Visualization Methods for Explainable Machine Learning

Statistics PhD Oral Prelim

Katherine Goode
Iowa State University
May 6, 2020

Personal Background

Education

B.A. in Mathematics

- Lawrence University (Appleton, WI)
- Graduated in June 2013

M.S. in Statistics

- University of Wisconsin, Madison
- Graduated in May 2015

Ph.D. in Statistics (in progress)

- Iowa State University
- Started in January 2016

Teaching

- Teaching assistant at UW Madison
- Lecturer at Lawrence University
- Lecturer at ISU

Consulting

- AES Statistical Consultant
- NREM Research Assistant

Internship

- Sandia National Labs: Statistical Sciences Research and Development Intern

Overview of Talk

1. Background and Overview of Thesis
2. Detailed explanation of Chapter 1
    - Visual Diagnostics of a Model Explainer -- Tools for the Assessment of LIME Explanations
3. Plan for Chapter 2
    - Explaining Random Forests using Clustering of Trees
4. Ideas for Chapter 3
    - Extensions of Neural Network Explanation Tools to Tabular Data Applications
5. Timeline for Completion
6. Discussion Points

Background and Overview of Thesis

Explainable Machine Learning

- Machine learning models:
  - Good in prediction problems
  - Many considered "black-boxes" since too complex to directly interpret
- Led to research area of explainable machine learning
  - Goal: provide methods to explain predictions made by black-box models
  - Method overview papers/books: (Gilpin, Bau, Yuan, Bajwa, Specter, and Kagal, 2018; Guidotti, Monreale, Ruggieri, Turini, Pedreschi, and Giannotti, 2018; Ming, 2017; Mohseni, Zarei, and Ragan, 2018; Molnar, 2019).
- European General Data Protection Regulation (GDPR) implemented in 2018 includes a "right to explanation"

> Goodman and Flaxman (2016): "It is reasonable to suppose that any adequate explanation would, at a minimum, provide an account of how input features relate to predictions, allowing one to answer questions such as: Is the model more or less likely to recommend a loan if the applicant is a minority?"

Explainability versus Interpretability

No accepted definitions for explainability and interpretability (Gilpin, Bau, Yuan, et al., 2018; Lipton, 2016; Molnar, 2019; Montavon, Samek, and Müller, 2017; Murdoch, Singh, Kumbier, Abbasi-Asl, and Yu, 2019)

My definitions (implicitly used by Rudin (2018) and Ribeiro, Singh, and Guestrin (2016)):

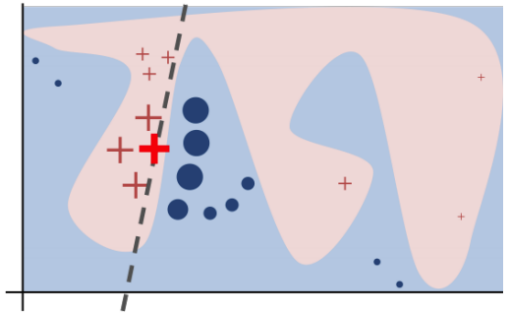
Interpretability is the ability to directly use model parameters to understand the mechanism of how the model makes predictions.

- Linear regression model

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p$$

Explainability is the ability to use the model in an indirect manner to understand the relationships in the data captured by the model.

- LIME: local interpretable model-agnostic explanations (Ribeiro, Singh, and Guestrin, 2016)



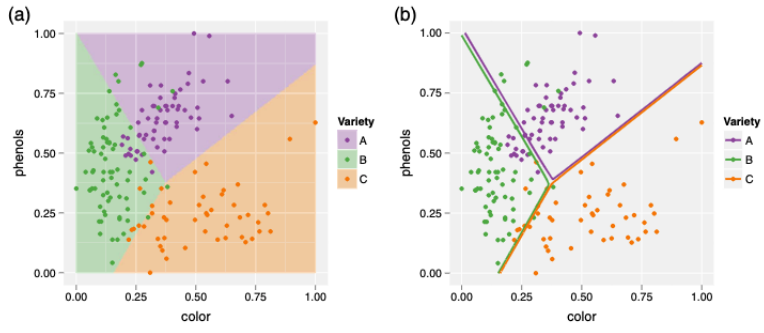
Model Agnostic Methods

General Model Visualizations: Strategies for understanding any model

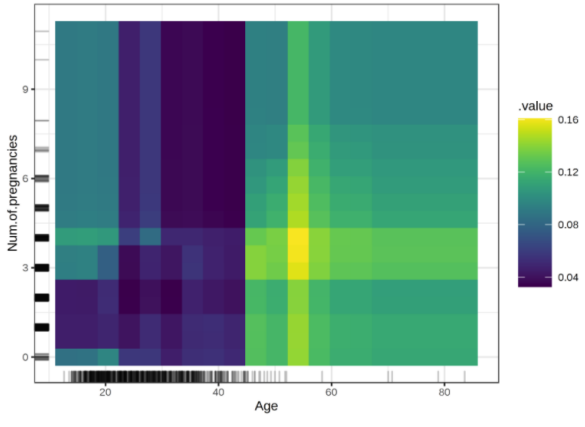
- Removing the blindfold (Wickham, Cook, and Hofmann, 2015)

Global Methods: Explanation for model as a whole

- Partial dependence plots (Friedman, 2001) and extensions:
  - Interactive partial dependence plots (Krause, Perer, and Ng, 2016)
  - Individual conditional expectation plots (Goldstein, Kapelner, Bleich, and Pitkin, 2013)
  - Accumulated local effect plots (Apley and Zhu, 2016)
  - Feature interaction plots (Friedman and Popescu, 2008; Greenwell, Boehmke, and McCarthy, 2018; Hooker, 2004)
- Global feature importance plots (Fisher, Rudin, and Dominici, 2018; Altmann, Toloşi, Sander, and Lengauer, 2010; Casalicchio, Molnar, and Bischl, 2019)
- Global surrogate models (Molnar, 2019)



Model in data-space from Wickham, Cook, and Hofmann (2015).



Partial dependence plot from Molnar (2019).

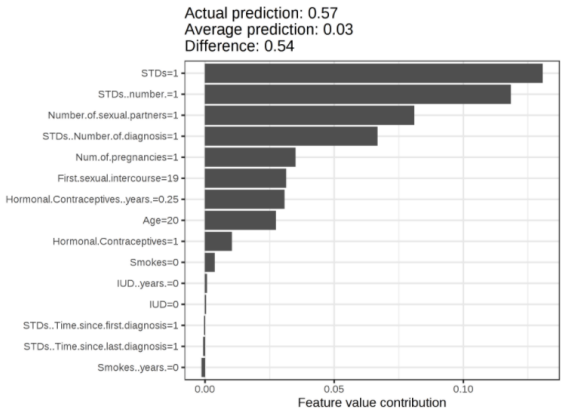
Model Agnostic Methods

Local Methods: Explanation for an individual prediction

- Individual conditional importance plots (Casalicchio, Molnar, and Bischl, 2019)
- LIME (Ribeiro, Singh, and Guestrin, 2016)
- Anchors (scoped rules) (Ribeiro, Singh, and Guestrin, 2018)
- Shapely values
- SHAP (Lundberg and Lee, 2017)
- breakDown (Staniak and Biecek, 2018)

Example Based: Explanations based on examples from the data

- Counterfactual examples (Wachter, Mittelstadt, and Russell, 2017; Martens and Provost, 2014; Looveren and Klaise, 2019; Laugel, Lesot, Marsala, Renard, and Detyniecki, 2017)
- Adversarial examples (Szegedy, Zaremba, Sutskever, Bruna, Erhan, Goodfellow, and Fergus, 2013; Goodfellow, Shlens, and Szegedy, 2014; Biggio and Roli, 2018; Su, Vargas, and Sakurai, 2019)
- Prototypes and criticisms
- Influential instances (Koh and Liang, 2017)



Bar chart of shapley values from Molnar (2019).

Adversarial example where one pixel change affects prediction from Su (2019).

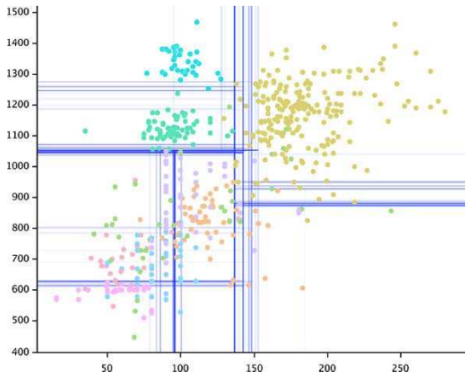
Model Specific Methods

Random Forests

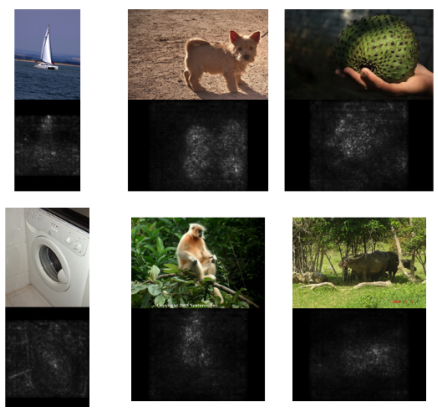
- Random forest impurity based feature importance (Breiman, 2001)
- Sectioned scatterplots (Urbanek, 2008)
- Trace plots of trees (Urbanek, 2008)
- Simplified model (Hara and Hayashi, 2016a)
- Forest floor visualizations (Welling, Refsgaard, Brockhoff, and Clemmensen, 2016)
- Interactive visualizations (Beckett, 2018; da Silva, Cook, and Lee, 2017)

Neural Networks

- Extracting tree structures (Craven and Shavlik, 1996)
- Saliency maps (Simonyan, Vedaldi, and Zisserman, 2013)
- Feature visualization (Olah, Mordvintsev, and Schubert, 2017)
- Grand tours (Li, Zhao, and Scheidegger, 2020)
- Flows (Halnaut, Giot, Bourqui, and Auber, 2020)



Sectioned scatterplot from Urbanek (2008).



Saliency maps from Simonyan, Vedaldi, and Zisserman (2013).

Assessments of Explainable Machine Learning

General

Argument against black box model explanations (Rudin, 2018):

- "Explanations must be wrong."
- Explanations may not:
  - be faithful to the original model
  - make sense
  - be detailed enough to understand the "black-box" model
- Debunks accuracy and interpretability trade-off myth
- Use interpretable models for high-stakes decisions

Method Specific

Assessment of LIME (Laugel, Renard, Lesot, Marsala, and Detyniecki, 2018):

- How to choose a local region?

