Visualization Methods for Explainable Machine Learning

Statistics PhD Oral Prelim

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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. Plan for Chapter 3
    - Extensions of Neural Network Explanation Tools to Functional Data
5. Timeline and 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
- **Explainable machine learning**
  - **Goal**: Explain predictions made by black-box models
  - **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)):

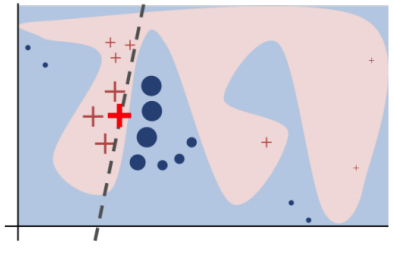
Interpretability is the ability to directly use model parameters to understand the mechanism of how the model makes predictions.

- 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)



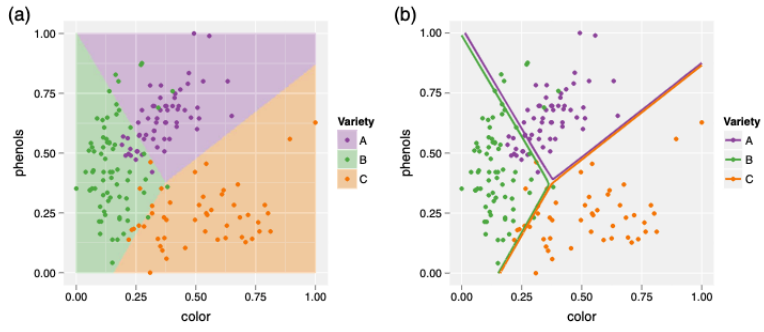
Model Agnostic Methods

General Model Visualizations: Strategies for understanding any model

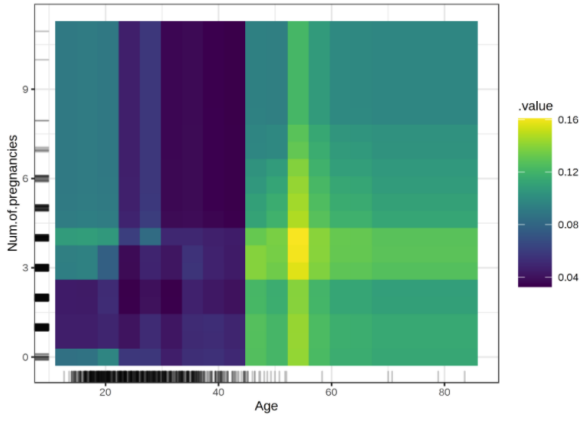
- Removing the blindfold (Wickham, Cook, and Hofmann, 2015)

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).

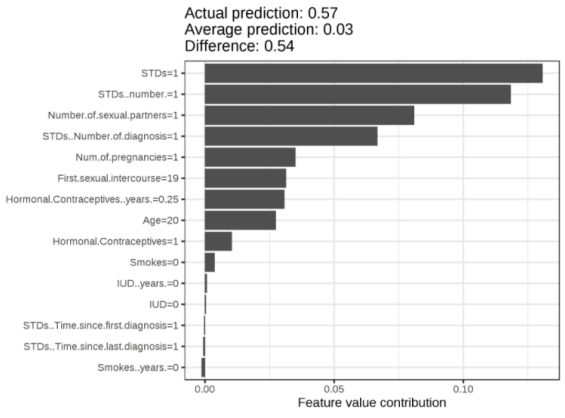
Model Agnostic Methods

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).

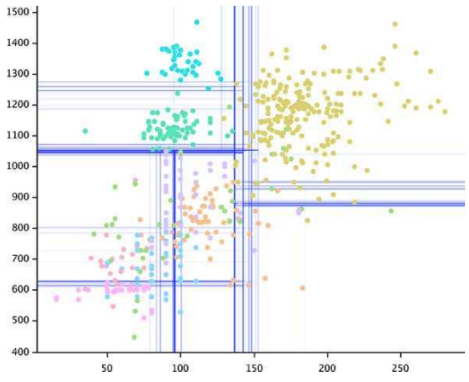
Model Specific Methods

Random Forests

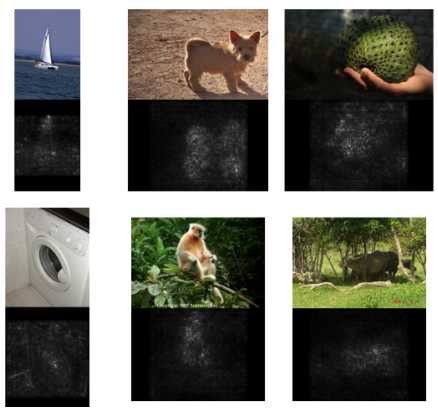
- Random forest impurity based feature importance (Breiman, 2001)
- Sectioned scatterplots (Urbanek, 2008)
- Trace plots of trees (Urbanek, 2008)
- Simplified model (Hara and Hayashi, 2016a)
- Forest floor visualizations (Welling, Refsgaard, Brockhoff, and Clemmensen, 2016)
- Interactive visualizations (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):

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

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

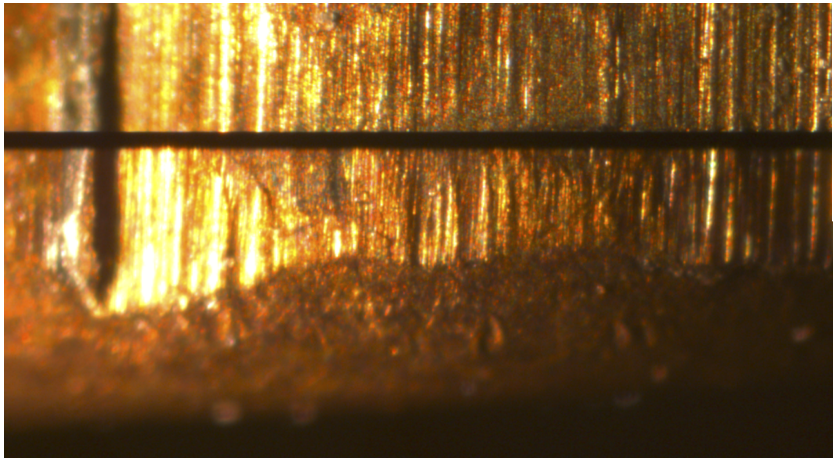
Chapter 1

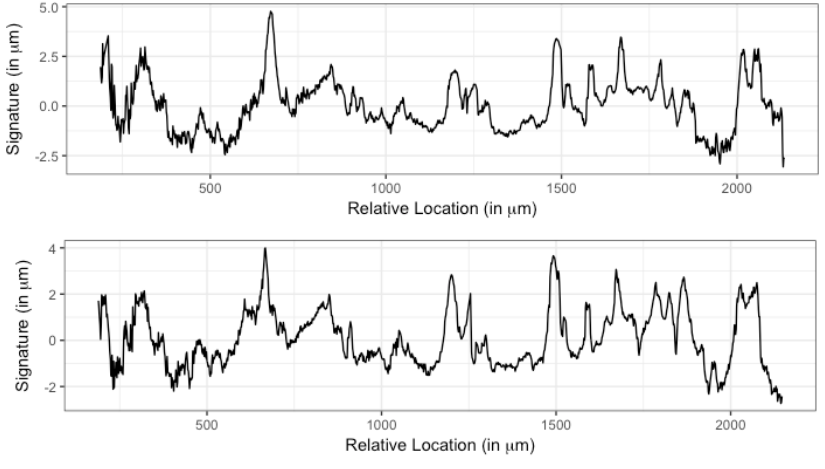
Visual Diagnostics of a Model Explainer -- Tools for the Assessment of LIME Explanations

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

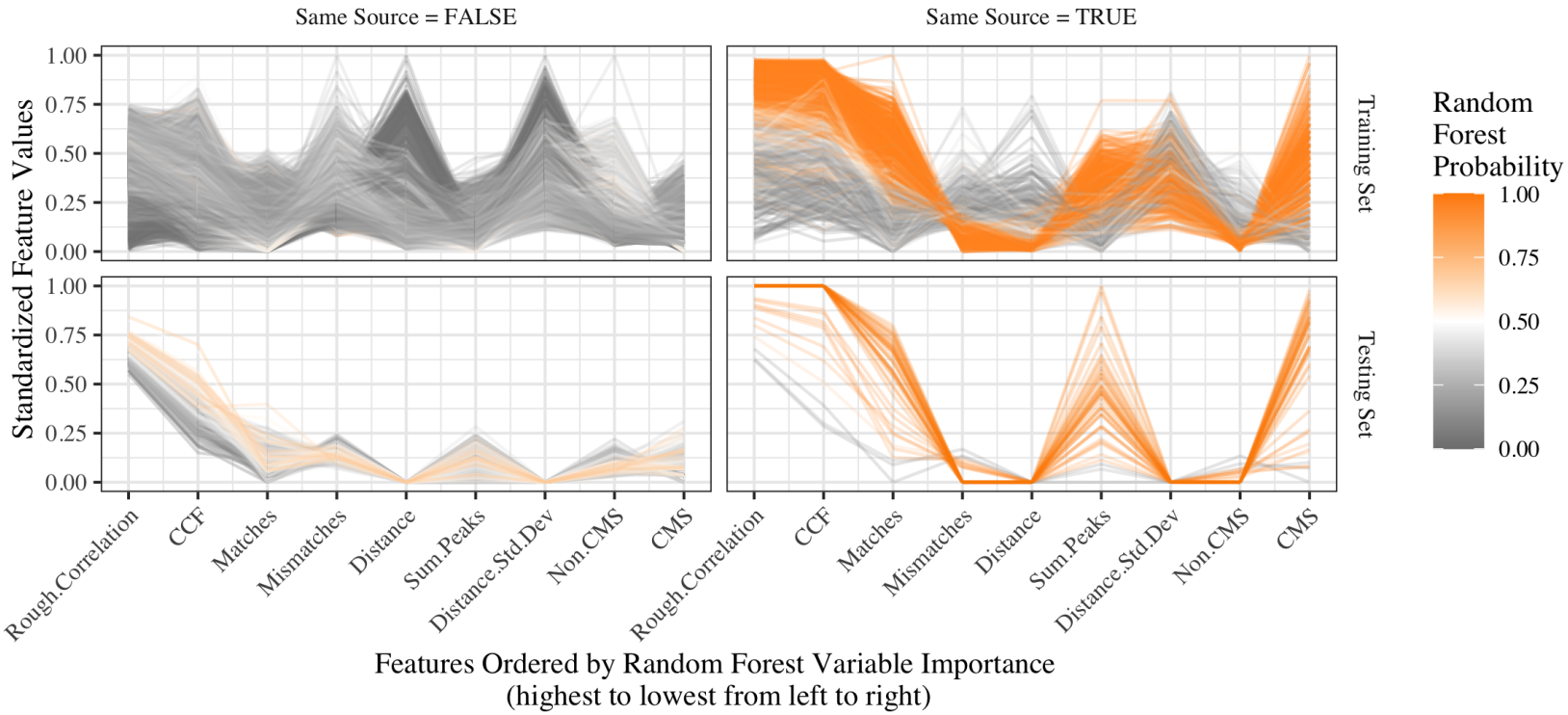




Motivation

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
- Explanations

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

- **Interpretability**: Easy to interpret the explainer model
- **Faithfulness**: Explainer model captures relationship between complex model predictions and features (in local region)
- **Linearity**: Ridge regression assumes linear relationship between complex model predictions and features
- **Localness**: Explanations are local in regards to 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**

Note: We focus on binary response variable and continuous predictor variables

Sine Example Data

Training data: 500 observations

Testing data: 100 observations

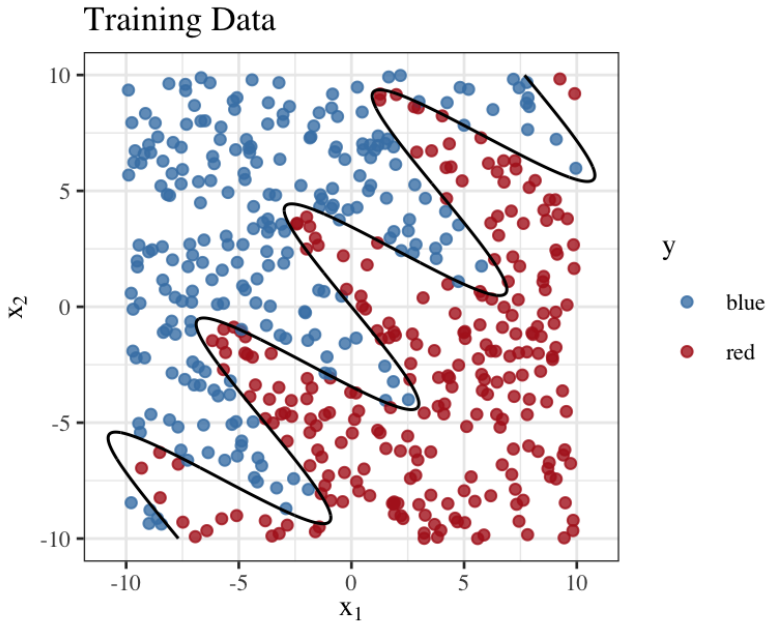
Black-box model: random forest

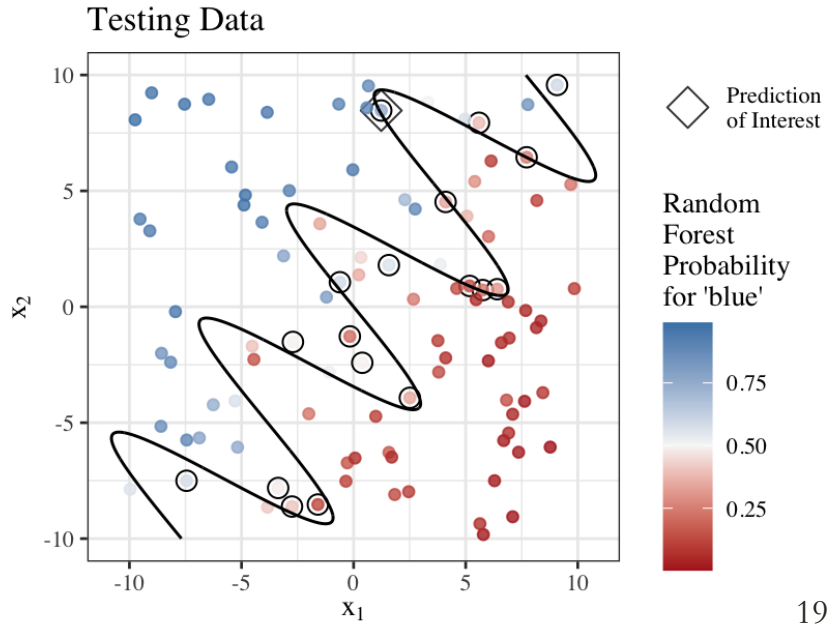
$$x_1 \sim Unif(\text{ -10, 10 })$$
$$x_2 \sim Unif(\text{ -10, 10 })$$
$$x_3 \sim \text{N}(0, 1)$$

