Responsible Machine Learning*

Lecture 1: Interpretable Machine Learning Models

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Contents

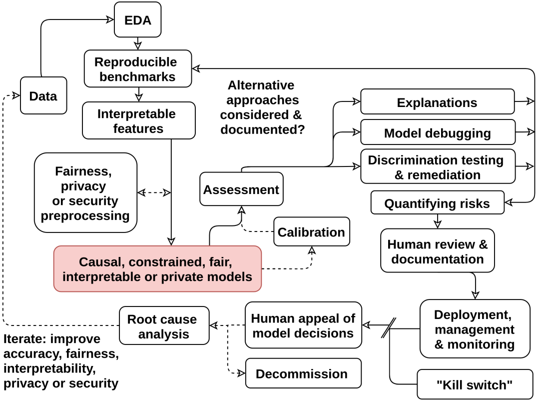
Grading and Policy

- Grading:
  - $\frac{1}{3}$ Participation
  - $\frac{1}{3}$ Project GitHub or Kaggle kernel
  - $\frac{1}{3}$ Public Kaggle leaderboard score
- Project:
  - Kaggle competition using techniques from class
  - Individual or group (no more than 4 members)
  - Select team members ASAP
- Syllabus
- Webex office hours: Thurs. 5-6 pm or by appointment
- Class resources: https://jphall663.github.io/GWU_rml/

Overview

- **Class 1**: Interpretable Models
- **Class 2**: Post-hoc Explanations
- **Class 3**: Fairness
- **Class 4**: Security
- **Class 5**: Model Debugging
- **Class 6**: Best Practices

A Responsible Machine Learning Workflow[†]



[†] *A Responsible Machine Learning Workflow*

Notation

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 $\hat{\mathcal{Y}}$.

Notation

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 $\mathbf{x}^{(i)} = [x_0^{(i)}, x_1^{(i)}, \dots, x_{P-1}^{(i)}]$, 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: $[(\mathbf{x}^{(0)}, \mathbf{y}^{(0)}), (\mathbf{x}^{(1)}, \mathbf{y}^{(1)}), \dots, (\mathbf{x}^{(N-1)}, \mathbf{y}^{(N-1)})]$.
- Each j-th input column vector of $\mathbf{X}$ is denoted as $X_j = [x_j^{(0)}, x_j^{(1)}, \dots, x_j^{(N-1)}]^T$.

Notation

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, tested for discrimination, or debugged is denoted as g.

Background

We will frequently refer to following terms and definitions today:

- Pearson correlation
  - Measurement of the linear relationship between two input X_j; values between -1 and +1, including 0.
- Shapley value
- Partial dependence and individual conditional expectation (ICE)
- Gradient boosting machine (GBM)

Shapley Value

Shapley explanations, including TreeSHAP and even certain implementations of LIME, are a class of additive, locally accurate feature contribution measures with long-standing theoretical support (Lundberg and Lee, 2017).

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

$$\phi_j = \underbrace{\sum_{S \subseteq \mathcal{P} \setminus \{j\}} \frac{|S|!(\mathcal{P} - |S| - 1)!}{\mathcal{P}!}}_{\text{weighted average over all subsets in } \mathbf{X}} \underbrace{(S \cup \{j\}) - g_x(S)]}_{g \text{ "without" } x_j} \tag{1}$$

$$g(\mathbf{x}) = \phi_0 + \sum_{j=0}^{j=\mathcal{P}-1} \phi_j \mathbf{z}_j \tag{2}$$

Partial Dependence and ICE

- Following Friedman, Hastie, and Tibshirani, 2001, 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 components 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 $x \in \mathcal{X}$ (Goldstein et al., 2015).

Gradient Boosting Machine

$$g^{\text{GBM}}(\mathbf{x}) = \sum_{b=0}^{B-1} T_b(\mathbf{x}; \Theta) \tag{3}$$

A GBM is a sequential combination of decision trees, T_b, where T_0 is trained to predict $\mathbf{y}$, but all subsequent T are trained to reduce the errors of T_{b-1}.

Anatomy of Elastic Net Regression: L1 and L2 Penalty

Same basic functional form as more traditional linear models, e.g. ...

$$g^{\text{GLM}}(\mathbf{x}) = \beta_0 + \beta_1 x_0 + \beta_2 x_1 + \cdots + \beta_P x_{P-1} \tag{4}$$

... but more robust to correlation, wide data, and outliers.

