a template workflow for important machine learning applications that require high accuracy and interpretability and low disparate impact.

Keywords: Machine Learning; Neural Network; Gradient Boosting Machine; Interpretable; Explanation; Fairness; Disparate Impact; Python

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0. Introduction

1. Materials and Methods

1.1. Notation

To facilitate descriptions of data, modeling, explanatory, and social bias techniques, notation for input and output spaces, datasets, and models is defined.

1.1.1. Spaces

- Input features come from the set $\mathcal{X}$ contained in a P-dimensional input space, $\mathcal{X} \subset \mathbb{R}^P$. An arbitrary, potentially unobserved, or future instance of $\mathcal{X}$ is denoted $\mathbf{x}$, $\mathbf{x} \in \mathcal{X}$.
- Labels corresponding to instances of $\mathcal{X}$ come from the set $\mathcal{Y}$.
- Learned output responses come from the set $\hat{\mathcal{Y}}$.

1.1.2. Datasets

- The input dataset $\mathbf{X}$ is composed of observed instances of the set $\mathcal{X}$ with a corresponding dataset of labels $\mathbf{Y}$, observed instances of the set $\mathcal{Y}$.

- Each i-th observation of $\mathbf{X}$ is denoted as $\mathbf{x}^{(i)} = [x_0^{(i)}, x_1^{(i)}, \ldots, x_{P-1}^{(i)}]$, with corresponding i-th labels in $\mathbf{Y}$, $\mathbf{y}^{(i)}$, and corresponding predictions in $\hat{\mathbf{Y}}$, $\hat{\mathbf{y}}^{(i)}$.
- $\mathbf{X}$ and $\mathbf{Y}$ consist of N tuples of observations: $[(\mathbf{x}^{(0)}, \mathbf{y}^{(0)}), (\mathbf{x}^{(1)}, \mathbf{y}^{(1)}), \ldots, (\mathbf{x}^{(N-1)}, \mathbf{y}^{(N-1)})]$.
- Each j-th input column vector of $\mathbf{X}$ is denoted as $X_j = [x_j^{(0)}, x_j^{(1)}, \ldots, x_j^{(N-1)}]^T$.

1.1.3. Models

- A type of machine learning model g, selected from a hypothesis set $\mathcal{H}$, is trained to represent an unknown signal-generating function f observed as $\mathbf{X}$ with labels $\mathbf{Y}$ using a training algorithm $\mathcal{A}$: $\mathbf{X}, \mathbf{Y} \xrightarrow{\mathcal{A}} g$, such that $g \approx f$.
- g generates learned output responses on the input dataset $g(\mathbf{X}) = \hat{\mathbf{Y}}$, and on the general input space $g(\mathcal{X}) = \hat{\mathcal{Y}}$.
- The model to be explained and tested for unwanted social bias is denoted as g.

1.2. Data Description

1.3. Model Description

1.3.1. Explainable Neural Network

Explainable neural networks (XNNs) are an alternative formulation of additive index models in which the ridge functions are neural networks [1]. XNNs also bare a strong resemblance to generalized additive models (GAMs) and so-called explainable boosting machines (EBMs or GA^{2}M), i.e. GAMs which consider main effects and a small number of 2-way interactions and incorporate boosting in their training [2], [3]. Hence, XNNs enable users to tailor interpretable neural network architectures to a given prediction problem and to visualize model behavior by plotting ridge functions. XNNs are composed of a global bias term, μ_0, K individually specified neural networks, n_k with scale parameters γ_k, and the inputs to each n_k are themselves a linear combination of modeling inputs, $\sum_{j=0}^{J} \beta_{k,j} x_j$.

$$g^{\text{XNN}}(\mathbf{x}) = \mu_0 + \sum_{k=1}^{K} \gamma_k n_k \left(\sum_{j=1}^{J} \beta_{k,j} x_j\right) \tag{1}$$

g^{XNN} is comprised of 3 meta-layers:

1. The first and deepest meta-layer, composed of K linear $\sum_j \beta_{k,j} x_j$ hidden units, is known as the *projection layer* and is fully connected to each input feature, X_j.
2. The second meta-layer contains K hidden and separate n_k ridge functions, or *subnetworks*. Each n_k is a neural network, which can be parameterized to suite a given modeling task. To facilitate direct visualization, the input to each subnetwork is the 1-dimensional output of its associated projection layer hidden unit, $\sum_j \beta_{k,j} x_j$.
3. The output meta-layer, called the *combination layer*, is another linear unit comprised of a global bias term, μ_0, and the K weighted 1-dimensional outputs of each subnetwork, $\gamma_k n_k(\sum_j \beta_{k,j} x_j)$. Again, subnetwork output is restricted to 1-dimension for visualization purposes.

g^{XNN} is typically trained by mini-batch stochastic gradient descent (SGD). L_1 regularization is often applied to both the projection and combination layers to induce a sparse and interpretable model, where each n_k subnetwork and corresponding combination layer γ_k are ideally associated with an important X_j or combination thereof.