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

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

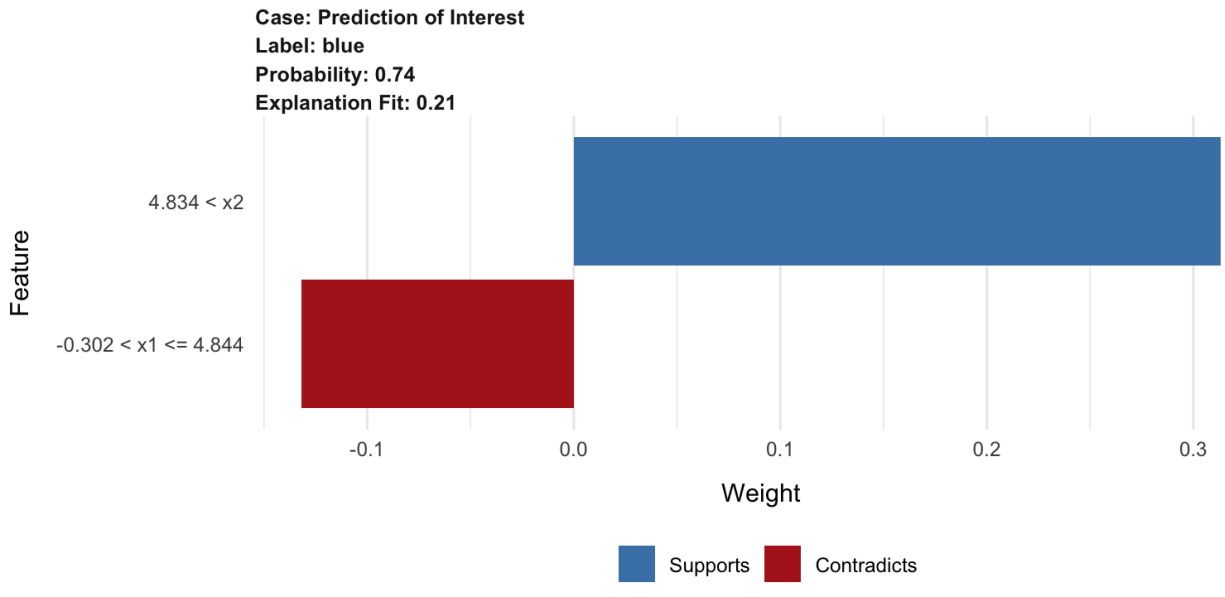
Diagnostics for Individual Explanations

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

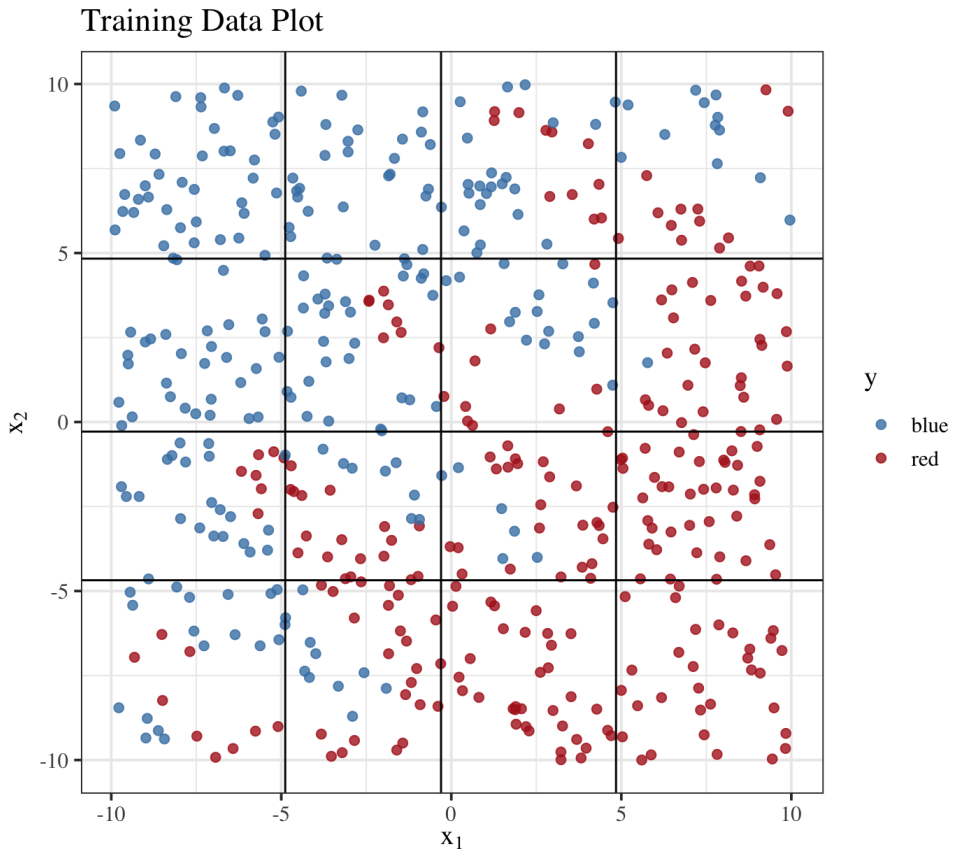
Step 1a: Data Simulation

- 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

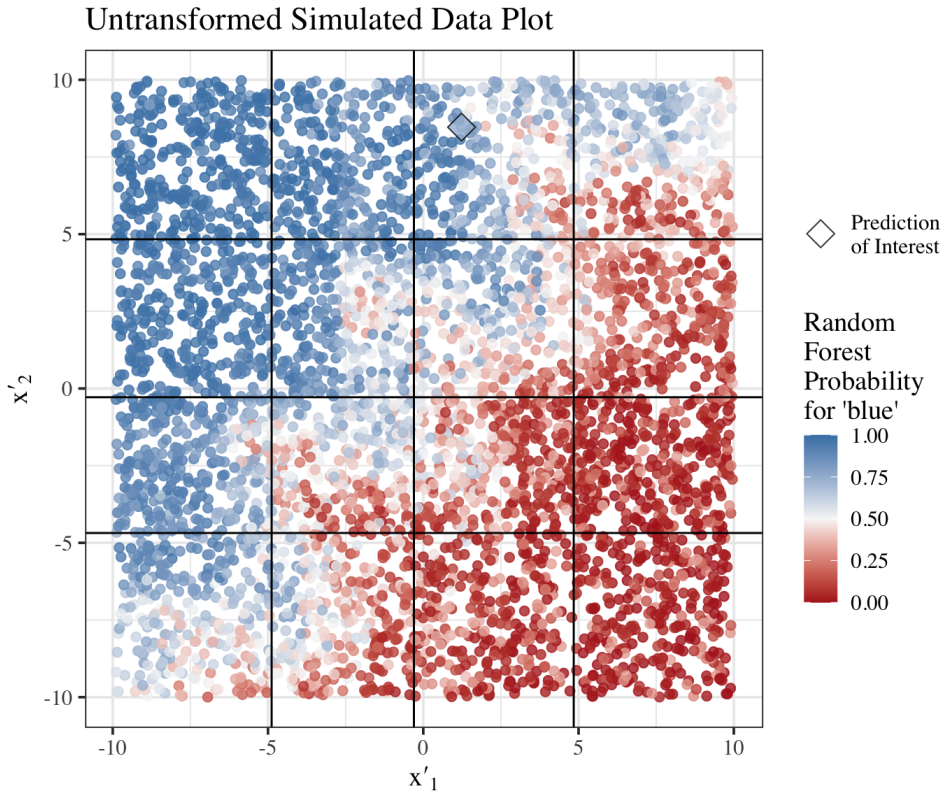
Step 1b: Complex Model Predictions

- Apply complex model to simulated data to obtain predictions

Corresponding Diagnostic:

Untransformed Simulated Data Plot

- Axes: simulated data features
  - denoted as x_1' and x_2')
- Points: simulated data
- Diamond: prediction of interest
- Color: random forest prediction (for 'blue')
- Lines: 4 quantile bins boundaries