Assessment of counterfactual examples (Laugel, Renard, Lesot, et al., 2018):

- Issues with unjustified counterfactual examples

Assessment of saliency maps (Kindermans, Hooker, Adebayo, Alber, Schütt, Dähne, Erhan, and Kim, 2017):

- Transformation to input data affects saliency map but not model

Overview of Dissertation Chapters

Chapter 1: Visual Diagnostics for LIME

- Discuss importance of assessing LIME
- Suggest the use of visualizations for assessment and provide example visualizations

Chapter 2: Visualizations for Explaining Random Forests

- Use clustering to identify key tree structures within the random forest
- Improve visualizations for use of trees as global surrogate models

Chapter 3: Visualizations for Explaining Neural Networks

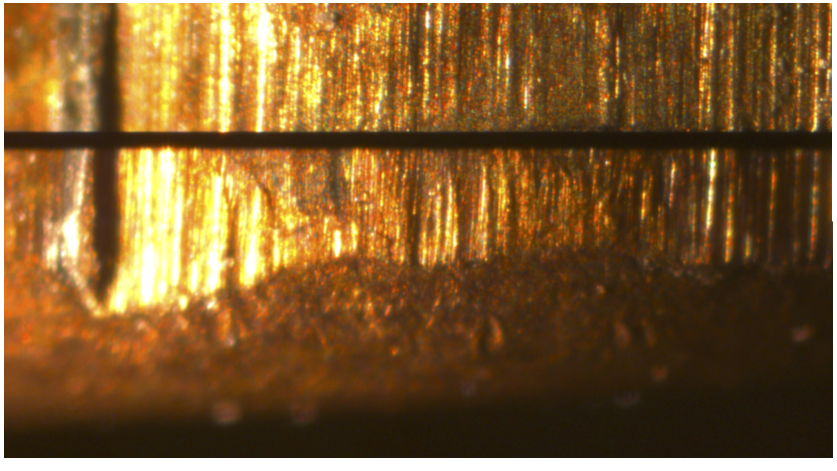
- Project for my internship with Sandia National Labs
- Application with functional data
- Visualizations for the explaining and understanding the models

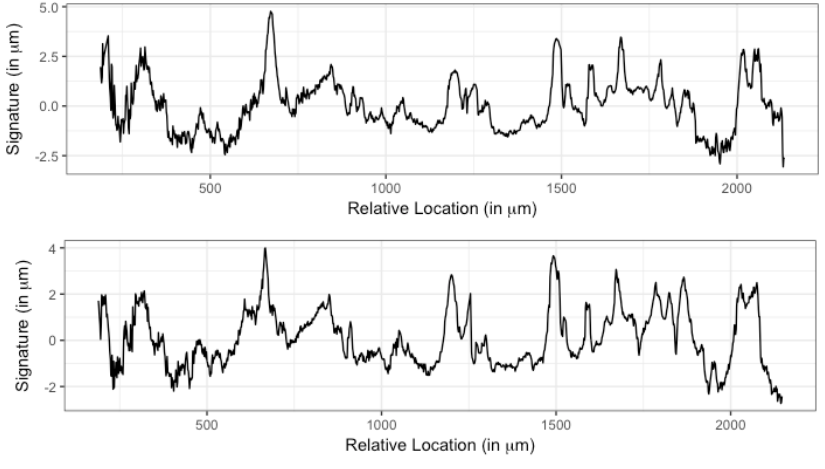
Chapter 1: Visual Diagnostics of a Model Explainer -- Tools for the Assessment of LIME Explanations

Motivation

Hare, Hofmann, and Carriquiry (2016):

- Want to provide quantitative evidence for whether two bullets were fired from the same gun
- Use high definition scans of striations on bullet lands to extract "signatures"
- Compute similarity features to compare two signatures

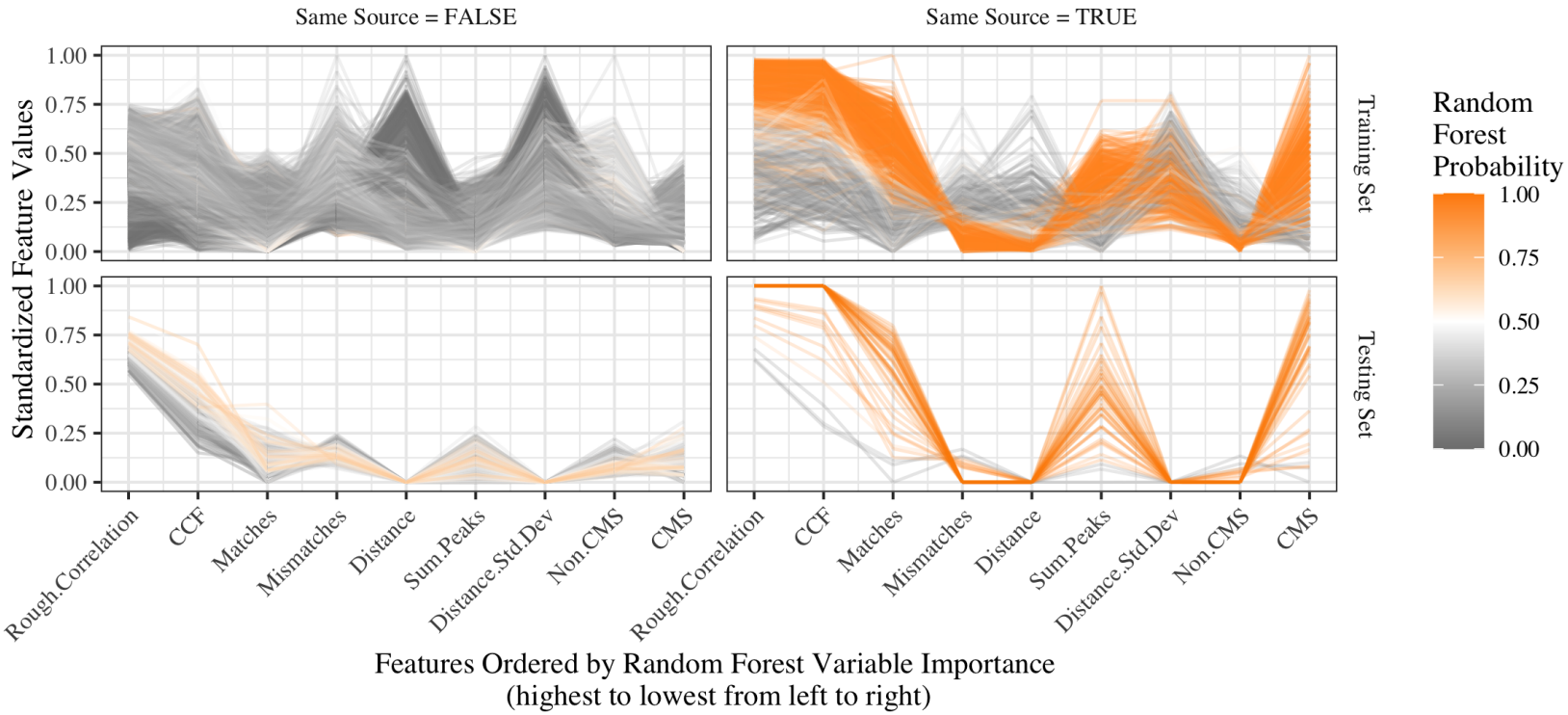




Motivation

Hare, Hofmann, and Carriquiry (2016) approach:

- Random forest model
- 9 signature similarity features
- Returns a score for the comparison of two lands



Motivation

Our Original Goal: Provide explanations for specific signatures comparisons

Attempt: Applied LIME

Result: Unreasonable explanations (e.g., LIME explanation does not agree with random forest prediction)

Example: Known non-match

Conceptual Depiction of LIME

LIME (Ribeiro, Singh, and Guestrin, 2016):

- Local
- Interpretable
- Model-agnostic
- Explanation

Concept: For *one prediction of interest*

- Focus on a neighborhood around the prediction of interest
- Use an inherently interpretable model
- Understand the complex model
- Capture the relationship between the complex model predictions and predictor variables

Importance of Assessing LIME

Additional layer of complexity:

- Start with a complex model
- LIME uses another model
- End with two models to assess

Questions raised:

- Explainer model a good approximation?
- Appropriate local region?
- Relationship linear in the local region?
- Which tuning parameter settings to use when applying LIME?

Visualizations for Model Assessment

Claims made about LIME (Ribeiro, Singh, and Guestrin, 2016):

- **Interpretability**: Easy to interpret the explainer model to provide meaningful explanations
- **Faithfulness**: Explainer model sufficiently captures the relationship between the complex model predictions and the features in the local region around a prediction of interest
- **Linearity**: Using a ridge regression as the explainer model assumes a linear relationship between complex model predictions and the features
- **Localness**: Explanations are local in regards to a prediction of interest

We suggest visual diagnostics to assess these claims:

- **Diagnostics for individual explanations**
- **Diagnostics for sets of explanations**
- **Diagnostics for comparisons of tuning parameters**

Sine Example Data

Training data: 500 observations

Testing data: 100 observations

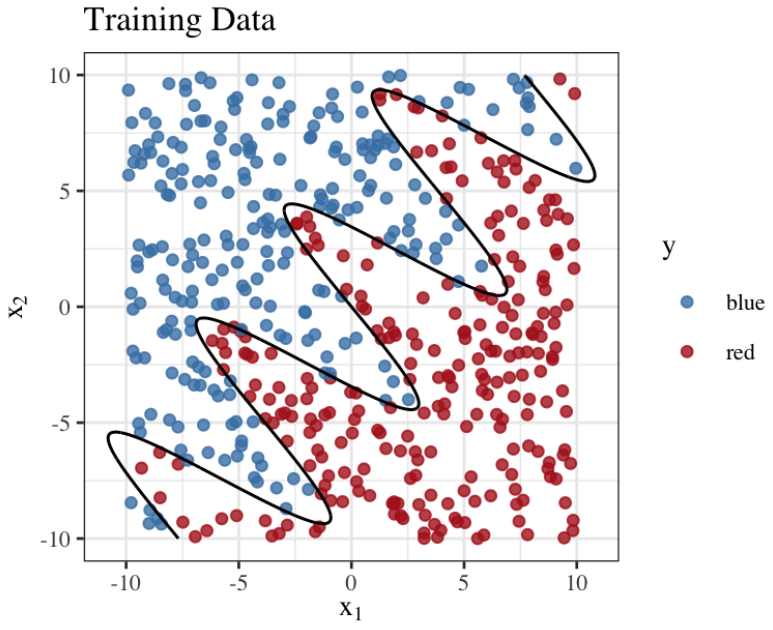
Black-box model: random forest

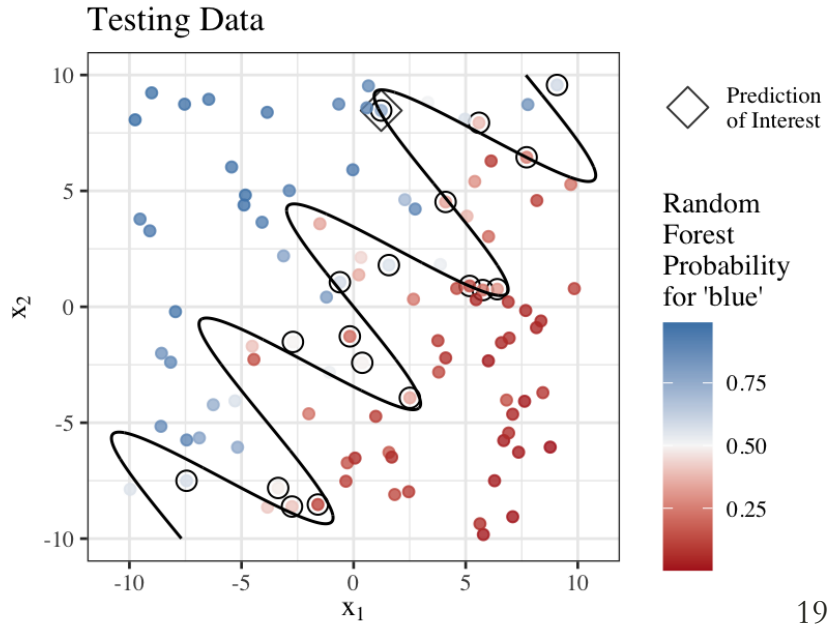
$$x_1 \sim Unif(\text{ -10, 10 })$$
$$x_2 \sim Unif(\text{ -10, 10 })$$
$$x_3 \sim \text{N}(0, 1)$$

$$y = \begin{cases} \text{blue} & \text{if } x_2' > \sin(x_1') \\ \text{red} & \text{if } x_2' \leq \sin(x_1') \end{cases}.$$

where

$$x_1' = x_1 \cos(\theta) - x_2 \sin(\theta)$$
$$x_2' = x_1 \sin(\theta) + x_2 \cos(\theta)$$
$$\theta = -0.9$$