1.3.2. Monotonically Constrained Gradient Boosting Machine

Monotonic gradient boosting machines (M-GBMs) constrain typical GBM training to consider only tree splits that obey user-defined positive and negative monotonicity constraints. The M-GBM

remains an additive combination of B trees trained by gradient boosting, T_b, but each tree learns a set of splitting rules that respect monotonicity constraints, Θ_b^{mono}.

$$g^{\text{mono}}(\mathbf{x}) = \sum_{b=1}^{B} T_b\left(\mathbf{x}; \Theta_b^{\text{mono}}\right) \tag{2}$$

As in unconstrained GBM, Θ_b^{mono} is selected in a greedy, additive fashion by minimizing a regularized loss function that considers known target labels, $\mathbf{y}$, the predictions of all subsequently trained trees in the M-GBM, $g_{b-1}^{\text{mono}}(\mathbf{X})$, and a regularization term that penalizes complexity in the current tree, $\Omega(T_b)$. For the b-th iteration, the loss function, $\mathcal{L}_b$, can generally be defined as:

$$\mathcal{L}_b = \sum_{i=0}^{N-1} l(y^{(i)}, g_{b-1}^{\text{mono}}(\mathbf{x}^{(i)}), T_b(\mathbf{x}^{(i)}; \Theta_b^{\text{mono}})) + \Omega(T_b) \tag{3}$$

In addition to $\mathcal{L}_b$, g^{mono} training is characterized by additional splitting rules and constraints on tree node weights. Each binary splitting rule, $\theta_{b,j,k} \in \Theta_b$, is associated with a feature, X_j, is the k-th split associated with X_j in T_b, and results in left and right child nodes with a numeric weights, $\{w_{b,j,k,L}, w_{b,j,kR}\}$. For terminal nodes, $\{w_{b,j,k,L}, w_{b,j,kR}\}$ can be direct numeric components of some g^{mono} prediction. For two values of some feature X_j, $x_j^{\alpha} \leq x_j^{\beta}$, where the prediction for each value results in $T_b(x_j^{\alpha}; \Theta_b) = w_{\alpha}$ and $T_b(x_j^{\beta}; \Theta_b) = w_{\beta}$, Θ_b is restricted to be positive monotonic w.r.t. X_j by the following rules and constraints.

1. For the first and highest split in T_b involving X_j, any $\theta_{b,j,0}$ resulting in the left child weight being greater than the right child weight, $T(x_j; \theta_{b,j,0}) = \{w_{b,j,0,L}, w_{j,0,R}\}$ where $w_{b,j,0,L} > w_{b,j,0,R}$, is not considered.
2. For any subsequent left child node involving X_j, any $\theta_{b,j,k\geq 1}$ resulting in $T(x_j; \theta_{b,j,k\geq 1}) = \{w_{b,j,k\geq 1,L}, w_{b,j,k\geq 1,R}\}$ where $w_{b,j,k\geq 1,L} > w_{b,j,k\geq 1,R}$, is not considered.
3. Moreover, for any subsequent left child node involving X_j, $T(x_j; \theta_{b,j,k\geq 1}) = \{w_{b,j,k\geq 1,L}, w_{b,j,k\geq 1,R}\}$, $\{w_{b,j,k\geq 1,L}, w_{b,j,k\geq 1,R}\}$ are bound by the parent set of node weights, $\{w_{b,j,k-1,L}, w_{b,j,k-1,R}\}$, such that $\{w_{b,j,k\geq 1,L}, w_{b,j,k\geq 1,R}\} \leq \frac{w_{b,j,k-1,L} + w_{b,j,k-1,R}}{2}$.
4. (1) and (2) are also applied to all right child nodes, except that for right child nodes $\{w_{b,j,k\geq 1,L}, w_{b,j,k\geq 1,R}\} \geq \frac{w_{b,j,k-1,L} + w_{b,j,k-1,R}}{2}$.