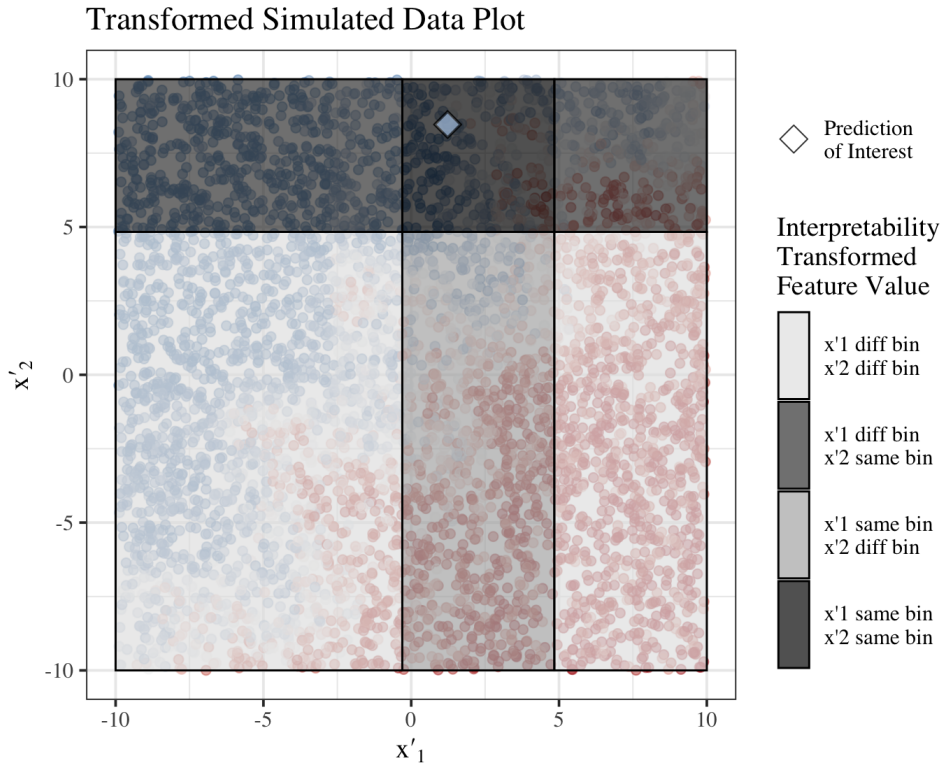
Diagnostics for Individual Explanations

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

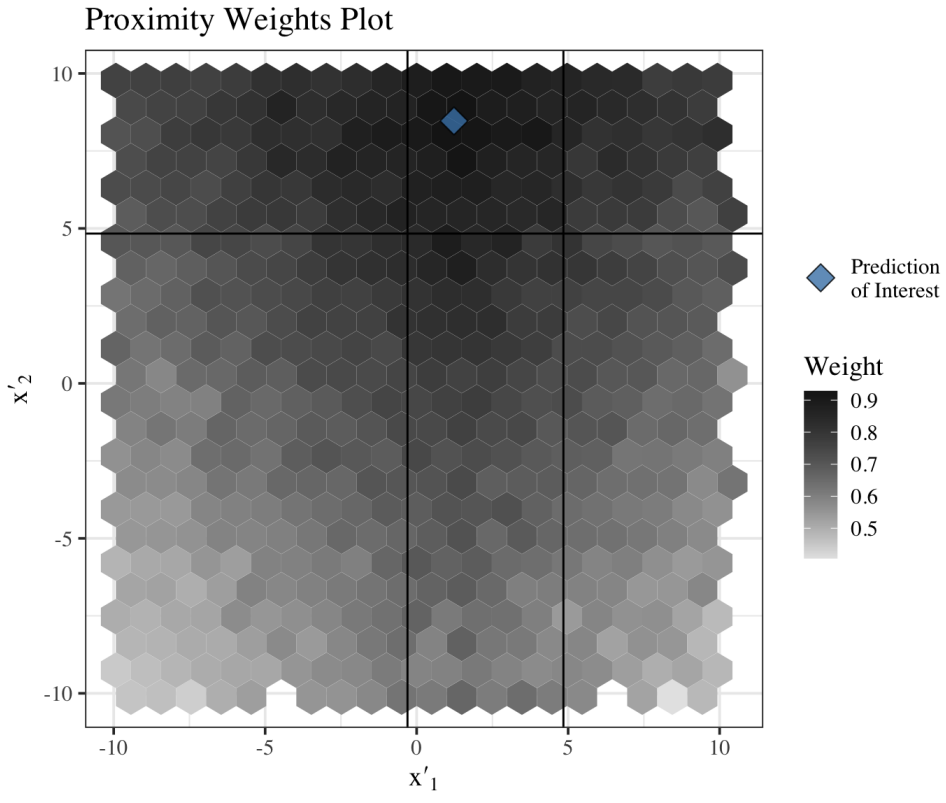
Step 2a: Assign Weights

- 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

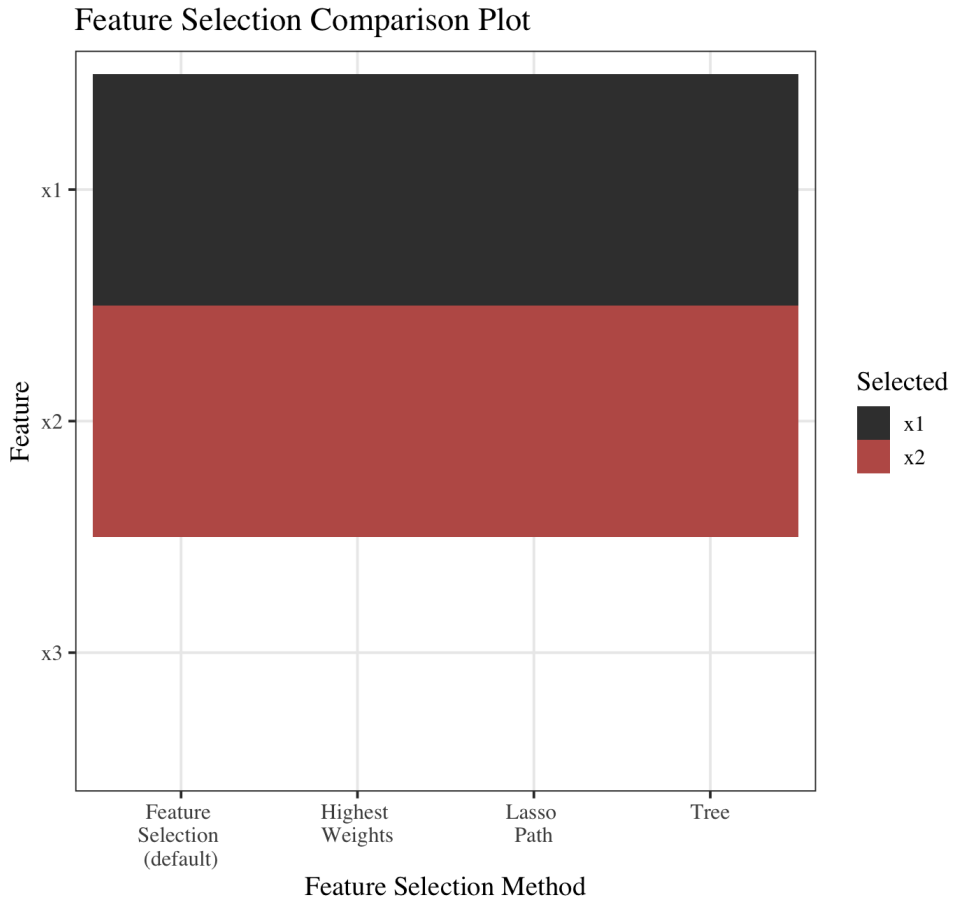
Step 2b: Feature Selection

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

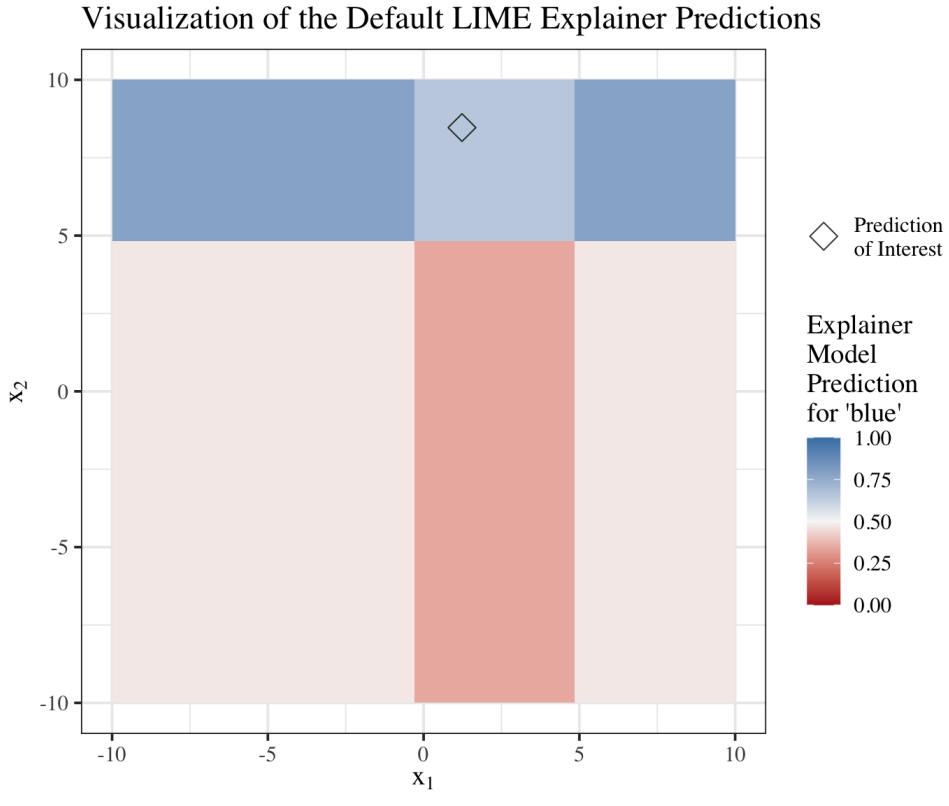
Step 2c: Fit Explainer Model

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

Corresponding Diagnostic:

Explainer Model Prediction Plot

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



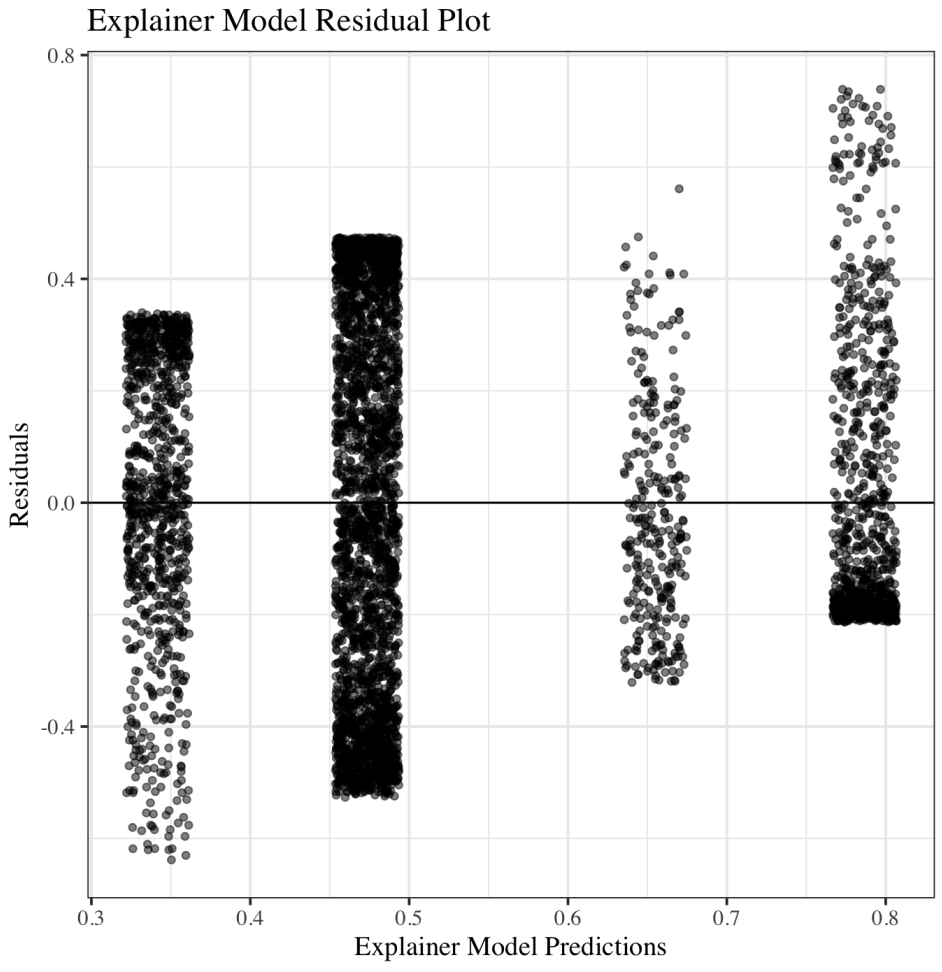
Diagnostics for Individual Explanations

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



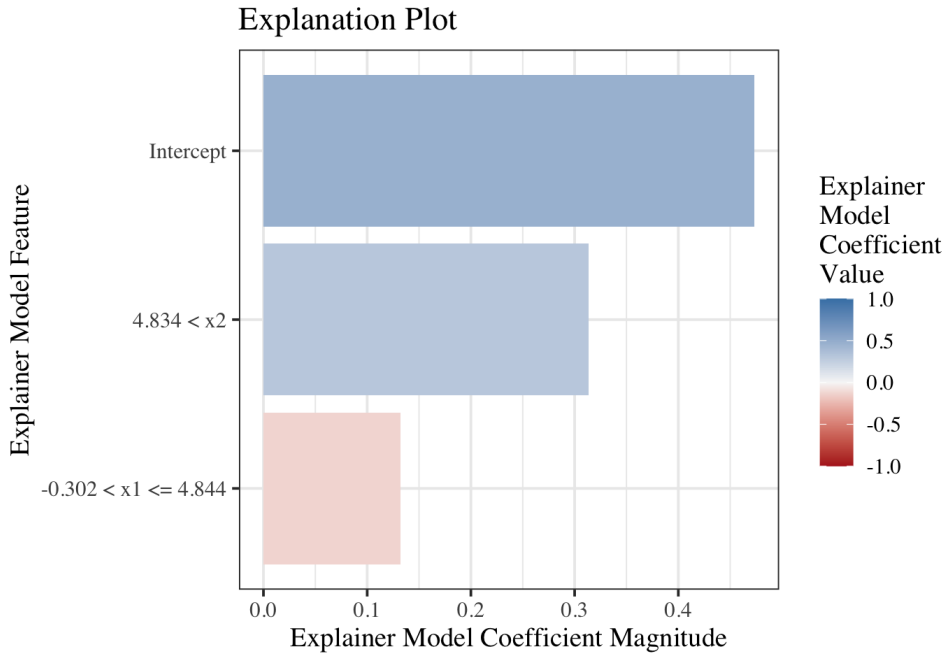
Diagnostics for Individual Explanations

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

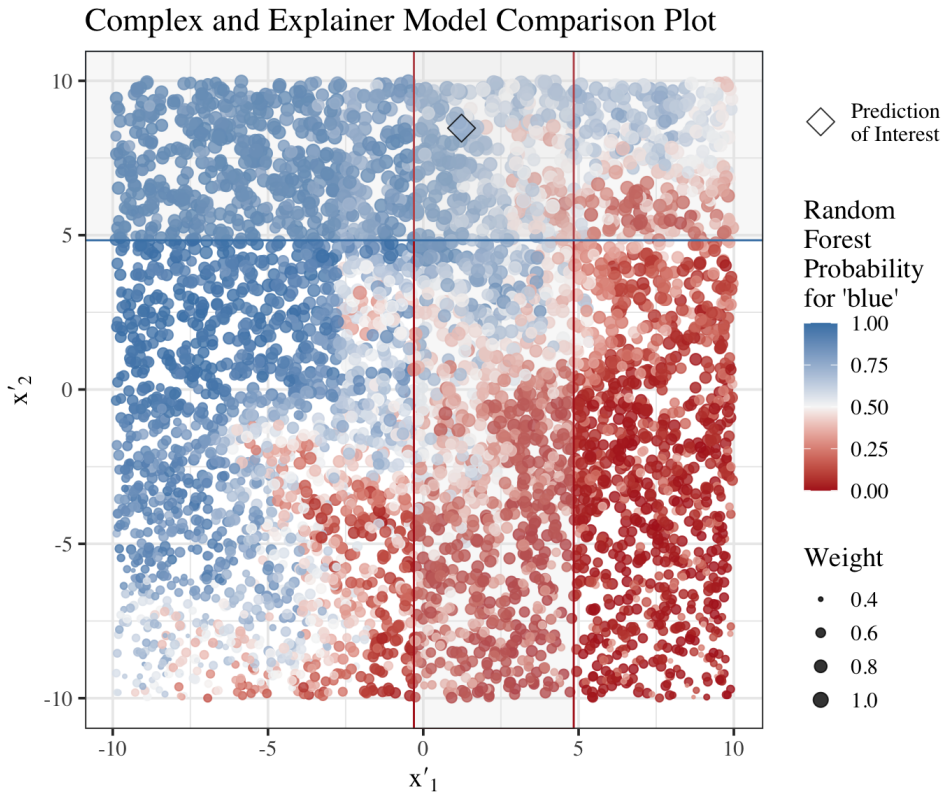


Diagnostics for Individual Explanations

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)