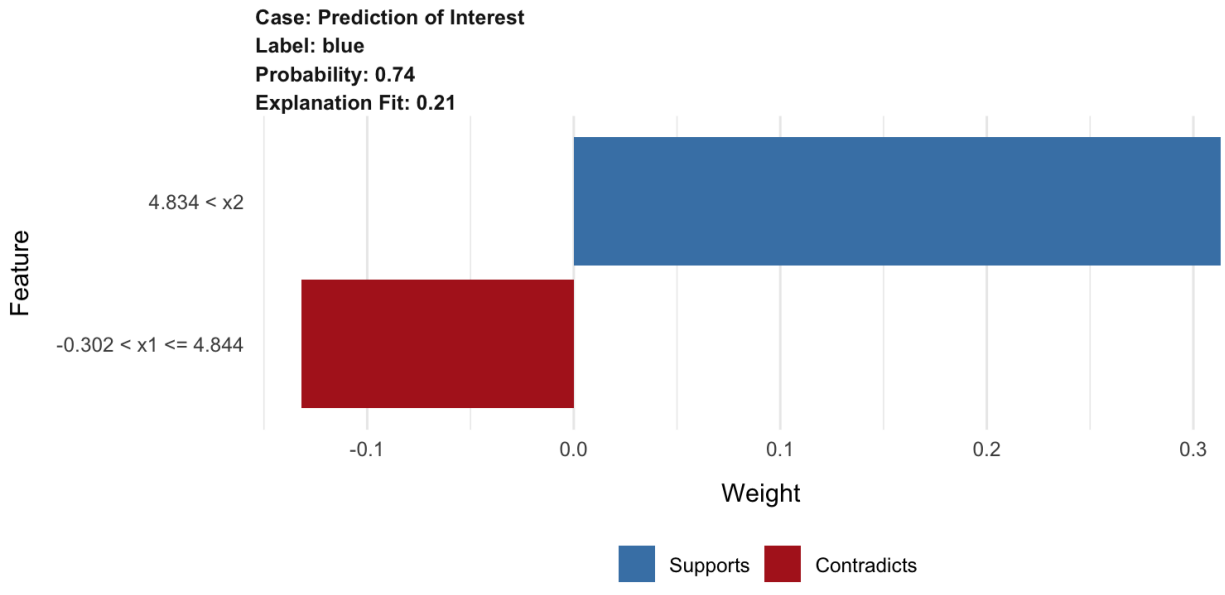
Set 1 of Visualizations: Diagnostics for Individual Explanations

Diagnostics for Individual Explanations

Applied LIME using *lime* R package (Pedersen and Benesty, 2020)

- To prediction of interest
- Number of features to return in explanation: 2
- Default tuning parameters settings

lime R package visualization of the explanation:



Diagnostics for Individual Explanations

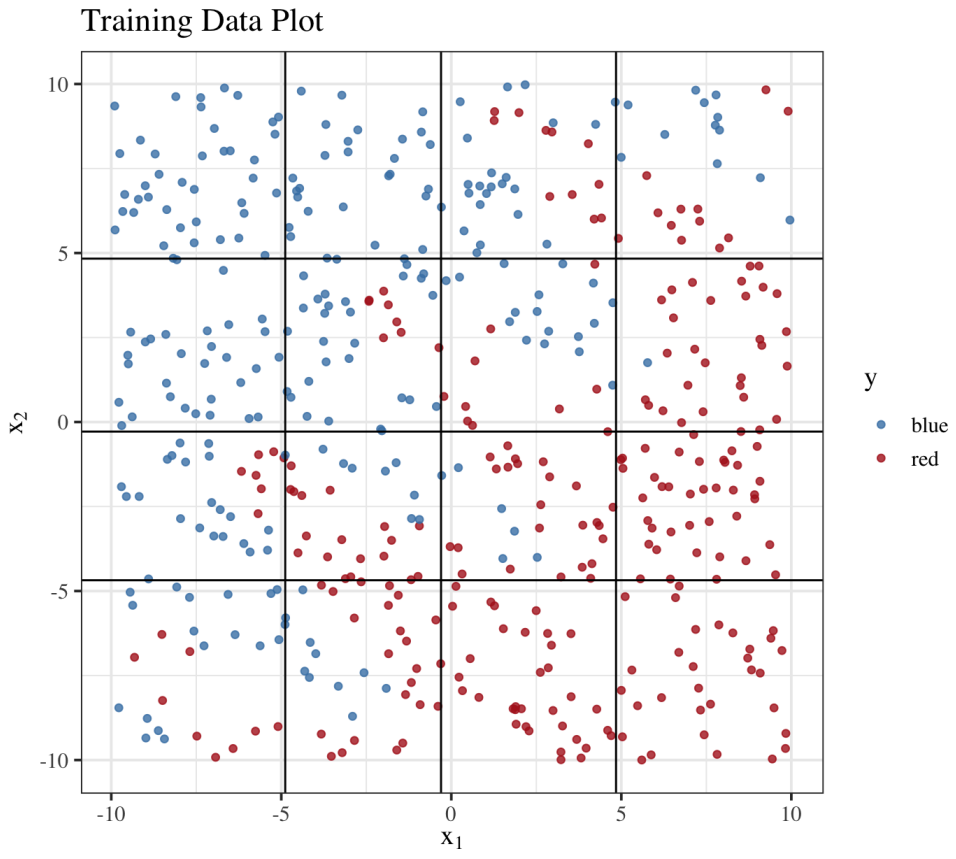
Step 1a: Data Simulation

- Sample 4999 observations uniformly from 4 quantile bins for each feature in the training data

Corresponding Diagnostic:

Training Data Plot

- Axes: two features selected by LIME
- Points: training data
- Color: observed response
- Lines: 4 quantile bins boundaries



Diagnostics for Individual Explanations

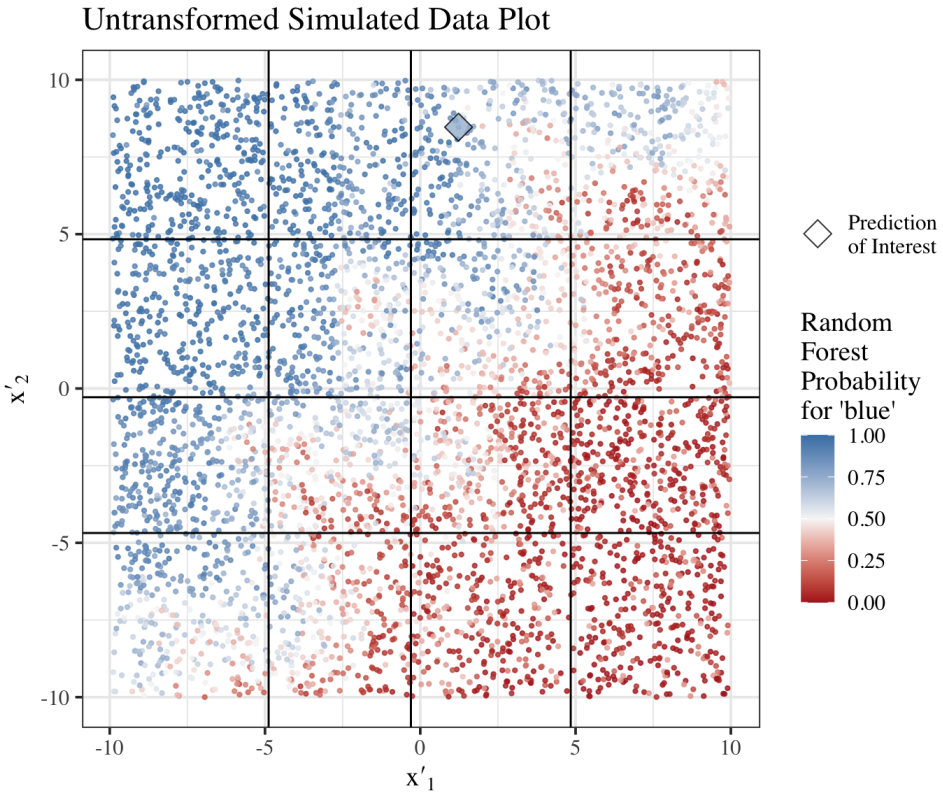
Step 1b: Complex Model Predictions

- Apply complex model to simulated data to obtain predictions

Corresponding Diagnostic:

Untransformed Simulated Data Plot

- Axes: simulated data features (x'_1 and x'_2)
- Points: simulated data
- Diamond: prediction of interest
- Color: random forest prediction (for 'blue')
- Lines: 4 quantile bins boundaries



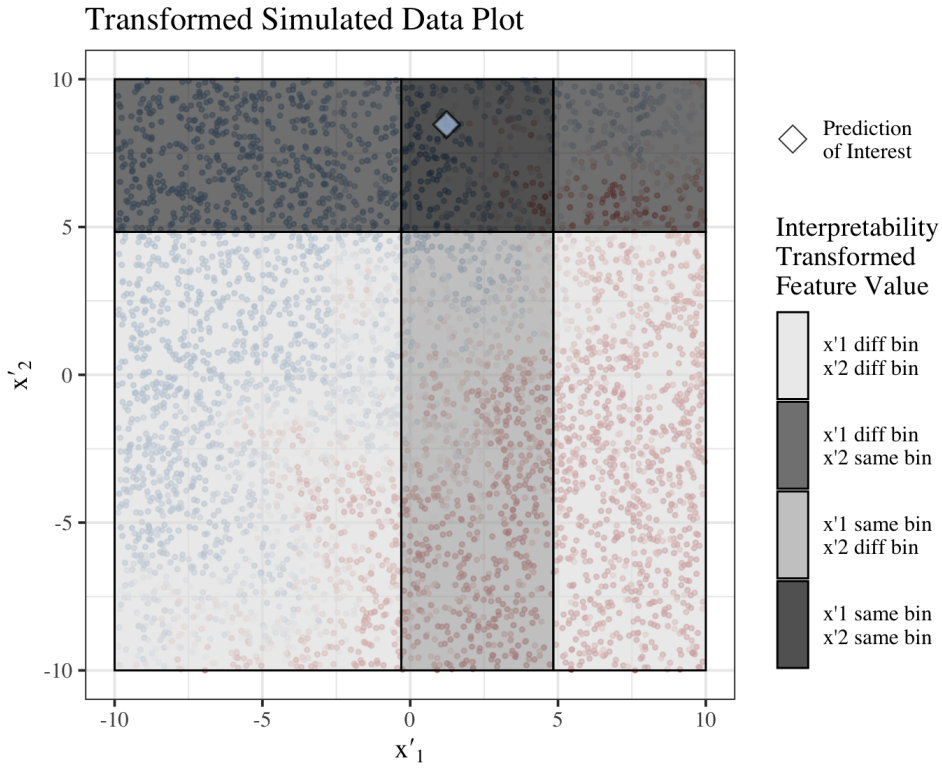
Diagnostics for Individual Explanations

Step 1c: Interpretability Transformation

- Convert continuous features to binary variables based on whether the observation falls in the same quantile bin as the prediction of interest or not

Corresponding Diagnostic: *Transformed Simulated Data Plot*

- Axes: Simulated data features
- Points: simulated data
- Diamond: prediction of interest
- Color: random forest prediction (for 'blue')
- Rectangle Shades: interpretability transformed feature regions