Note that for any one X_j and $T_b \in g^{\text{mono}}$ left subtrees will alway produce lower predictions than right subtrees, and that any $g^{\text{mono}}(\mathbf{x})$ is an addition of each T_b output, with the application of a monotonic logit or softmax link function for classification problems. Moreover, each tree's root node corresponds to some constant node weight that by definition obeys monotonicity constraints, $T(x_j^{\alpha}; \theta_{b,0}) = T(x_j^{\beta}; \theta_{b,j,0}) = w_{b,0}$. Together these additional splitting rules and node weight constraints ensure that $g^{\text{mono}}(x_j^{\alpha}) \leq g^{\text{mono}}(x_j^{\beta}) \; \forall \; x_j^{\alpha} \leq x_j^{\beta} \in X_j$. For a negative monotonic constraint, i.e. $g^{\text{mono}}(x_j^{\alpha}) \geq g^{\text{mono}}(x_j^{\beta}) \; \forall \; x_j^{\alpha} \leq x_j^{\beta} \in X_j$, left and right splitting rules and node weight constraints are switched.

1.4. Explanatory Method Description

1.4.1. Partial Dependence and Individual Conditional Expectation

Partial dependence (PD) plots are a widely-used method for describing the average predictions of a complex model g across some partition of data $\mathbf{X}$ for some interesting input feature X_j [2]. Individual conditional expectation (ICE) plots are a newer method that describes the local behavior of g for a single instance $\mathbf{x} \in \mathcal{X}$. Partial dependence and ICE can be combined in the same plot to compensate for known weaknesses of partial dependence, to identify interactions modeled by g, and to create a holistic portrait of the predictions of a complex model for some X_j [4].

Following Friedman *et al.* [2] a single feature $X_j \in \mathbf{X}$ and its complement set $\mathbf{X}_{(-j)} \in \mathbf{X}$ (where $X_j \cup \mathbf{X}_{(-j)} = \mathbf{X}$) is considered. $\text{PD}(X_j, g)$ for a given feature X_j is estimated as the average output of the learned function $g(\mathbf{X})$ when all the observations of X_j are set to a constant $x \in \mathcal{X}$ and $\mathbf{X}_{(-j)}$ is left unchanged. $\text{ICE}(x_j, \mathbf{x}, g)$ for a given instance $\mathbf{x}$ and feature x_j is estimated as the output of $g(\mathbf{x})$ when x_j is set to a constant $x \in \mathcal{X}$ and all other features $\mathbf{x} \in \mathbf{X}_{(-j)}$ are left untouched. Partial dependence and ICE curves are usually plotted over some set of constants $x \in \mathcal{X}$.

1.4.2. Shapley Values

Shapley explanations, including Tree SHAP (SHapley Additive exPlanations) , are a class of additive, locally accurate feature contribution measures with long-standing theoretical support [5]. Shapley explanations are the only possible locally accurate and globally consistent feature contribution values, meaning that Shapley explanation values for input features always sum to $g(\mathbf{x})$ and that Shapley explanation values can never decrease for some x_j when g is changed such that x_j truly makes a stronger contribution to $g(\mathbf{x})$ [5].

For some observation $\mathbf{x} \in \mathcal{X}$, Shapley explanations take the form:

$$g(\mathbf{x}) = \phi_0 + \sum_{j=0}^{j=\mathcal{P}-1} \phi_j \mathbf{z}_j \tag{4}$$

In Equation 4, $\mathbf{z} \in \{0,1\}^{\mathcal{P}}$ is a binary representation of $\mathbf{x}$ where 0 indicates missingness. Each ϕ_j is the local feature contribution value associated with x_j and ϕ_0 is the average of $g(\mathbf{X})$.

Shapley values can be estimated in different ways. Tree SHAP is a specific implementation of Shapley explanations that relies on traversing internal tree structures to estimate the impact of each x_j for some $g(\mathbf{x})$ of interest [6].

$$\phi_j = \sum_{S \subseteq \mathcal{P} \setminus \{j\}} \frac{|S|!(\mathcal{P} - |S| - 1)!}{\mathcal{P}!} [g_x(S \cup \{j\}) - g_x(S)] \tag{5}$$

1.5. Social Bias Test Description

1.6. Software Resources

2. Results

2.1. Simulated Data Results

2.2. Loan Data Results

3. Discussion

4. Conclusions

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Conflicts of Interest:

Abbreviations

The following abbreviations are used in this manuscript:

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