Anatomy of Elastic Net Regression: L1 and L2 Penalty

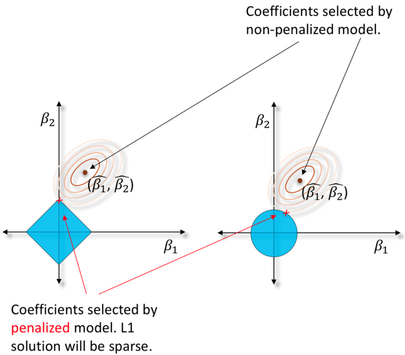
Iteratively reweighted least squares (IRLS) method with ridge (L_2) and LASSO (L_1) penalty terms:

$$\tilde{\beta} = \min_{\beta} \Big\{ \underbrace{\sum_{i=0}^{N-1} (y_i - \beta_0 - \sum_{j=1}^{P-1} x_{ij}\beta_j)^2}_{1} + \underbrace{\lambda}_{2} \sum_{j=1}^{P-1} (\underbrace{\alpha}_{3} \underbrace{\beta_j^2}_{4} + (1 - \underbrace{\alpha}_{3}) \underbrace{|\beta_j|}_{5}) \Big\} \tag{5}$$

- 1: Least square minimization
- 2: Controls magnitude of penalties
- 3: Tunes balane between L1 and L2
- 4: L_2/Ridge penalty term
- 5: L_1/LASSO penalty term

Graphical Illustration of Shrinkage/Regularization Method:

Penalized regression



Monotonic GBM (Gill et al., 2020)

MGBMs constrain typical GBM training to consider only tree splits that obey user-defined positive and negative monotone constraints, with respect to each input feature, X_j, and a target feature, $\mathbf{y}$, independently. An MGBM remains an additive combination of B trees trained by gradient boosting, T_b, and each tree learns a set of splitting rules that respect monotone constraints, Θ_b^{mono}. A trained MGBM model, g^{MGBM}, takes the form:

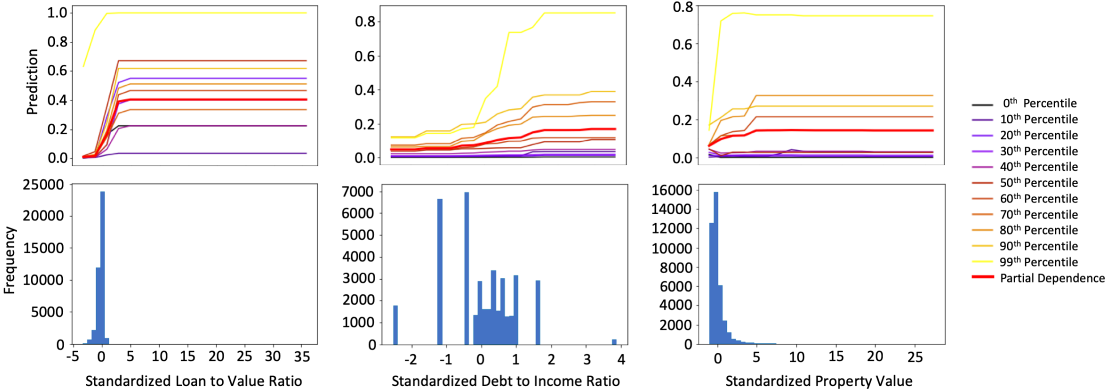
$$g^{\text{MGBM}}(\mathbf{x}) = \sum_{b=0}^{B-1} T_b\left(\mathbf{x}; \Theta_b^{\text{mono}}\right) \tag{6}$$

Monotone Constraints for GBM (Gill et al., 2020)

1. For the first and highest split in T_b involving X_j, any $\theta_{b,j,0}$ resulting in $T(x_j;\theta_{b,j,0}) = \{w_{b,j,0,L}, w_{b,j,0,R}\}$ 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 associated $\theta_{b,j,k-1}$ set of node weights, $\{w_{b,j,k-1,L}, w_{b,j,k-1,R}\}$, such that $\{w_{b,j,k\geq 1,L}, w_{b,j,k\geq 1,R}\} < \frac{w_{b,j,k-1,L}+w_{b,j,k-1,R}}{2}$.
4. (1) and (2) are also applied to all right child nodes, except that for right child nodes $w_{b,j,k,L} \leq w_{b,j,k,R}$ and $\{w_{b,j,k\geq 1,L}, w_{b,j,k\geq 1,R}\} \geq \frac{w_{b,j,k-1,L}+w_{b,j,k-1,R}}{2}$.

Note that $g^{\text{MGBM}}(\mathbf{x})$ is an addition of each full T_b prediction, 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, $T(x_j^{\alpha};\theta_{b,0}) = T(x_j^{\beta};\theta_{b,0}) = w_{b,0}$.

Partial Dependence and ICE:



A Burgeoning Ecosystem of Interpretable Machine Learning Models

- Generalized additive model (GAM) (Friedman, Hastie, and Tibshirani, 2001)
- GA2M/Explainable boosting machine (EBM) (Lou et al., 2013)
- Explainable Neural Network (XNN) (Vaughan et al., 2018)
- Rudin group:
    - *This looks like that* deep learning (Chen et al., 2019)
    - Scalable Bayesian rule list (Yang, Rudin, and Seltzer, 2017)
    - Optimal sparse decision tree (Hu, Rudin, and Seltzer, 2019)
    - Supersparse linear integer models (Ustun and Rudin, 2016)
    - and more ...
- RuleFit (Friedman and Popescu, 2008)

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