Diagnostics for Individual Explanations

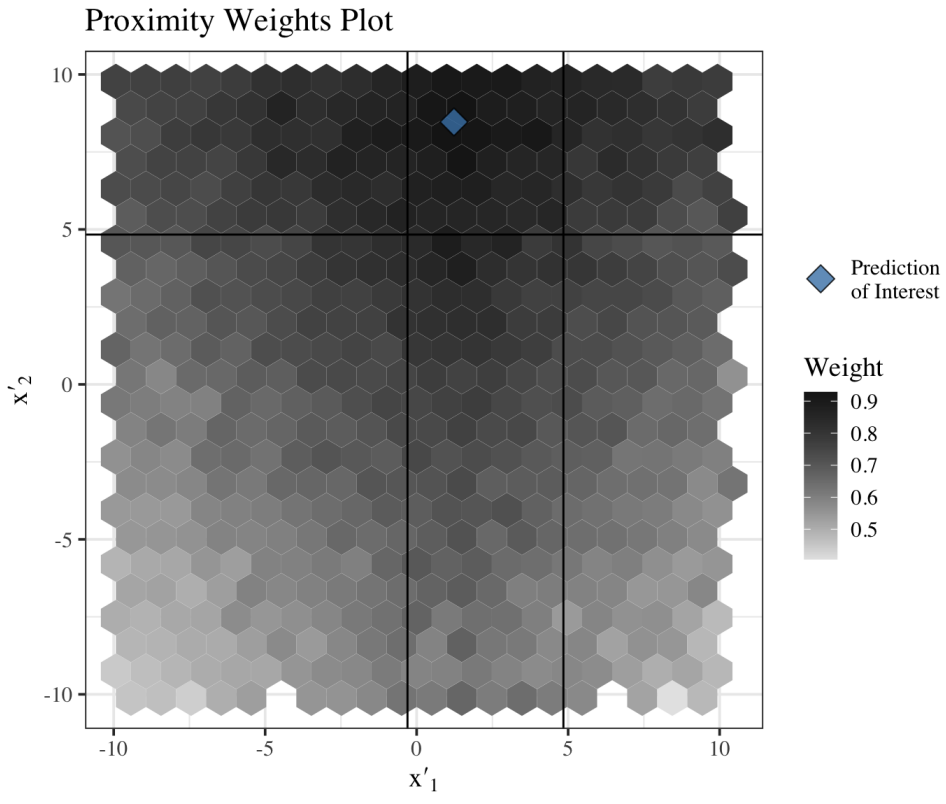
Step 2a: Assign Weights

- Assign weights to simulated data based on proximity to the prediction of interest (using untransformed feature values)
- Gower distance metric

Corresponding Diagnostic:

Proximity Weights Plot

- Axes: Simulated data features
- Rectangle Color: average weight within hexagon region
- Lines: interpretability transformation boundaries
- Diamond: prediction of interest



Diagnostics for Individual Explanations

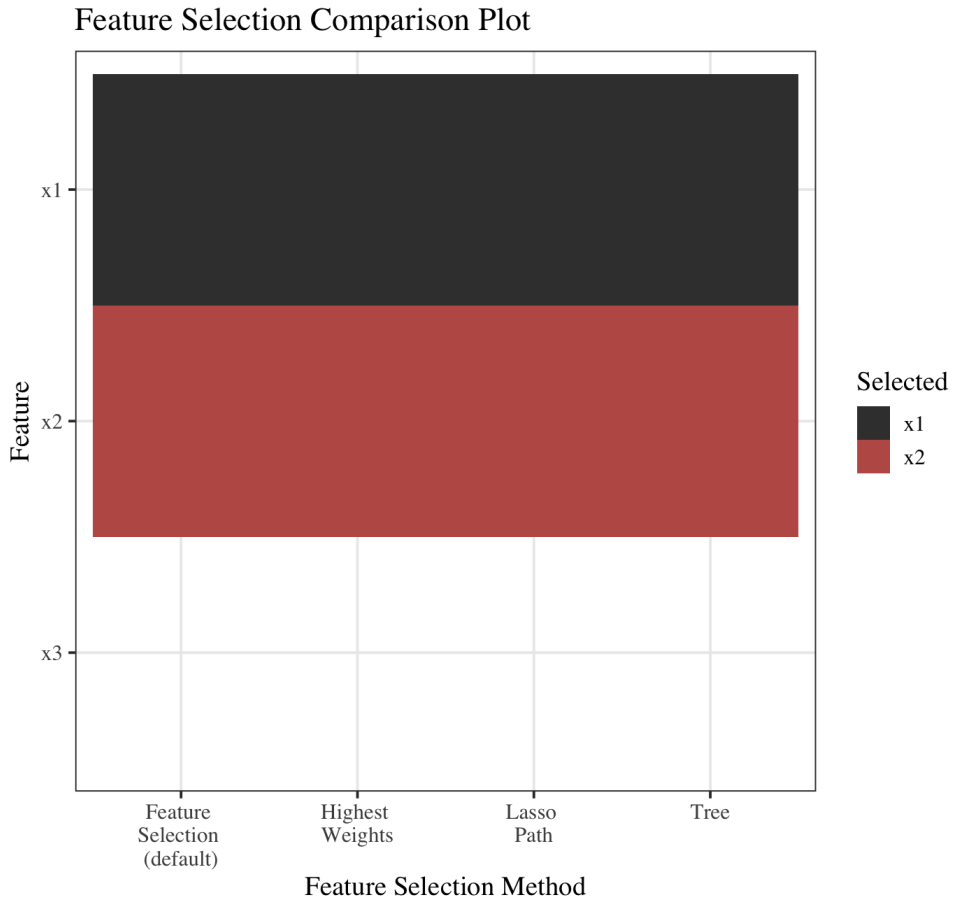
Step 2b: Feature Selection

- Ridge regression model fit to simulated data
  - Response: complex model predictions
  - Features: interpretability transformed features
- Forward selection (if less than 6 features specified)

Corresponding Diagnostic:

Feature Selection Comparison Plot

- Axes: Training data features versus feature selection method
- Tile Color: indicates if feature selected



Diagnostics for Individual Explanations

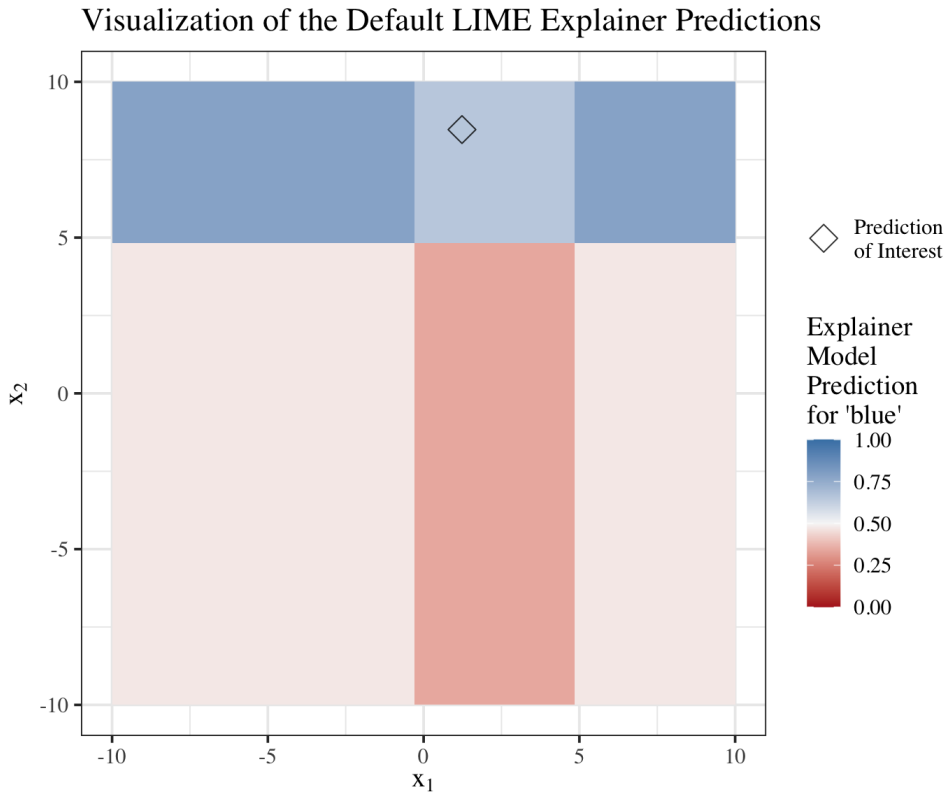
Step 2c: Fit Explainer Model

- Ridge regression model fit to simulated data
  - Response: complex model predictions
  - Features: selected interpretability transformed features

Corresponding Diagnostic:

Explainer Model Prediction Plot

- Axes: simulated data features
- Diamond: prediction of interest
- Rectangle: Interpretability transformed regions
- Color: explainer model prediction



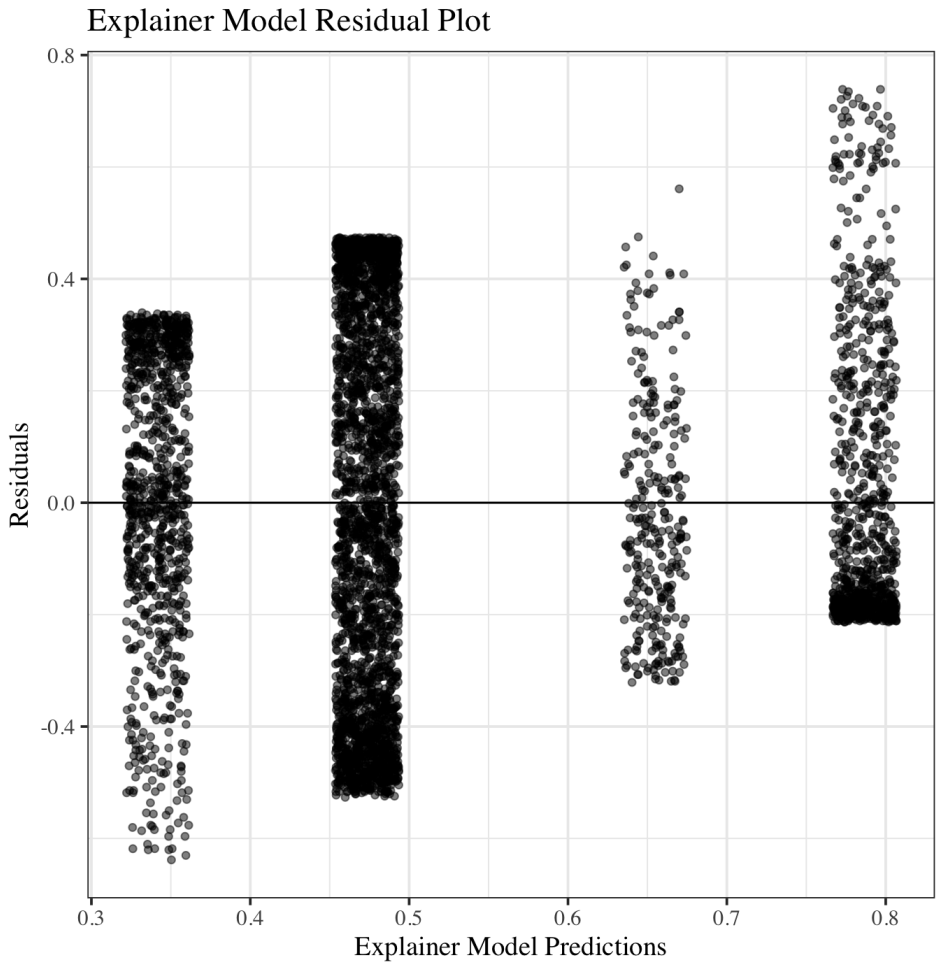
Diagnostics for Individual Explanations

Step 2c: Fit Explainer Model (continued)

Corresponding Diagnostic:

Explainer Model Residual Plot

- Residual plot for the explainer model
- Points have been jittered in the x-direction