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

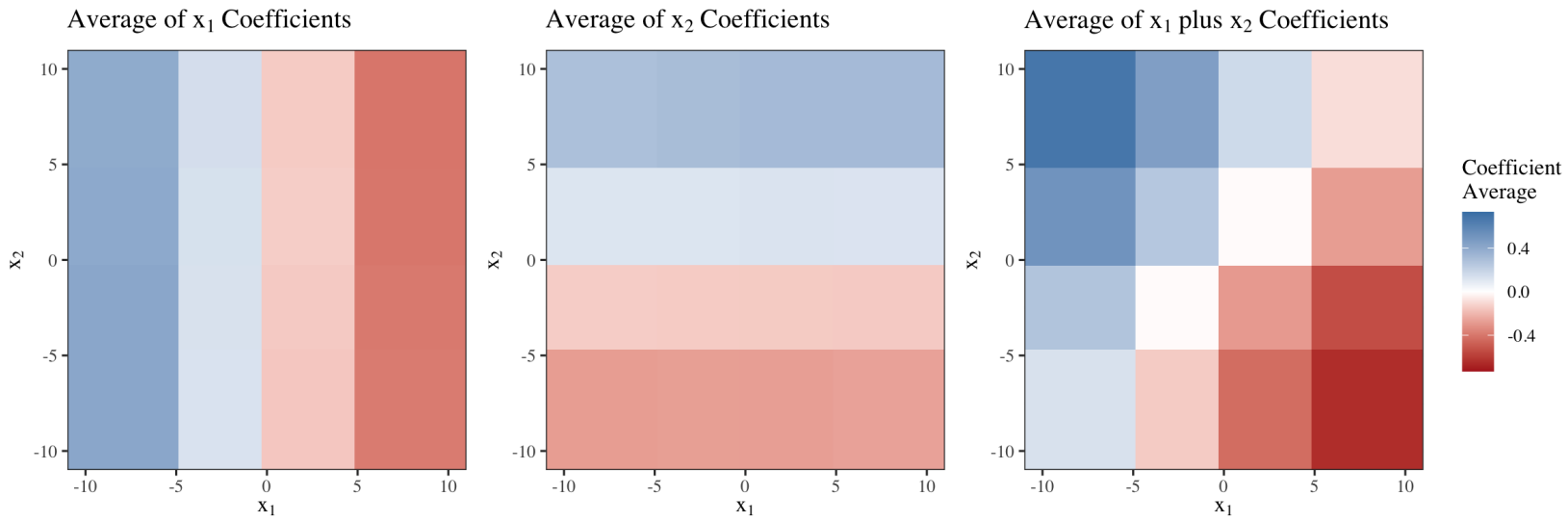
- Adaptation to the *lime* plot of all explanations
- Y-axis: Interpretability transformed features
- X-axis: Observation in the data set
- Tile Color: Ridge regression coefficient from the corresponding model

Diagnostics for Sets of Explanations

Average 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

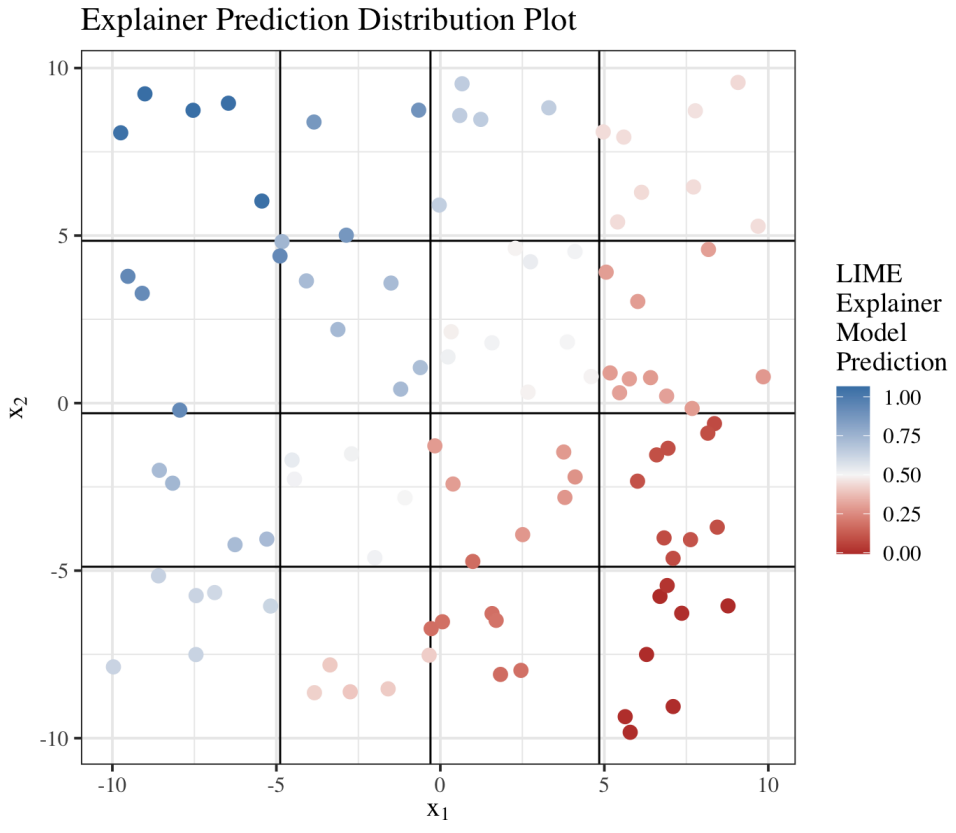


Diagnostics for Sets of Explanations

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

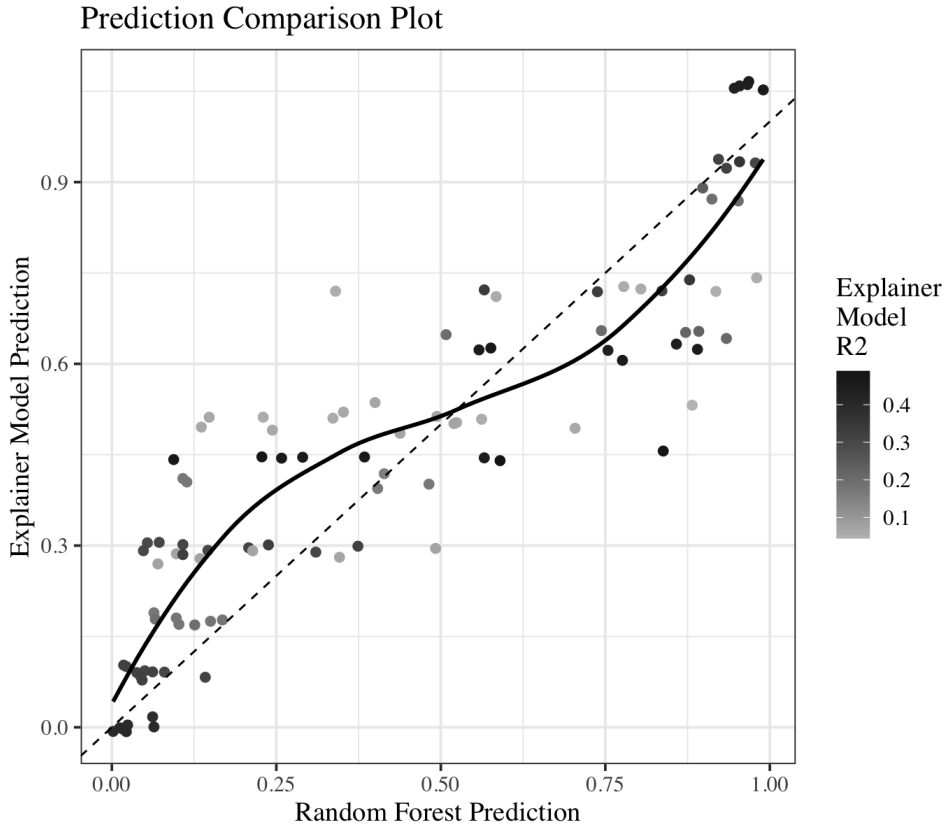


Diagnostics for Sets of Explanations

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
- Solid Line: Loess smoother fit to the points

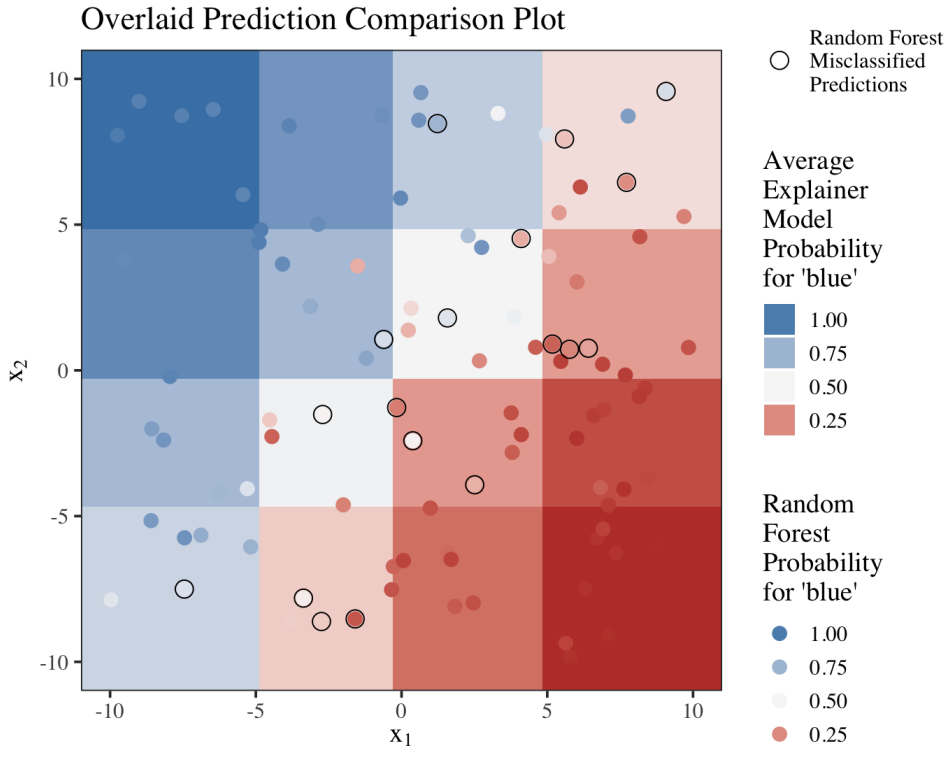


Diagnostics for Sets of Explanations

Overlaid 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

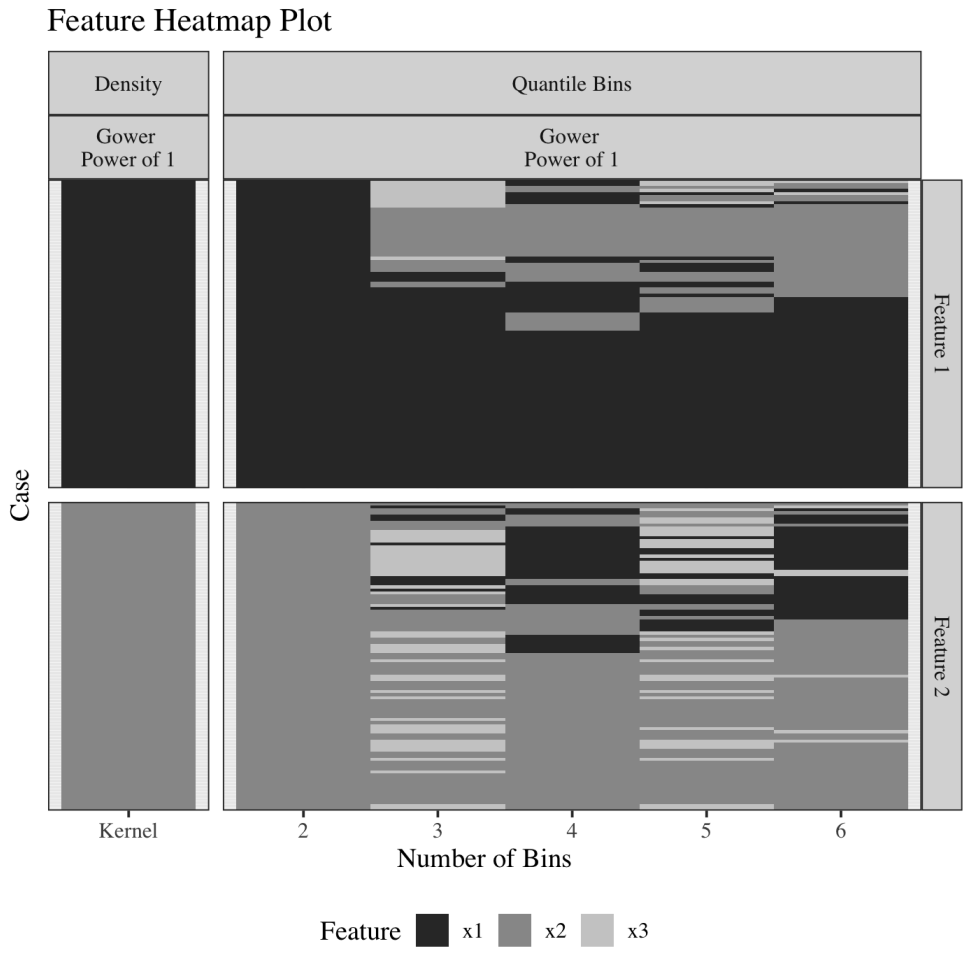
Plot of all explanations from *lime* R package:

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



Notation for Assessment Metrics

Data and Complex Model

For a set of E explanations

- $\mathbf{X}$ = matrix of observed data to be explained with K features and E observations
- x_e = observed feature vector for observation e
- f = complex model
- $f(x_e)$ = complex model prediction for observation e

Simulated and Transformed Data

For x_e and set of tuning parameters t

- $\mathbf{X}'_{e,t}$ = LIME simulated dataset with K features and S observations
- $x'_{e,t,s}$ = feature vector for simulated data observation s
- $\mathbf{Z}'_{e,t}$ = matrix of interpretability transformed simulated data with K features and S observations
- $z'_{e,t,s}$ = interpretability transformed feature vector
- $z_{e,t}$ = interpretability transformed x_e

Notation for Assessment Metrics

Weights and Explainer Model

For x_e and set of tuning parameters t

- π_t = proximity distance metric
- $\pi_t\left(x_e, x'_{e,t,s}\right)$ = weight assigned to $x'_{e,t,s}$ which are the proximity between x_e and $x'_{e,t,s}$
- $g_{e,t}$ = explainer model
- $g_{e,t}(z'_{e,s,t})$ = explainer model prediction for interpretability transformed simulated data observation s

Summary of Indices

- e = explanation $(e = 1, \ldots, E)$
- t = set of tuning parameters $(t = 1, \ldots, T)$
- s = simulated observation $(s = 1, \ldots, S)$

Metrics for the Assessment of LIME

Average R Squared: Average of explainer model R^2 values over a set of explanations with the same tuning parameters to assess the linearity claim where $R^2_{e,t}$ is the R^2 for $g_{e,t}$

$$R^2_{\text{ave}} = \frac{1}{E}\sum_{e=1}^{E} R^2_{e,t}$$

Average Fidelity: Average of fidelity metric introduced in Ribeiro, Singh, and Guestrin (2016) over a set of explanations with the same tuning parameters to assess the explainer model approximation to the complex model

$$\mathcal{L}_{\text{ave}} = \frac{1}{E}\sum_{e=1}^{E}\mathcal{L}(f,\, g_{e,t},\, \pi_t) = \frac{1}{E}\sum_{e=1}^{E}\sum_{s=1}^{S}\pi_t\left(x_e, x'_{e,t,s}\right)\left(f(x_e) - g_{e,t}\left(z'_{e,t,s}\right)\right)^2$$

Mean Squared Explanation Error (MSEE): Comparable to an MSE for comparing complex model predictions to explainer model predictions for each explanation

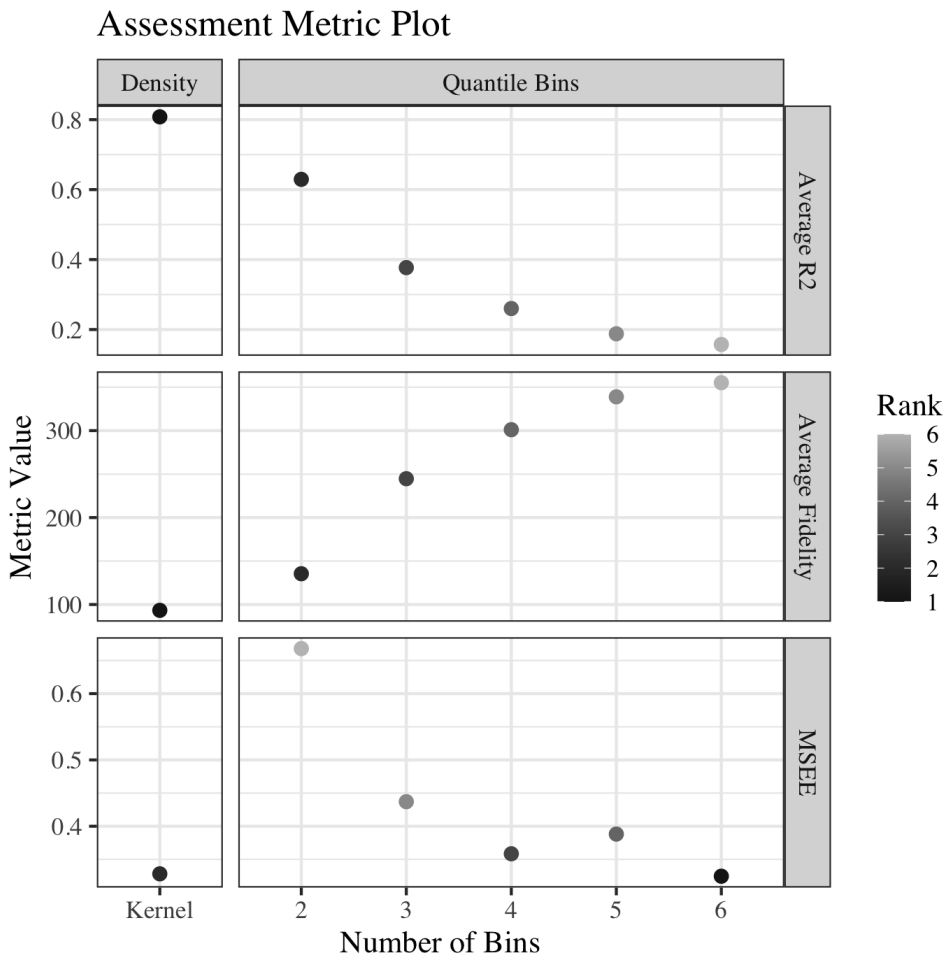
$$MSEE = \frac{1}{E}\sum_{e=1}^{E}\left(f\left(x_e\right) - g_{e,t}\left(z_{e,t}\right)\right)^2$$

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)



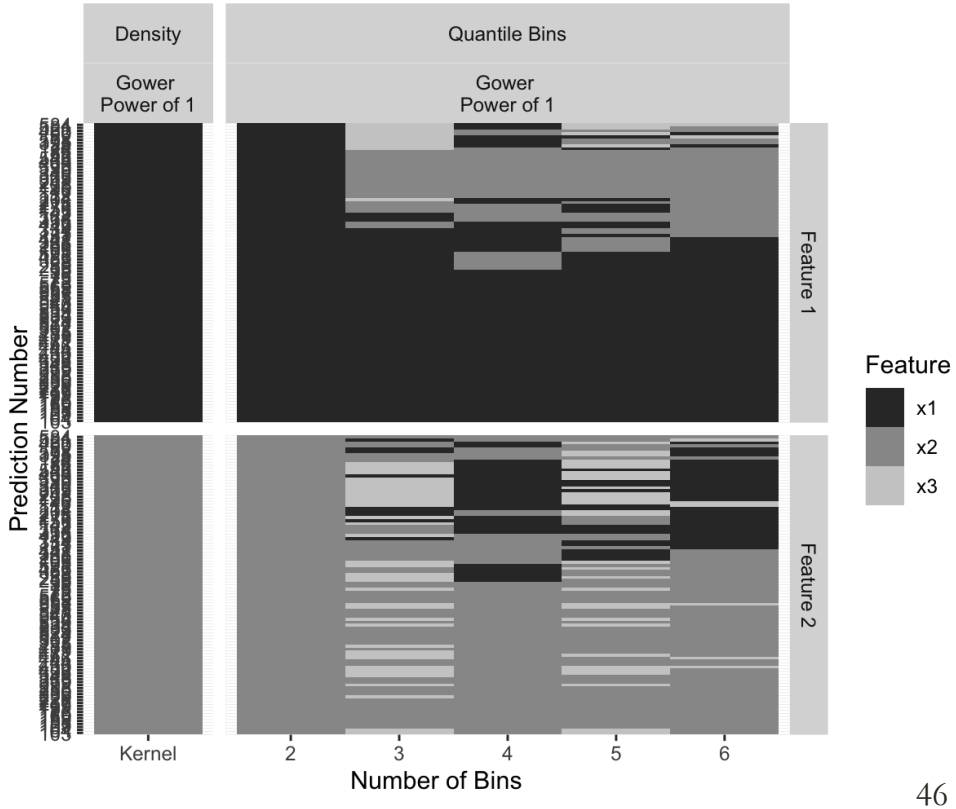
Implementation and Application

R package: limeaid

Our R package for visual LIME diagnostics:

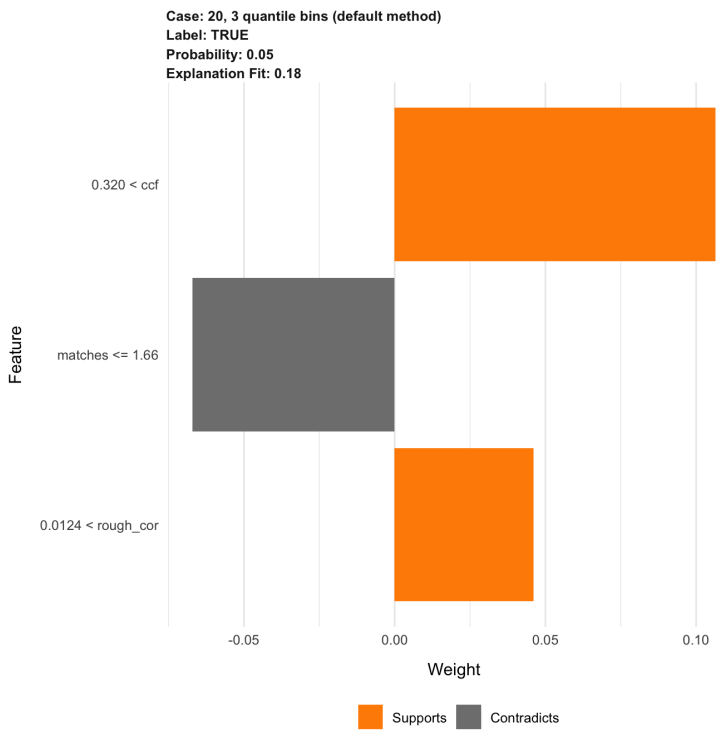
- Available on GitHub
  - github.com/goodekat/limeaid
- Functionality:
  - Applying LIME with multiple tuning parameters
  - Computing assessment metrics
  - Plots:
    - Complex and explainer model comparison plot
    - Feature Heatmap Plot
    - Assessment Metric Plot

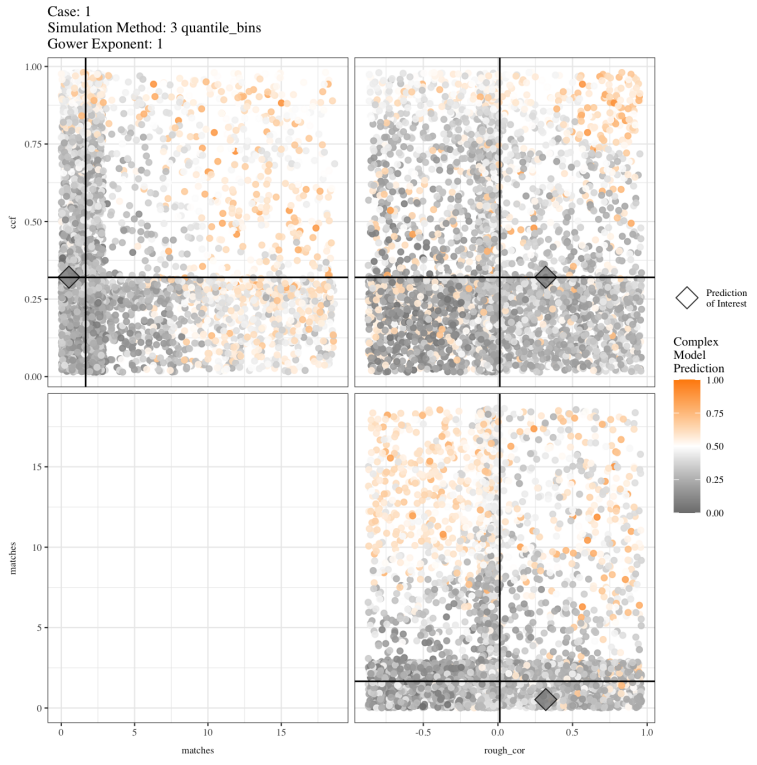
```
feature_heatmap(
  explanations = sine_lime_explain$explain,
  order_method = "PCA"
  )
```