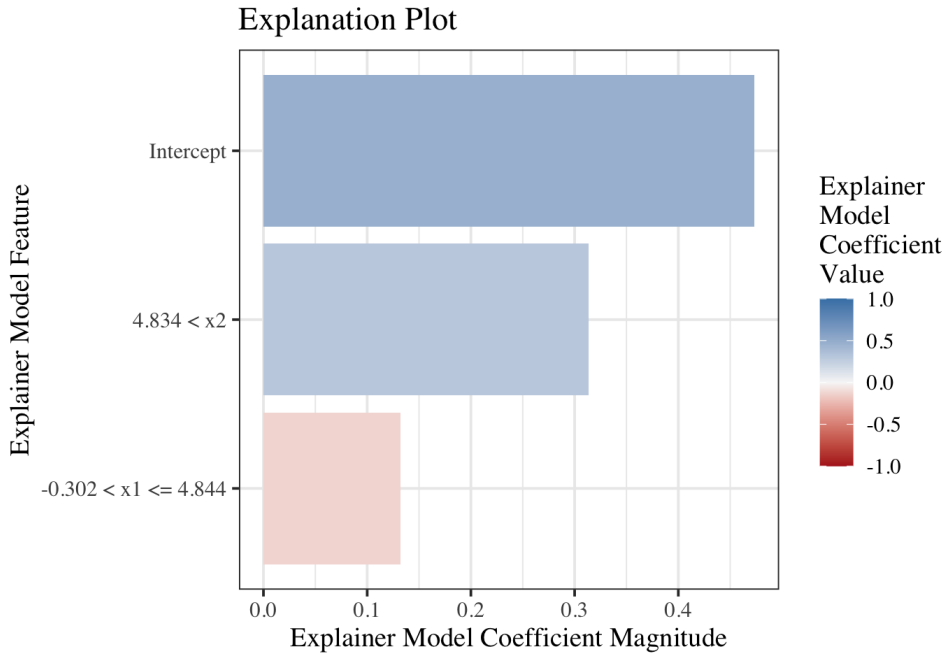
Diagnostics for Individual Explanations

Step 3a: Explainer Model Interpretation

- Interpret coefficients of explainer model
- Explains complex model prediction

Corresponding Diagnostic: *Explanation Plot*

- Adaptation of plot from *lime* R package
- Axes: Explainer model (interpretability transformed) feature versus explainer model coefficient
- Bar Length: magnitude of explainer model coefficients
- Bar Color: value of the explainer model coefficients

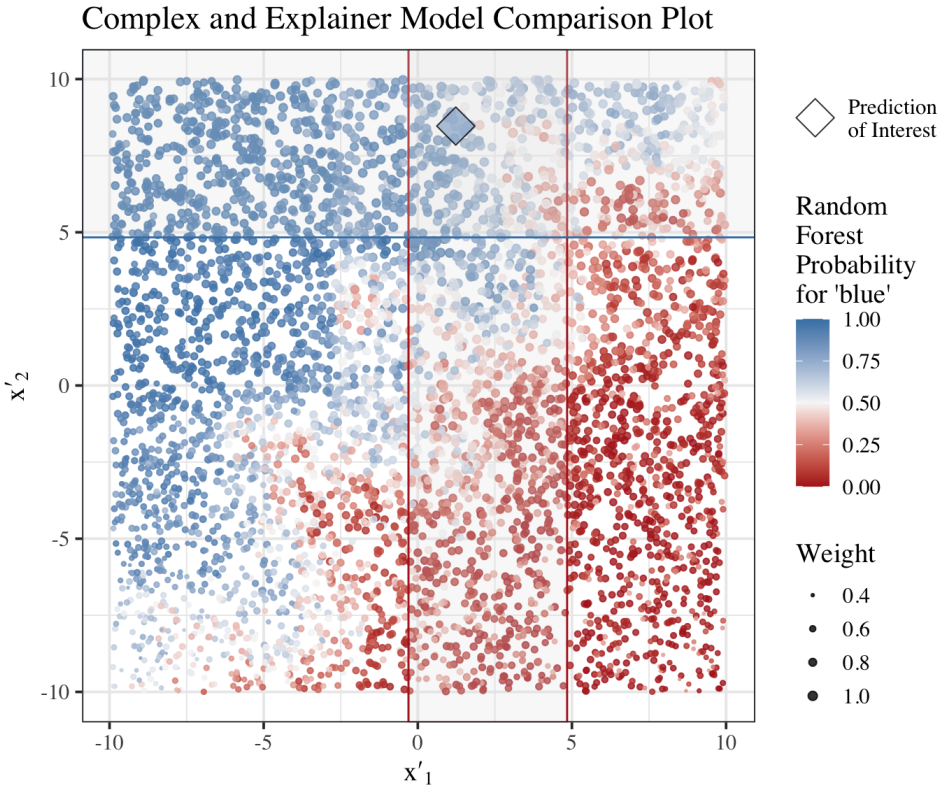


Diagnostics for Individual Explanations

Step 3b: Explainer Model Interpretation (continued)

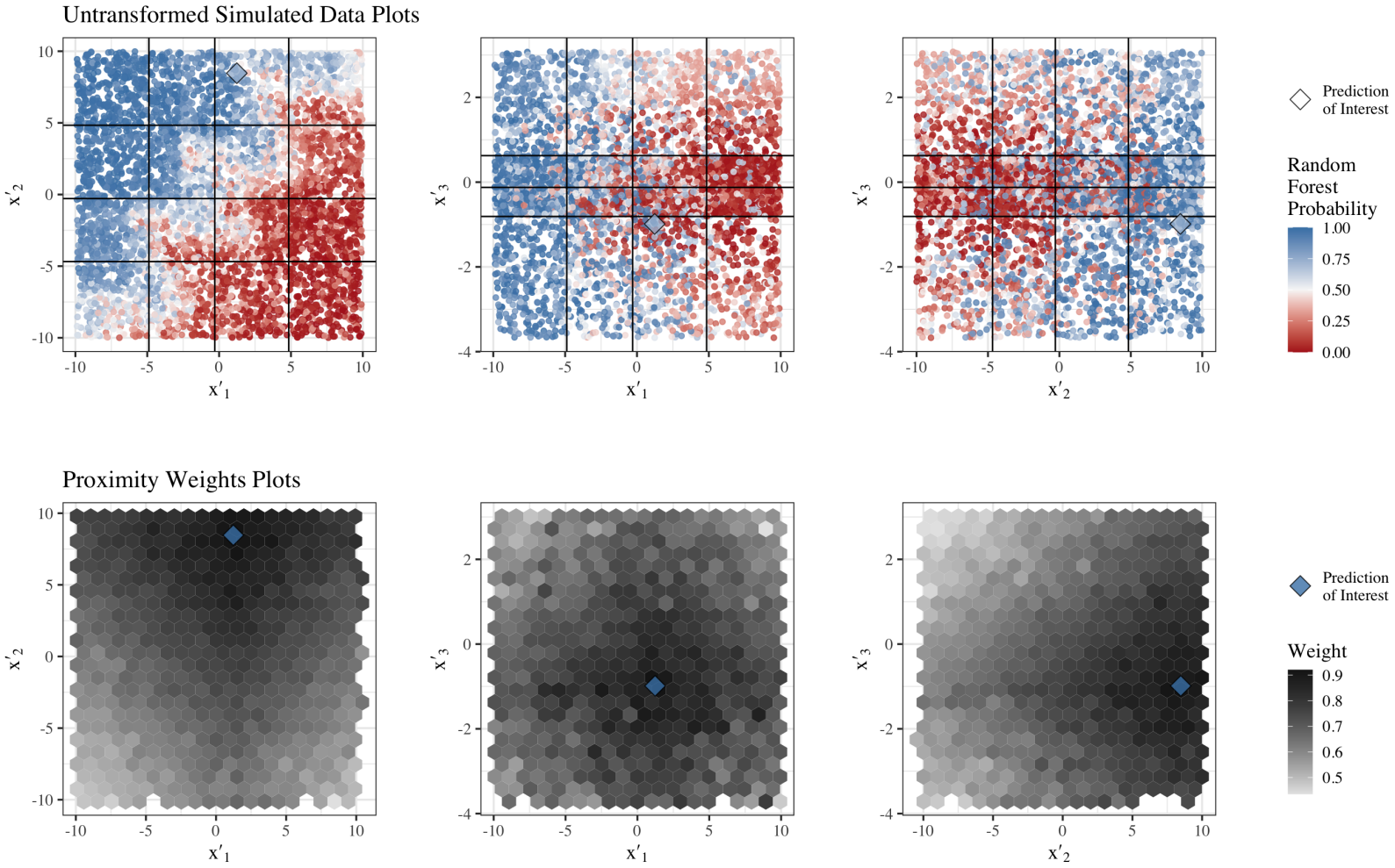
Corresponding Diagnostic: *Complex and Explainer Model Comparison Plot*

- Axes: simulated data features
- Points: simulated data
- Diamond: prediction of interest
- Point Color: random forest prediction (for 'blue')
- Point Size: proximity weight
- Lines: interpretability transformation boundaries
- Line Color: explainer coefficient supports a random forest prediction of 'blue' (blue) or not (red)



Diagnostics for Individual Explanations

Extensions to Higher Dimensions



Set 2 of Visualizations: Diagnostics for Sets of Explanations

Diagnostics for Sets of Explanations

Applied LIME using *lime* R package (Pedersen and Benesty, 2020)

- All test data observations
- Number of features to return in explanation: 2
- Default tuning parameters settings

Plot of all explanations from *lime* R package:

Diagnostics for Sets of Explanations

Explanation Set Plot

Provides an overview of groupings of LIME explanations

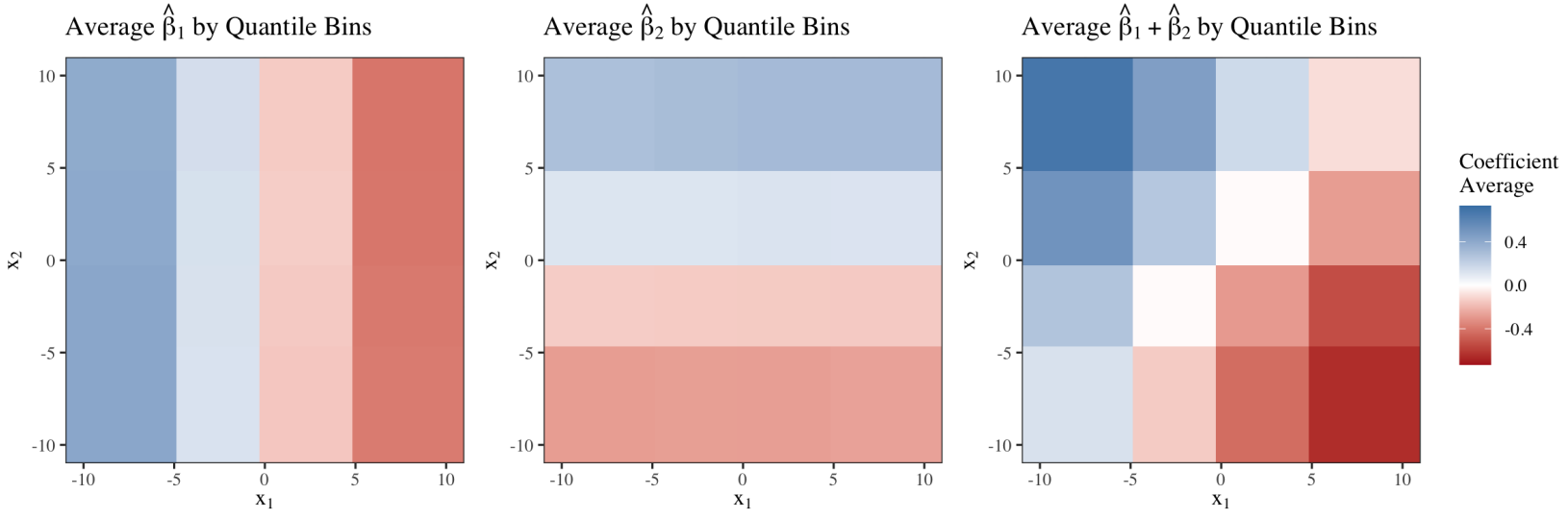
- Adaptation to the *lime* plot of all explanations
- Y-axis: Interpretability transformed features
- X-axis: Observation in the data set
- Tile Color: Ridge regression coefficient from the corresponding model