Application of Visual Diagnostics to Bullet Random Forest

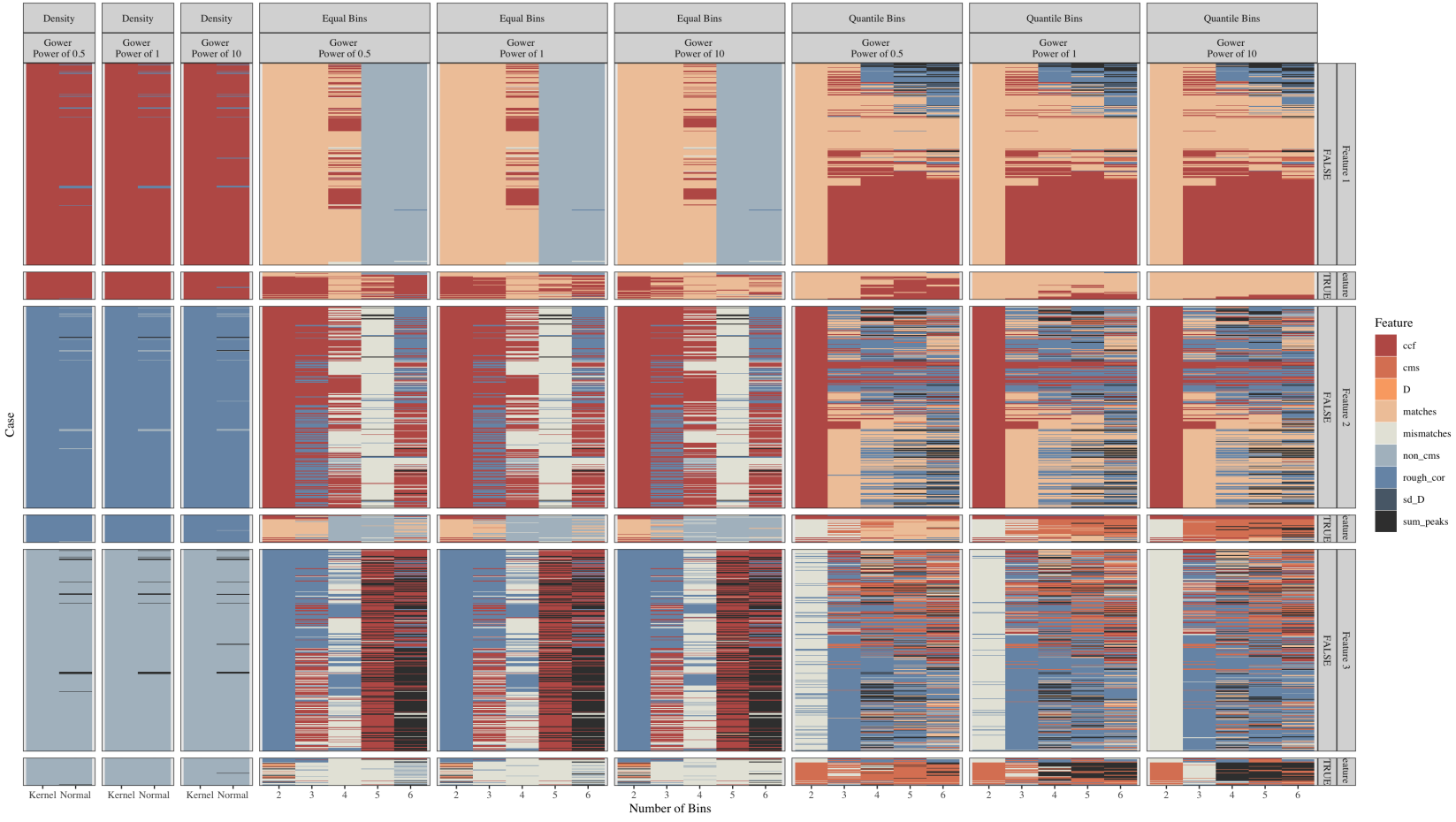
Bullet random forest prediction example from motivation with the complex and explainer model comparison plot





Application of Visual Diagnostics to Bullet Random Forest

Feature heatmap of LIME explanation from Hare, Hofmann, and Carriquiry (2016) bullet comparison forest model



Chapter 2

Explaining Random Forests using Clustering of Trees

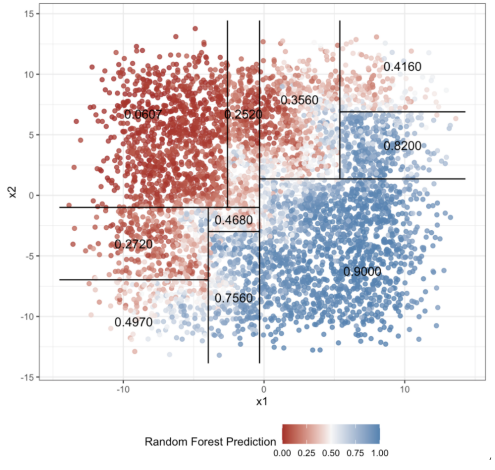
Current Plan

Motivation

- Still interested in gaining insights for the random forest from (Hare, Hofmann, and Carriquiry, 2016)
- Focus on visualizations of the random forest trees

Ideas

- Tree as a global explainer model
    - Plot global explainer on top of Urbanek (2008)'s trace plot
- Clustering to identify key trees in random forest
    - Use distance metric to compare trees



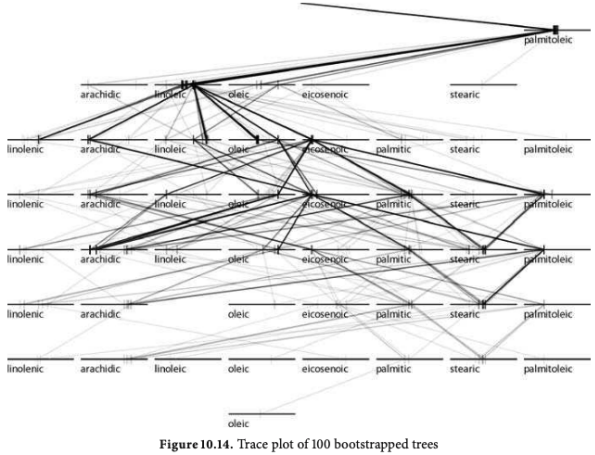


Figure 10.14. Trace plot of 100 bootstrapped trees

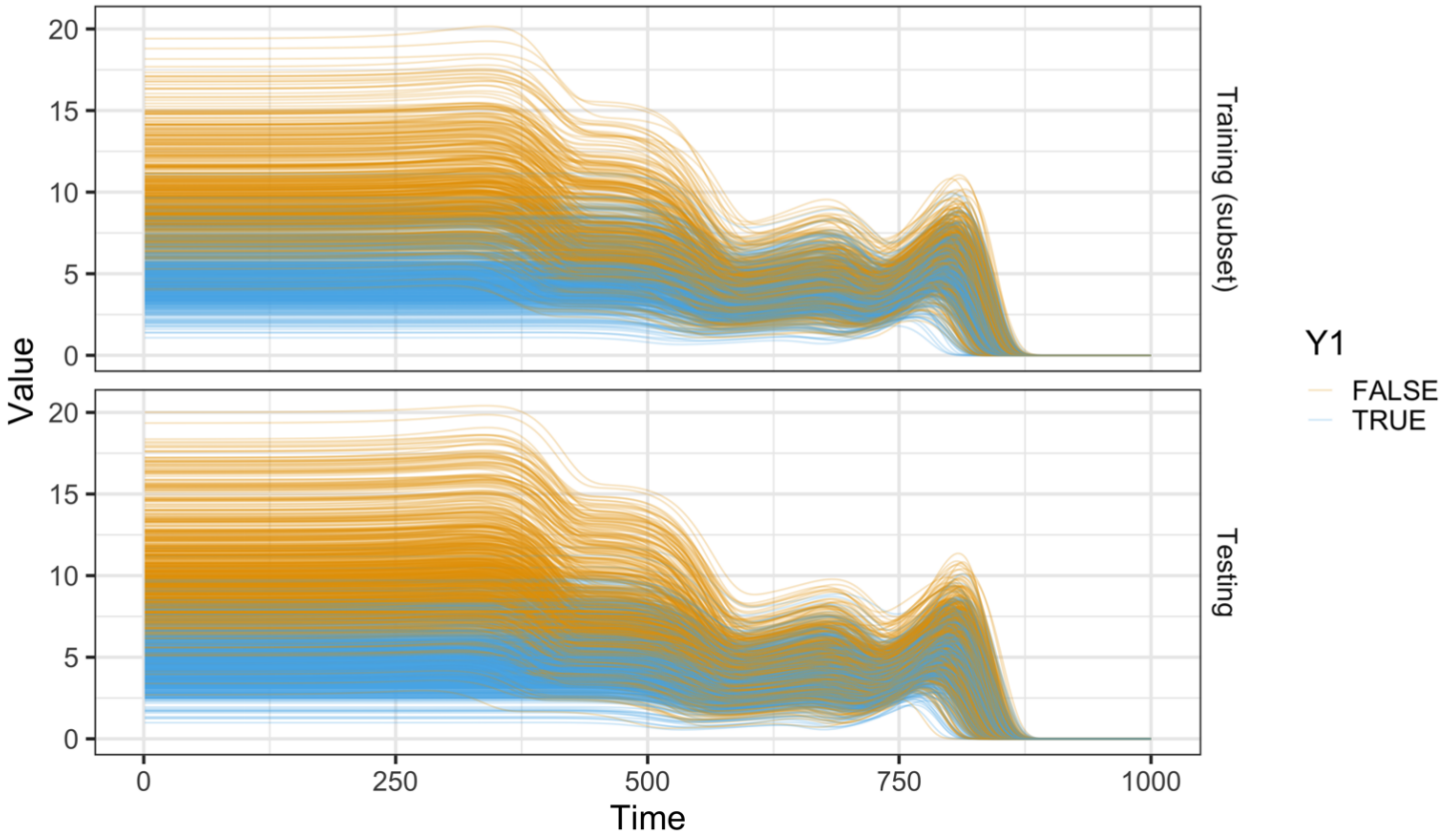
Trace plot from Urbanek (2008).

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 features that maximize the activation function
- Identify example observation that triggers a part of the network

Process

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

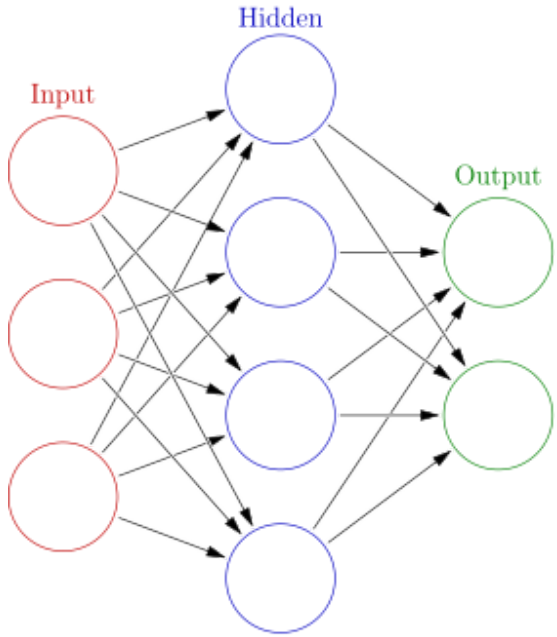
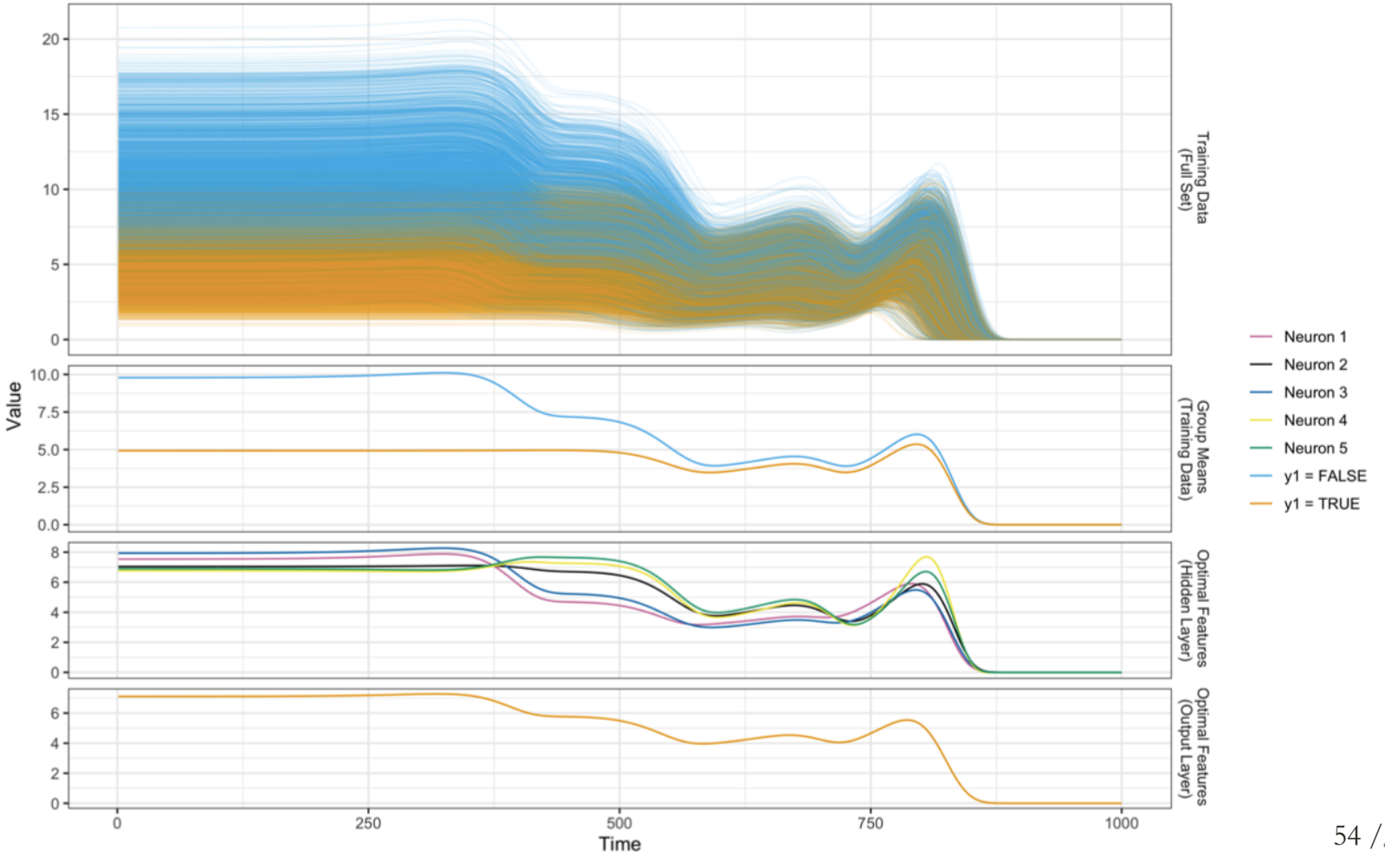