Diagnostics for Sets of Explanations

Aggregated Coefficient Plots

Provides a summary of explainer model coefficients across the set of explanations within quantile bin regions

- Axes: Test data features
- Cells: Intersections of quantile bins
- Color: Average of ridge regression coefficients (or sum of ridge regression coefficients) for observations within a cell

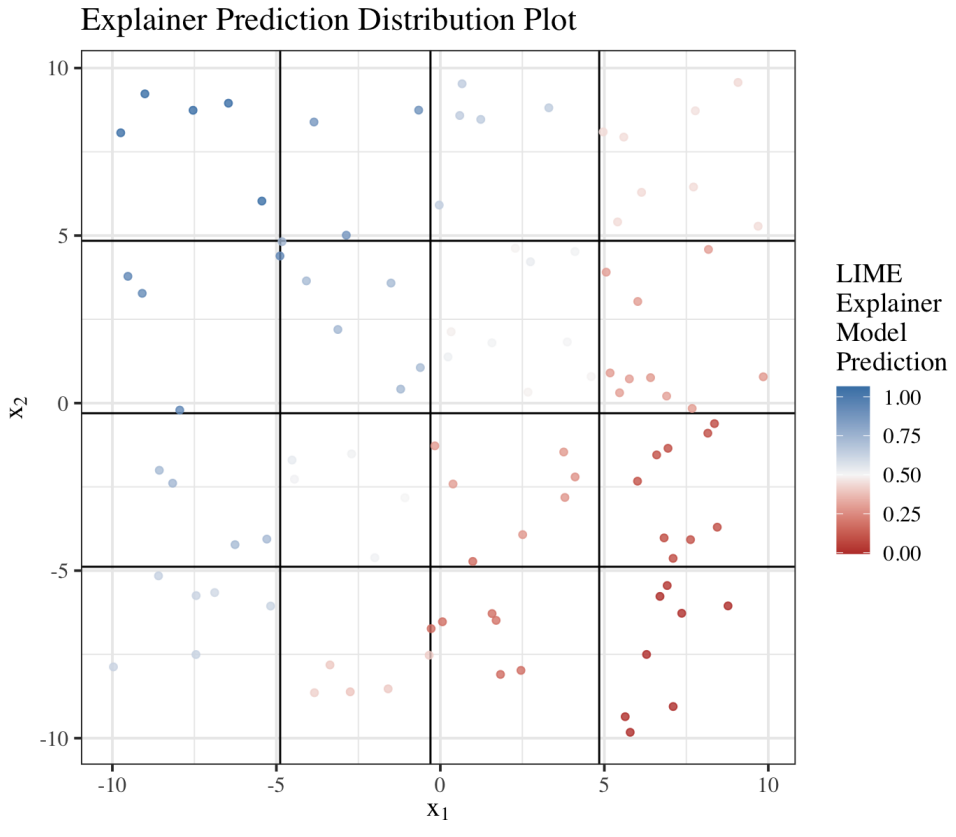


Diagnostics for Sets of Explanations

Explainer Prediction Distribution Plot

Shows the relationship between the explainer model predictions and the quantile bins

- Axes: Test data features
- Points: Test data observations
- Color: Explainer model prediction
- Lines: Quantile bin boundaries

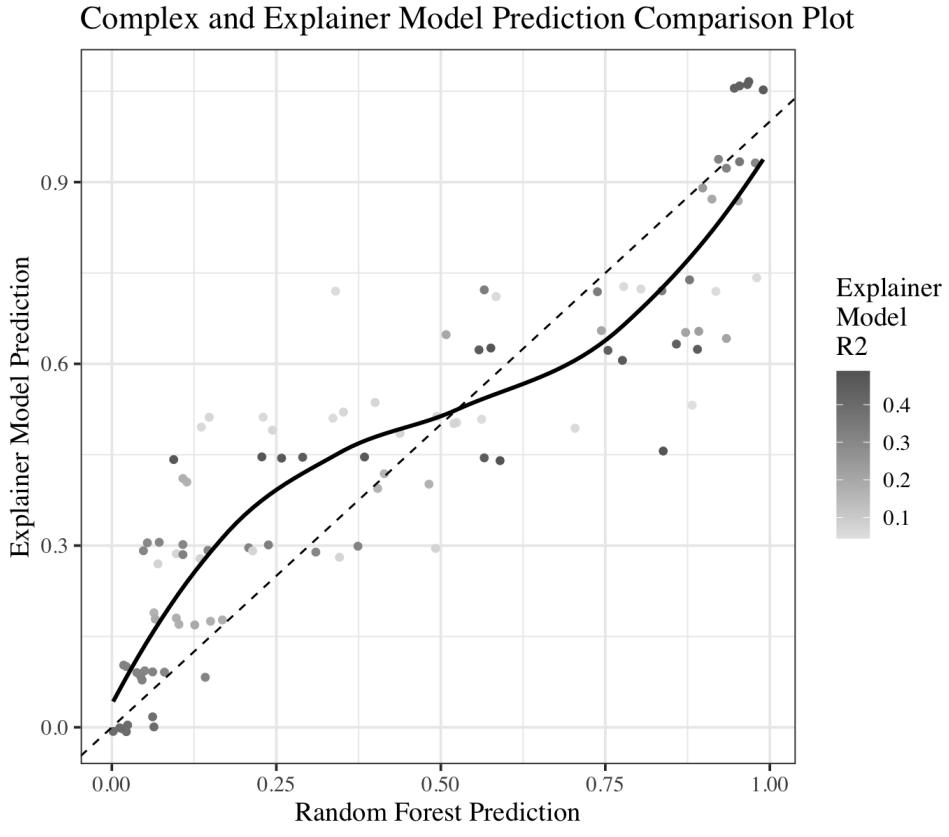


Diagnostics for Sets of Explanations

Complex and Explainer Model Prediction Comparison Plot

Shows the relationship between the explainer model and complex model predictions

- Y-Axis: Explainer model predictions
- X-Axis: Complex model predictions
- Points: Observations from the test data
- Color: Corresponding explainer model R^2
- Dashed Line: 1-1 line
- .red.[Solid Line]: Loess smoother fit to the points

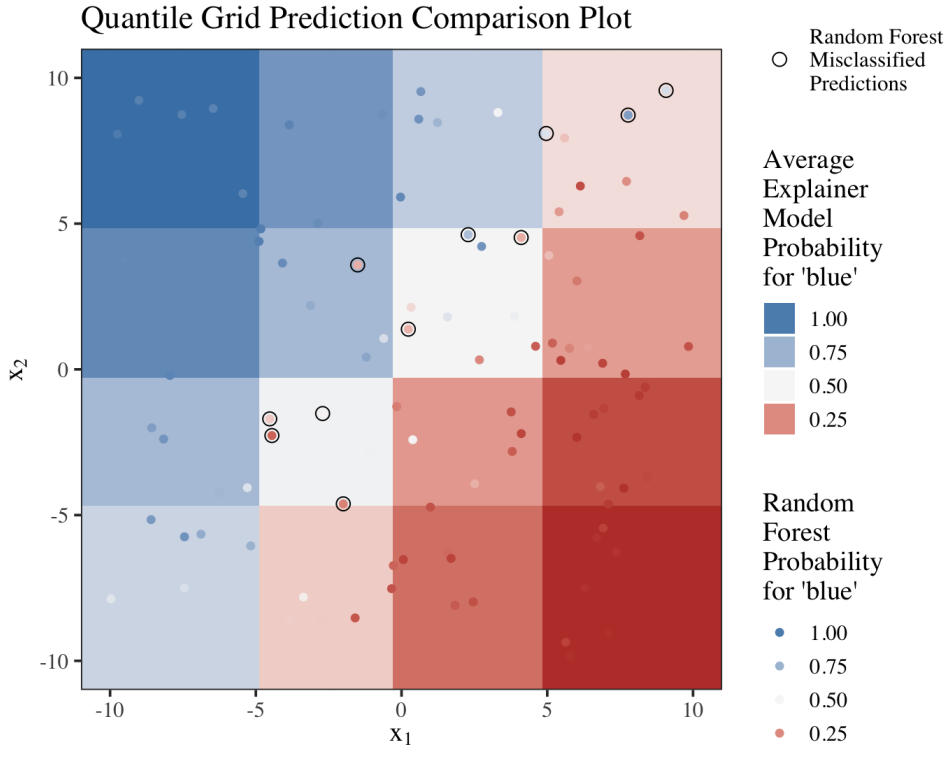


Diagnostics for Sets of Explanations

Quantile Grid Prediction Comparison Plot

Shows the relationship between the average explainer model predictions within a quantile bins cell and the complex model predictions

- Axes: Test data features
- Points: Test data observations
- Point Color: Explainer model prediction
- Cells: Intersections of quantile bins
- Cell Color: Average explainer model prediction
- Black Circles: Identify observations misclassified by the complex model



Set 3 of Visualizations: Diagnostics for Comparisons of Tuning Parameters

Diagnostics for Comparisons of Tuning Parameters

Applied LIME using *lime* R package (Pedersen and Benesty, 2020)

- All test data observations
- Number of features to return in explanation: 2
- Multiple applications of LIME for each observation
  - 2 to 6 quantile bins
  - Kernel density simulation

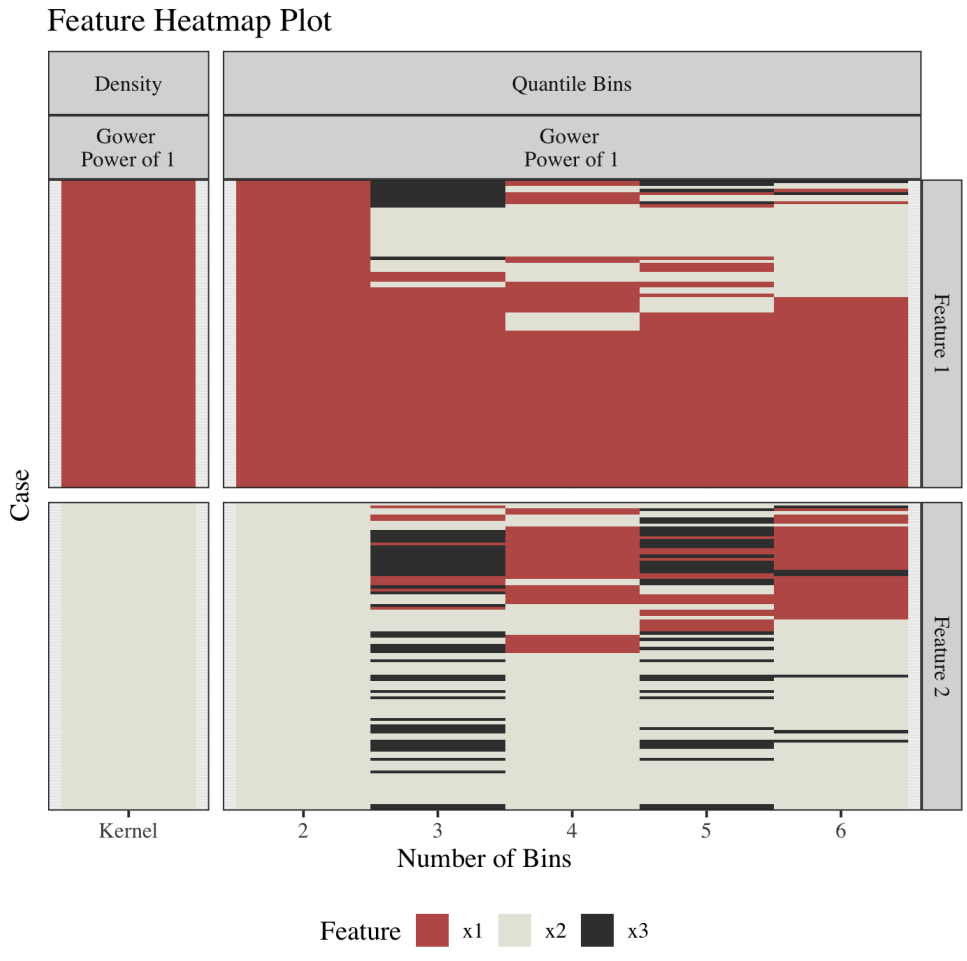
Plot of all explanations from *lime* R package:

Diagnostics for Comparisons of Tuning Parameters

Feature Heatmap Plot

Provides an overview of the features selected by LIME across observations and tuning parameters

- Y-Axis: Test data observation
- X-Axis: Data simulation method
- Y-Facet: LIME feature order selection (first, second, etc.)
- X-Facet: Density based or bin based simulation method
- Color: Feature selected



Metrics for the Assessment of LIME

Define the following:

Average Fidelity (Ribeiro, Singh, and Guestrin, 2016):

Average R^2:

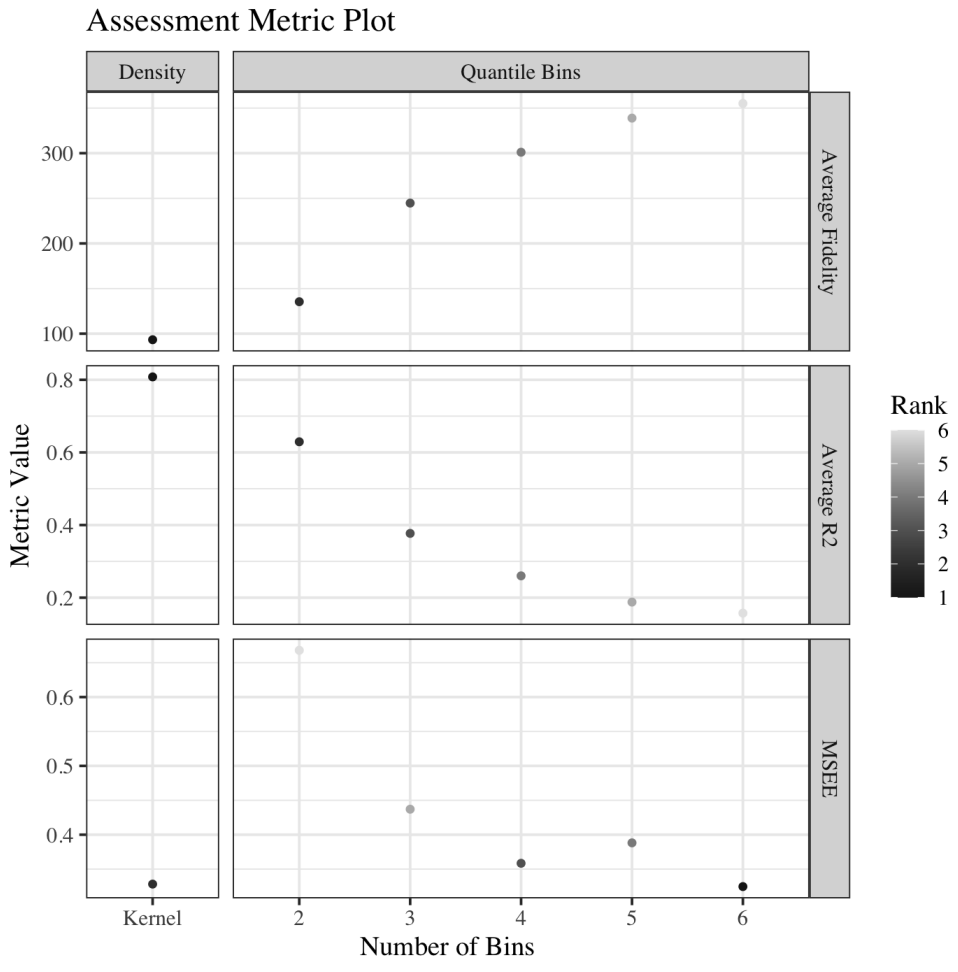
MSEE (Mean Squared Explanation Error):

Diagnostics for Comparisons of Tuning Parameters

Assessment Metric Plot

Visualization of assessment metrics for comparing tuning parameter performance

- Y-Axis: Metric value
- X-Axis: Data simulation method
- Y-Facet: Metric type
- X-Facet: Density based or bin based simulation method
- Point: Represents application of LIME to a set of observations
- Color: Rank of the application based on metric value (within a metric)



R package: limeaid

Application of Visual Diagnostics to Bullet

Chapter 2: Explaining Random Forests using Clustering of Trees

Motivation

- Since LIME did not provide reasonable explanations for the bullet matching random forest from the study by (Hare, Hofmann, and Carriquiry, 2016), it is still of interest to visualize the random forest to gain insight into the predictions.
- It is particularly of interest to provide explanations for incorrect predictions.

Current Ideas

Classification Tree as a Global Explainer Model

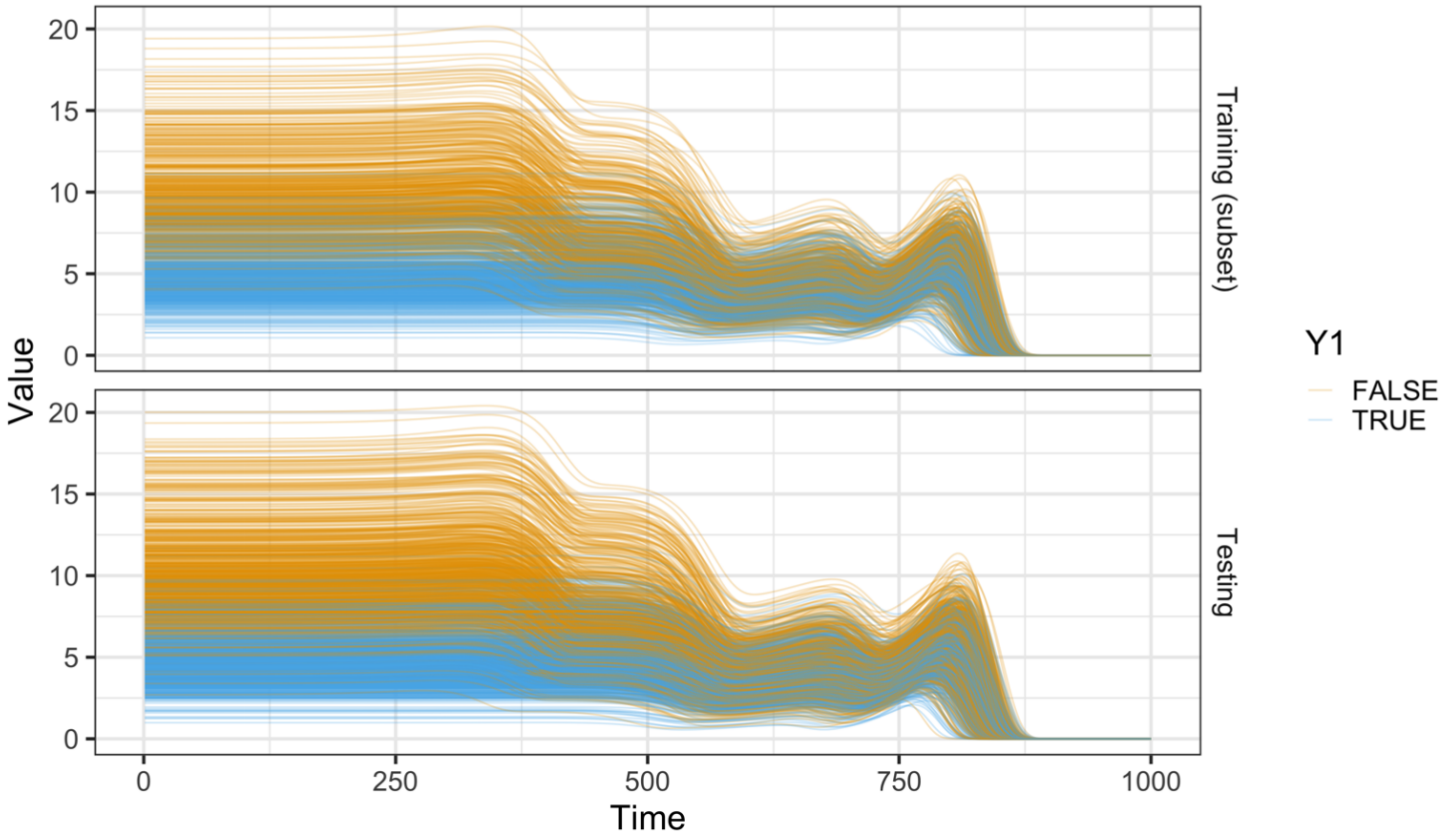
Current Ideas

Clustering to Identify Key Tree Paths in the Random Forest

Chapter 3: Extensions of Neural Network Explanation Tools to Functional Data

Application from Sandia National Labs

Plots of the training (randomly selected subset) and testing data



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Current Approach: Feature Visualization

Concept

- Focus on a "location" in the neural network
- Determine example observation that maximize the activation function

Process

1. Fit a model
2. Fix estimated parameter values
3. Determine values that maximized activation function at desired "location"

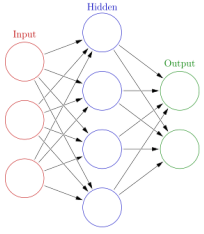


Image source: https://en.wikipedia.org/wiki/Artificial_neural_network

Example

- Response: $y \in \{0, 1\}$
- Features:

$$PC = (PC_1, PC_2, PC_3, PC_4, PC_5)$$

- Model: 1 hidden layer, 5 neurons
- Neuron i coefficients $(i = 1, \ldots, 5)$:

$$(\beta_{0,i}, \beta_{1,i}, \beta_{2,i}, \beta_{3,i}, \beta_{4,i}, \beta_{5,i})$$