Image source: https://en.wikipedia.org/wiki/Artificial_neural_network

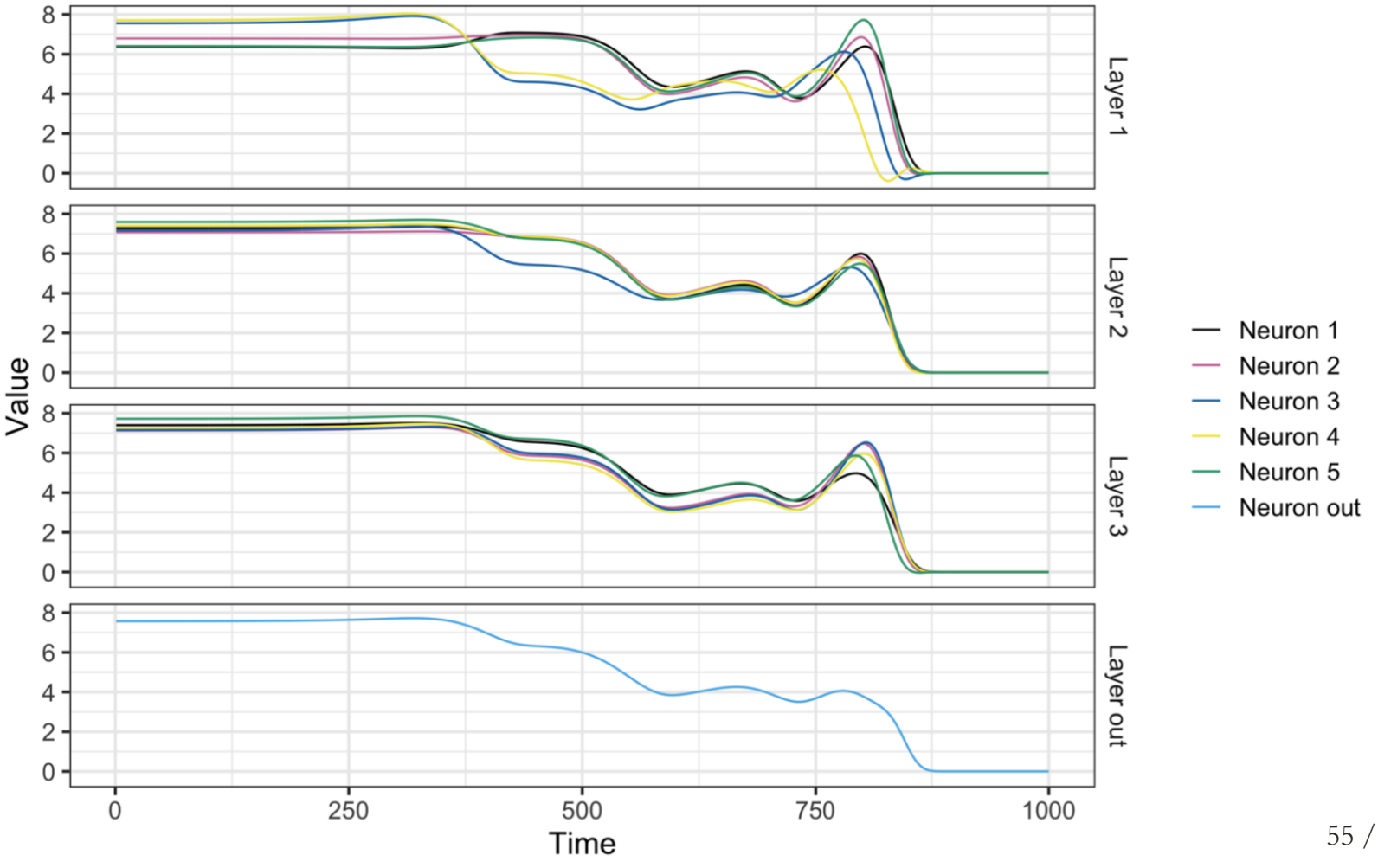
Feature Visualization

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)

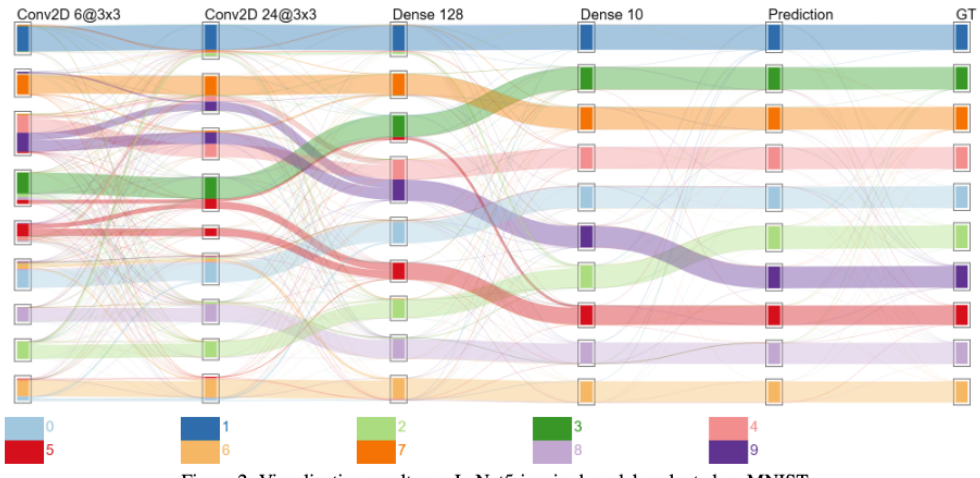


Figure 2: Visualization result on a LeNet5-inspired model evaluated on MNIST.

Timeline and Discussion Points

Timeline for Completion

Summer 2020

- Chapter 1: Finish writing (possibly submit paper)
- Chapter 2: Start on content (if time)
- Chapter 3: Work on content (Sandia internship)

Fall 2020

- Chapter 1: Submit paper (if not already done)
- Chapter 2: Work on content
- Chapter 3: Write up work

Spring 2021

- Chapter 1: Review process (if applicable)
- Chapter 2: Write up work
- Chapter 3: Submit paper (if ready)
- Defend dissertation

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)
- Present diagnostic plots
- Demonstrate issues found with LIME explanations

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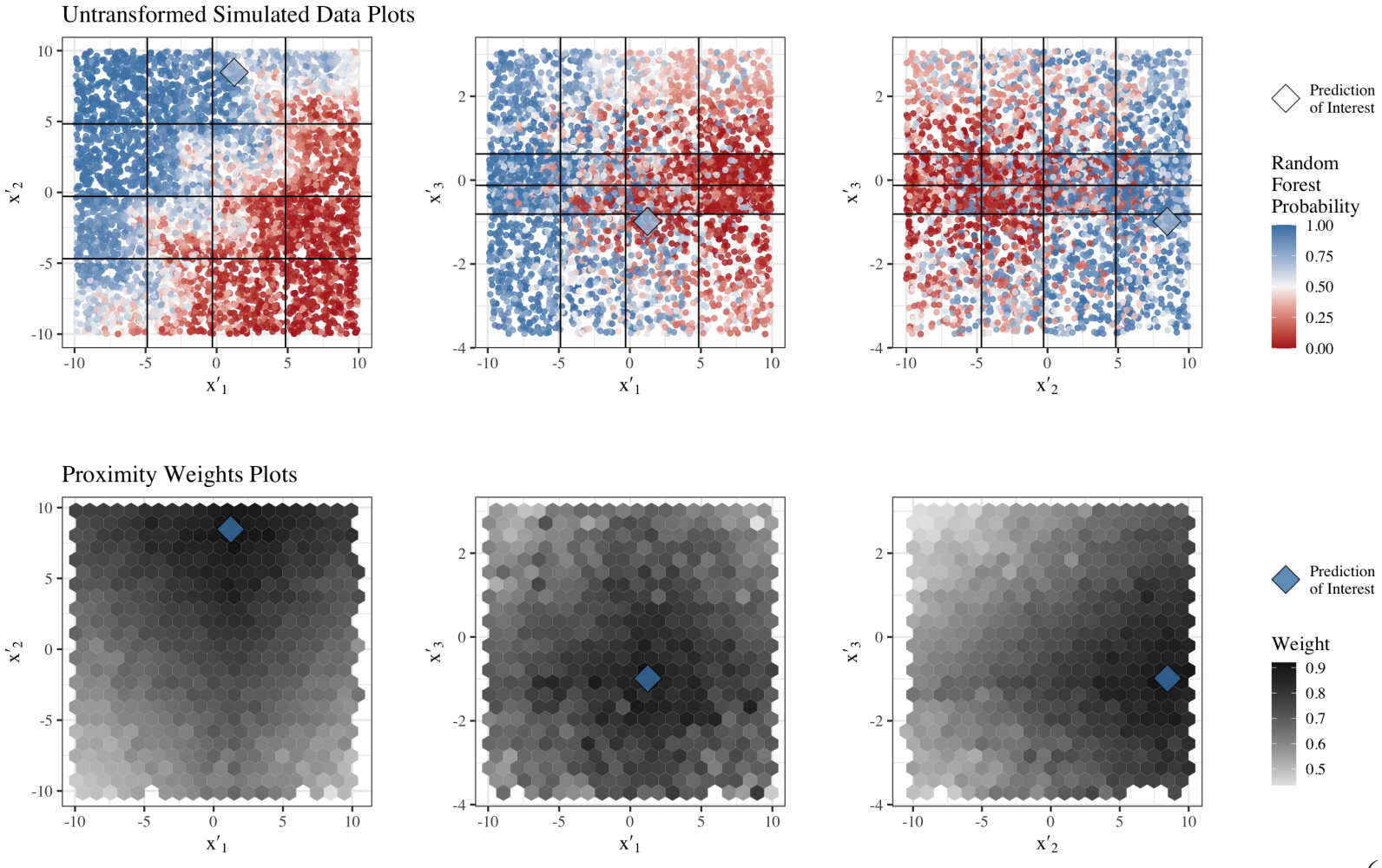
Appendix

Extensions to Diagnostics for Individual Explanations

Visualizations with more features



Additional Bullet Application Plots

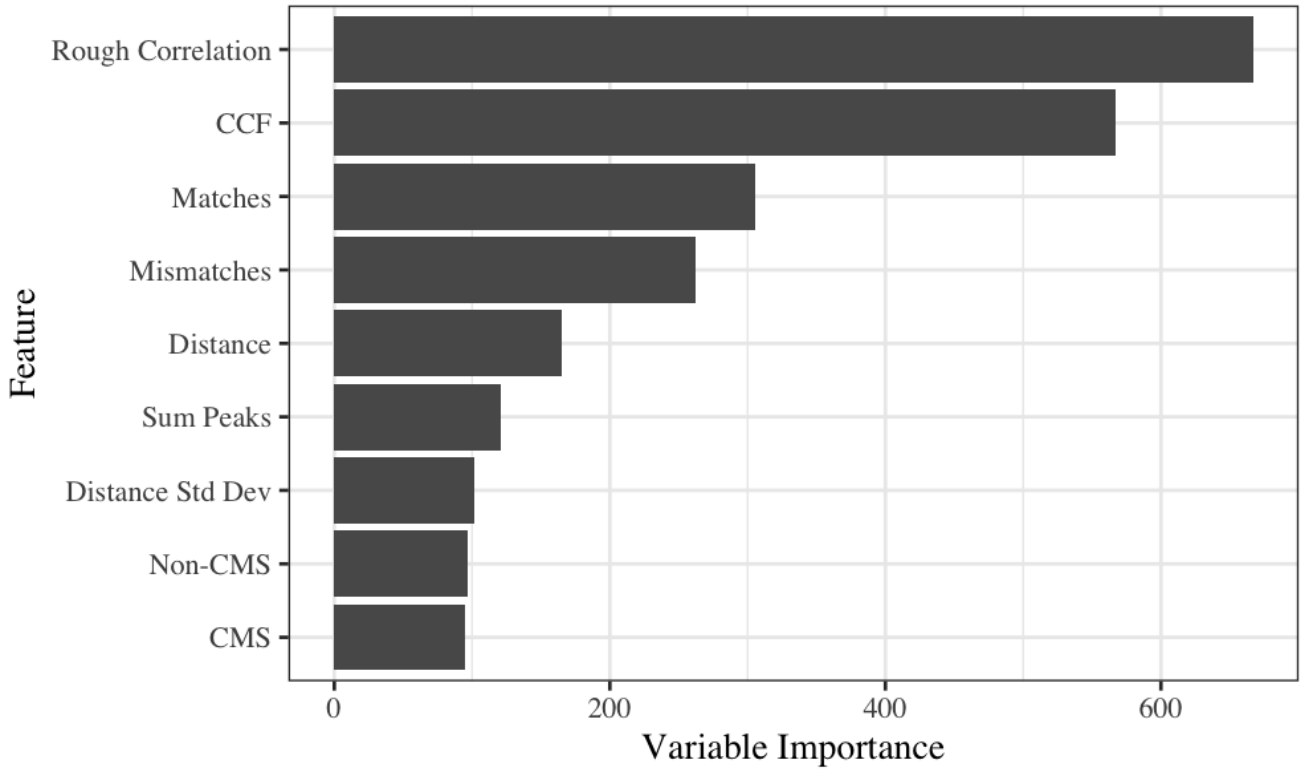
Distribution of the response variable for the random forest features

Additional Bullet Application Plots

Bivariate visualizations of the random forest training data

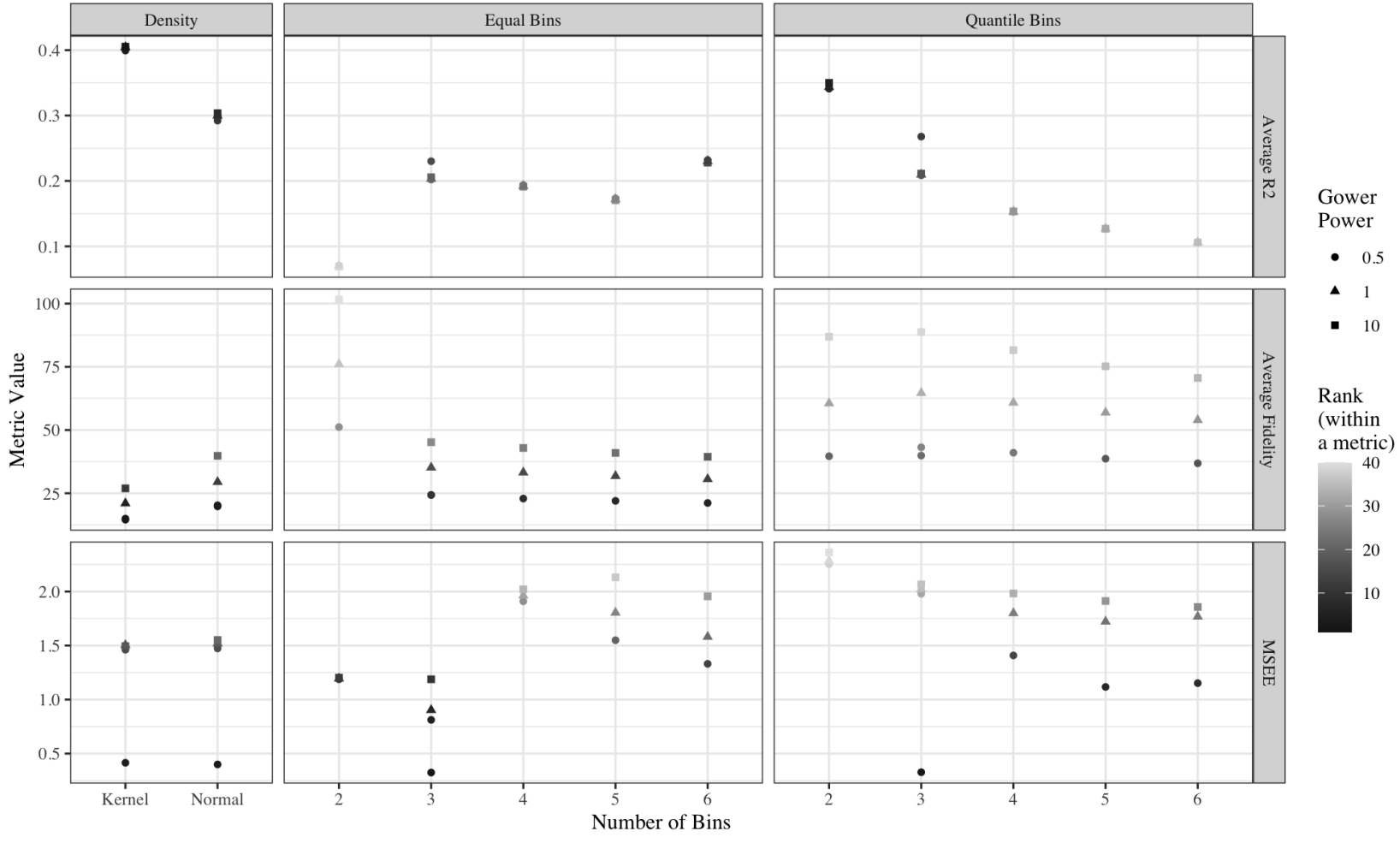
Additional Bullet Application Plots

Random forest variable importance plot



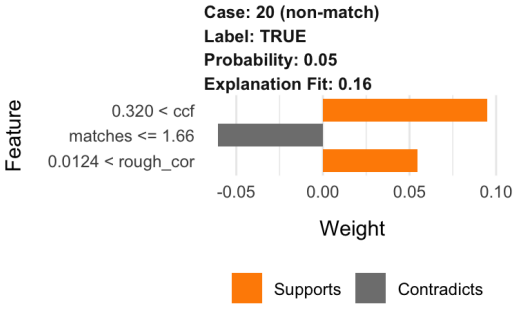
Additional Bullet Application Plots

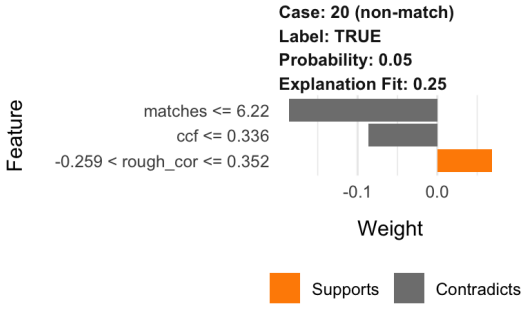
Assessment metric plot

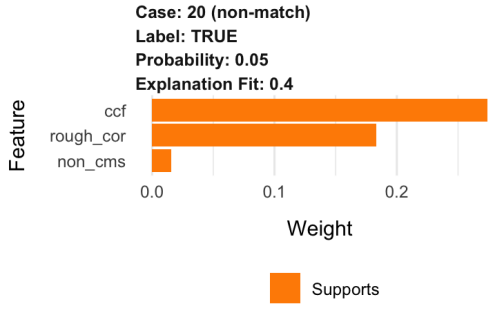


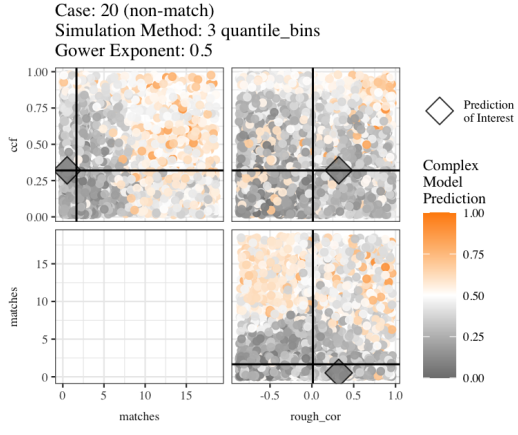
Additional Bullet Application Plots

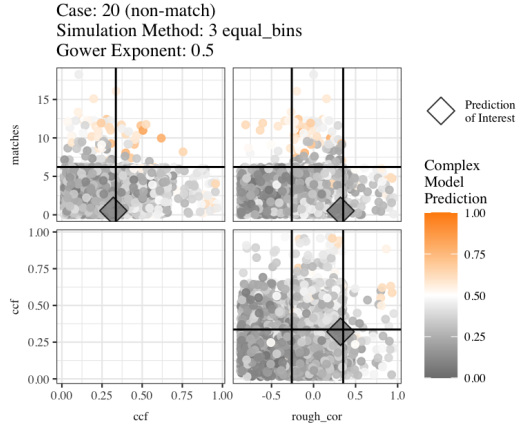
Plots of LIME explanations for one case in the test data that is a known non-match

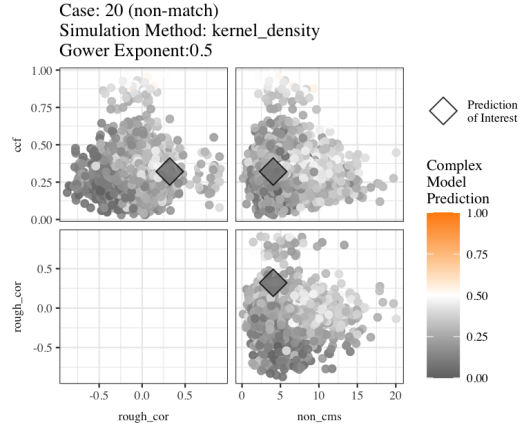






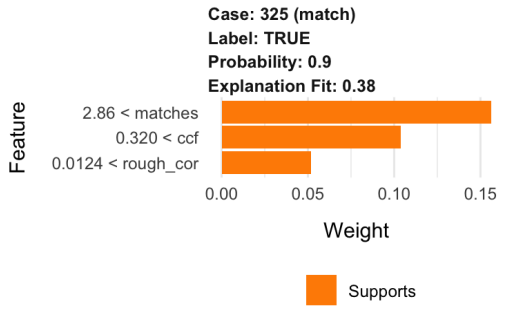


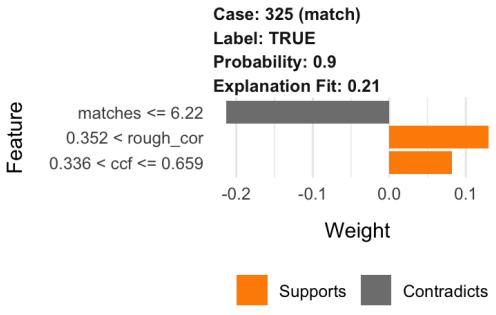


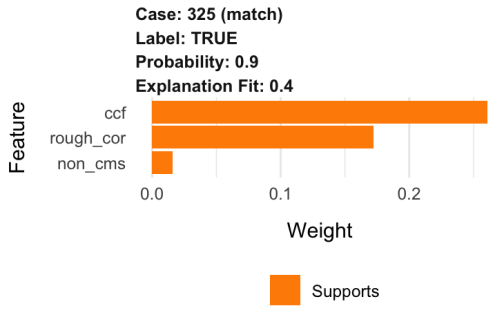


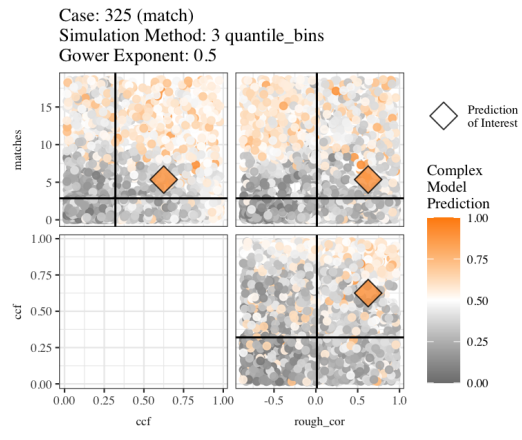
Additional Bullet Application Plots

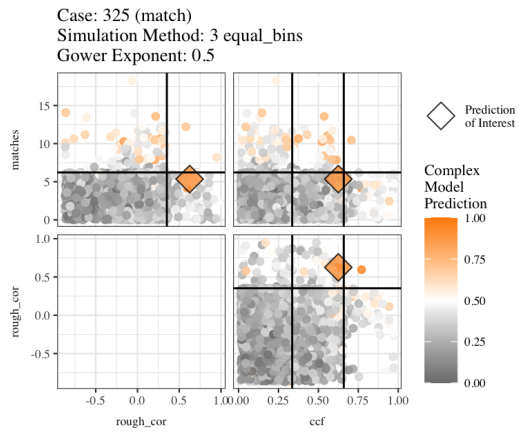
Plots of LIME explanations for one case in the test data that is a known match

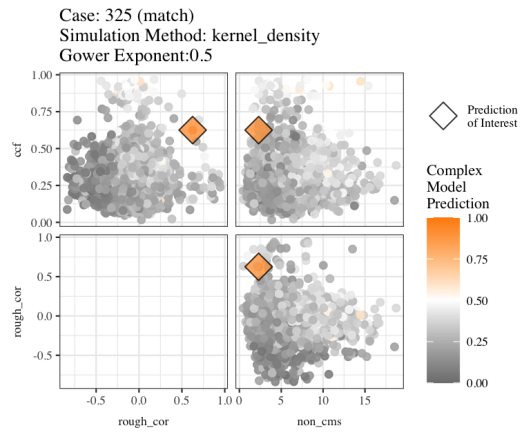












Feature Visualization Example Optimization Example

- 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:

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