- Activation Function: logistic

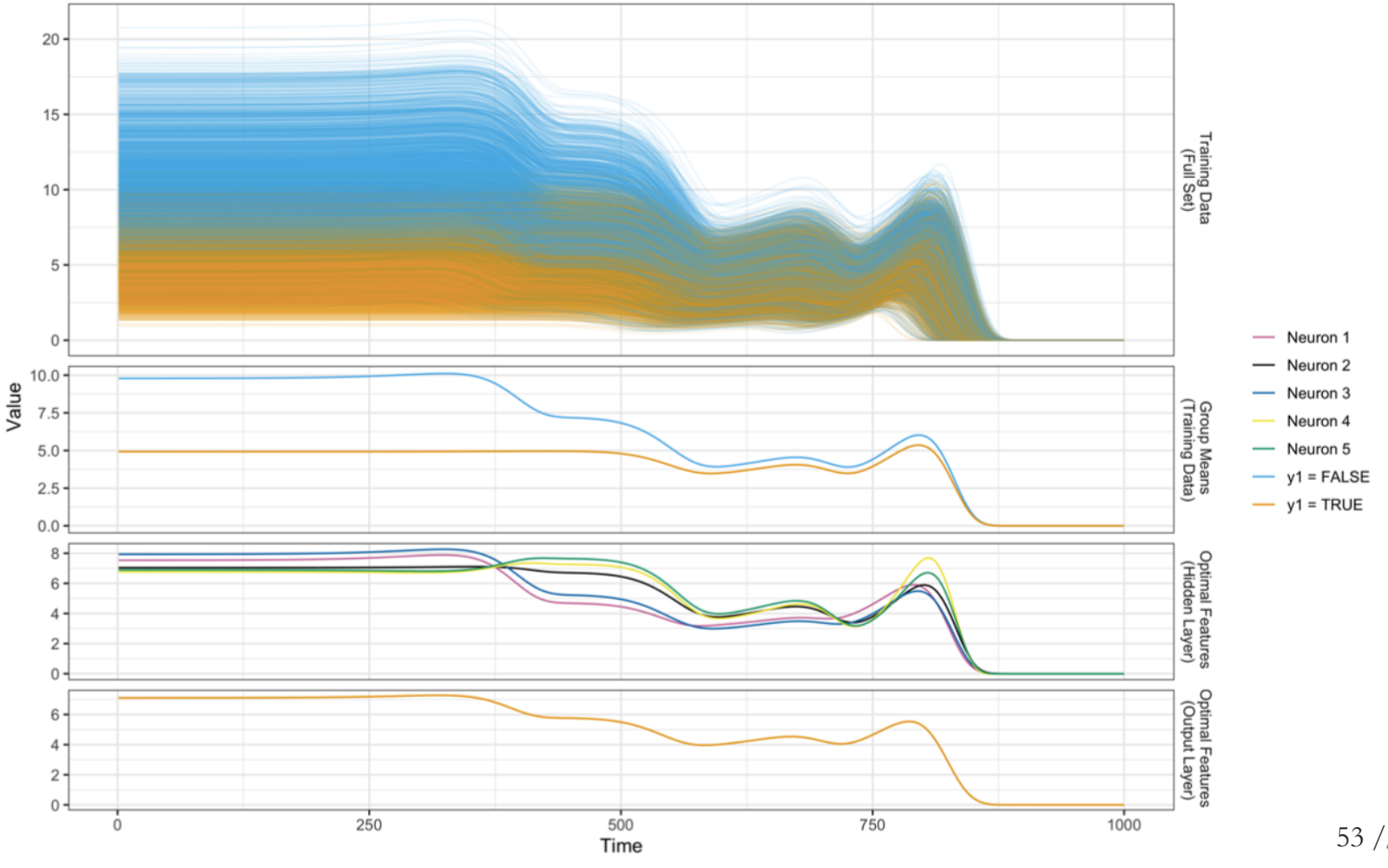
$$\sigma(v) = \frac{1}{1 + e^{-v}}$$

- Feature visualization optimization:

$$\arg\max_{PC} \ \sigma\left(\hat{\beta}_{0,i} + \hat{\beta}_{1,i} PC_1 + \cdots + \hat{\beta}_{5,i} PC_5\right)$$

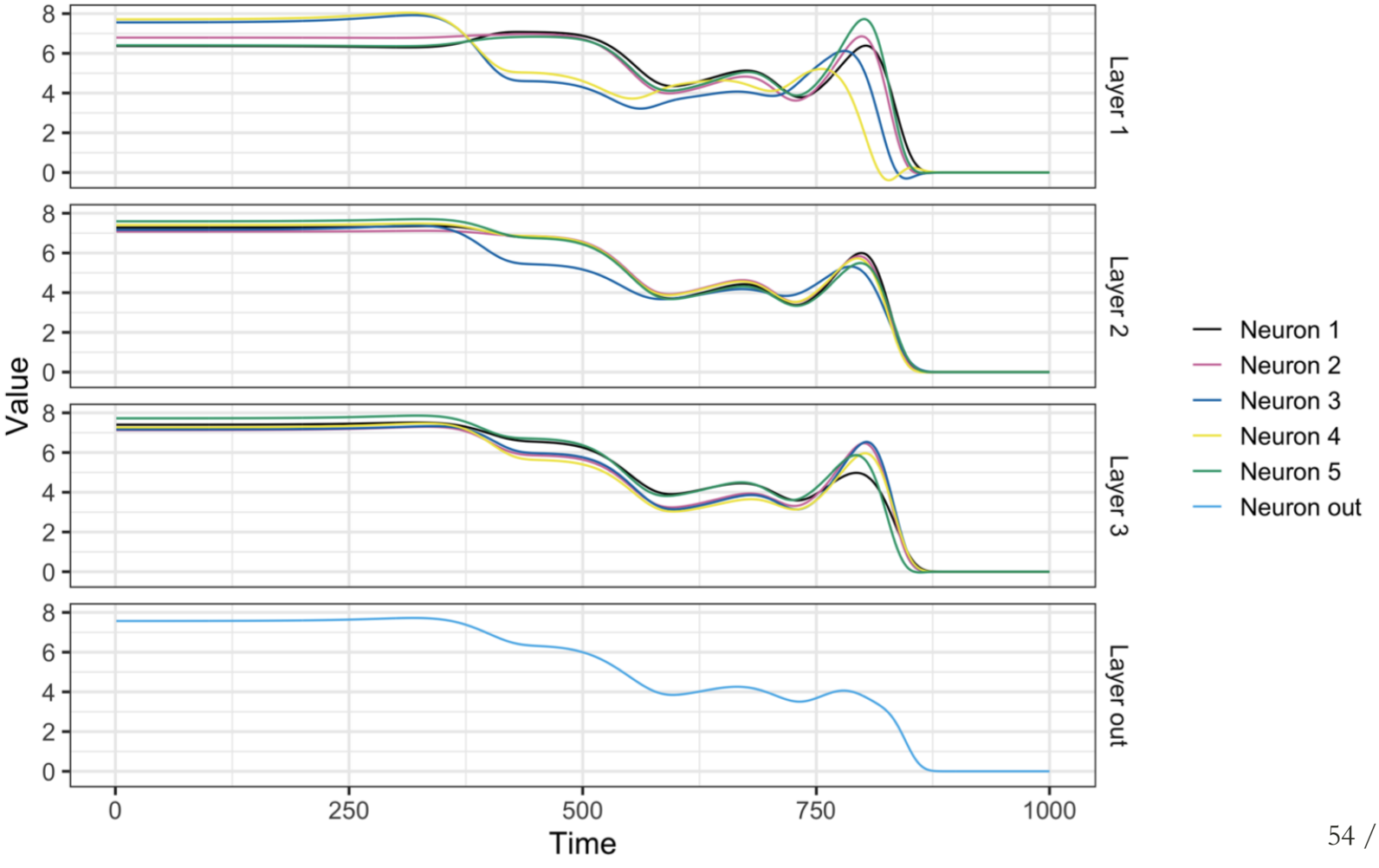
Feature Visualization

Comparing back-transformed optimal features to the observed data



Feature Visualization

Plots of the back transformed PCs that optimized the activation functions



Ideas for Future Work

Feature visualization adjustments

- Visualize the functional principal components

Applications/extensions of other methods

- Permutation feature importance, saliency maps, and partial dependence plots

Visualizations of the paths of an observation through the network

- Example: flow (Halnaut, Giot, Bourqui, et al., 2020)

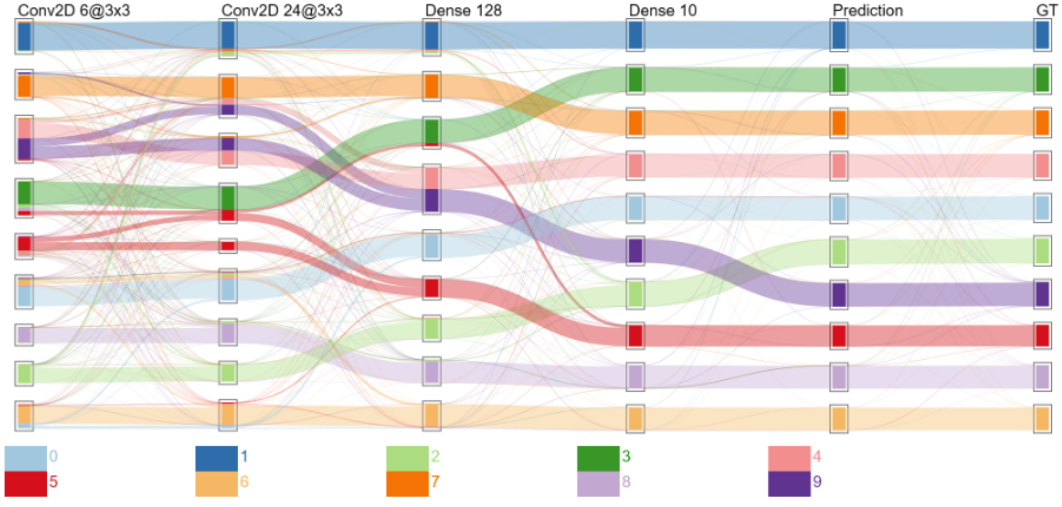


Figure 2: Visualization result on a LeNet5-inspired model evaluated on MNIST.

Timeline for Completion

Discussion Points

Publication of Chapter 1

How to divide up the material from chapter 1 for publication? Current ideas:

Paper 1: Survey paper on LIME

- Explain LIME in a statistical context
- Use visualizations to help explain the procedure
- Use diagnostic visualizations to assess LIME
- Highlight issues with LIME
- Use iris and sine data

Paper 2: Diagnostic plots for LIME

- Motivate assessment of LIME using the bullet matching data (example of high stakes decision using machine learning)
- Demonstrate issues found with LIME explanations using diagnostic plots
- LIME should not be trusted to explain machine learning models when making high stakes decisions

References

Need to format this eventually using `start` and `end` options

Altmann, A, L. Toloşi, O. Sander, et al. (2010). "Permutation importance: a corrected feature importance measure". In: *Bioinformatics* 26.10, pp. 1340-1347. ISSN: 1367-4803. DOI: 10.1093/bioinformatics/btq134.

Apley, D. W. and J. Zhu (2016). "Visualizing the Effects of Predictor Variables in Black Box Supervised Learning Models".

Beckett, C. (2018). "Rfviz: An Interactive Visualization Package for Random Forests in R". In: *DigitalCommons@USU All Graduate Plan B and otherReports*.

Biggio, B. and F. Roli (2018). "Wild Patterns: Ten Years After the Rise of Adversarial Machine Learning". In: *Pattern Recognition* 84, pp. 317-331. ISSN: 0031-3203. DOI: 10.1016/j.patcog.2018.07.023.

Breiman, L. (2001). "Random Forests". In: *Machine Learning* 45.1, pp. 5-32. ISSN: 0885-6125. DOI: 10.1023/a:1010933404324.

Casalicchio, G, C. Molnar, and B. Bischl (2019). "Visualizing the Feature Importance for Black Box Models" , pp. 655-670. ISSN: 2190-5053. DOI: 10.1007/978-3-030-10925-7_40.

Craven, M. W. and J. W. Shavlik (1996). "Extracting Tree-Structured Representations of Trained Networks". In: *Advances in Neural Information Processing Systems* 8.

Fisher, A, C. Rudin, and F. Dominici (2018). "Model Class Reliance: Variable Importance Measures for any Machine Learning Model Class, from the “Rashomon” Perspective".

Friedman, J. H. (2001). "Greedy function approximation: A gradient boosting machine." In: *The Annals of Statistics* 29.5. ISSN: 0090-5364. DOI: 10.1214/aos/1013203451.

Appendix

Add application of diagnostics to bullet examples