U-smile Shiny Application Help Documentation

Application Name: U-smile (User-centric Statistical Measures for Interpretable Learning Explanations)

1. Introduction

   The U-smile application is designed to visualize and quantify the usefulness of new predictors stratified by outcome class using the U-smile method. It provides a threshold-free and asymmetric approach to evaluating and comparing binary classification models, which is particularly useful for biomedical applications and imbalanced datasets.

2. How to Use the Application

   2.1. Standard Analysis Tab

   This tab allows you to perform a comparative analysis between two models. You have two main workflows:

   Build Models Automatically:

   <u>Upload Data:</u> Provide your training data (and optionally, separate test data) in CSV or Excel format.

   <u>Select Variables:</u> Choose your binary outcome/target variable and the predictor variables from your dataset.

   <u>Choose Models:</u> Select the types of models you want to build and compare (e.g., Logistic Regression vs. Logistic Regression, Logistic Regression vs. Random Forest).

   The application will train the models and generate the U-smile plot and related diagnostics.

   Use Pre-built Models:

   <u>Upload Models:</u> Upload your own previously saved model objects in .rds format. The application supports models from various algorithms (Logistic Regression, Random Forest, SVM, XGBoost, Neural Networks, Naive Bayes).

   <u>Upload Evaluation Data:</u> Provide the corresponding dataset (in .rda or other formats) that was used to generate the model predictions.

   The application will load the models, calculate predictions, and generate the comparative analysis.

   2.2. Interactive U-smile Editor Tab

   This tab provides an educational environment to explore how the U-smile visualization is constructed.

   Manually adjust the core coefficients (Y values for magnitude of change, I values for proportion of affected cases). Observe in real-time how changes to these values affect the shape and symmetry of the U-smile plot. This is ideal for understanding the methodology behind the plots generated in the Standard Analysis tab.

3. Data Requirements & Format

To use your own dataset with the U-smile application, please ensure it meets the following format requirements:

File Format: CSV or Excel (.xlsx, .xls) for the Standard Analysis tab. RDS (.rds) for models and RDA (.rda) for data in the Pre-built Models workflow.

Headers: The first row must contain column names (headers).

Outcome Variable: The dataset must include a binary outcome (target) variable.

Coding: The outcome variable must be coded with values 0 (indicating the absence of the event, e.g., no disease, healthy) and 1 (indicating the presence of the event, e.g., disease, ill).

Variable Types: The explanatory (predictor) variables should be primarily numeric (continuous or integers). Categorical variables are supported but may need to be converted into factors or properly specified within the application.

4. Default Dataset

The application includes a default heart disease dataset for demonstration and exploration purposes:

Source: Variables are based on real clinical and demographic data from the UCI Machine Learning Repository.

Cases: 661 complete cases (347 healthy controls, 314 with coronary artery disease).

Variables: 10 real variables and 34 synthetically generated variables.

Split: A predefined training set (331 cases) and test set (330 cases) are included.

This dataset is automatically loaded but can be easily replaced with your own data in the "Standard Analysis" tab.

5. Methodology & Interpretation of Results

5.1. Core Concept: Model Comparison

The U-smile method is always based on a comparison:

Single Model Evaluation: A new model is compared to a basic reference model of random class assignment (e.g., 50/50 chance).

Two Model Comparison: A new model of interest is directly compared to an existing reference model (e.g., a basic model with few predictors vs. an extended model with additional predictors).

5.2. Decoding the U-smile Plot

The resulting plot is a concise visualization that separates model performance for the event class and the non-event class.

X-Axis - Outcome Classes: The plot is split into the non-event class {0} (blue, left side) and the event class {1} (red, right side).

Subclassification: Within each class, instances are divided into those where the new model predicts better {+} (darker, outer points) or worse {-} (lighter, inner points) than the reference model.

Y-Axis - Magnitude of Change: The vertical position represents the quantitative change in prediction quality for a subgroup. This can be one of several coefficients:

rLR (Relative Likelihood Ratio)

BA (Brier Alteration)

RB (Relative Brier)

Point Size - Frequency of Change: The size of the points represents the I value, a qualitative coefficient indicating the proportion of individuals in the cohort that experienced that specific change (derived from the Net Reclassification Index framework). A larger point means the change affected more people.

5.3. The Story of the Smile: Symmetry and Significance

A Symmetrical Smile: Indicates that the new model performs better than the reference model in both classes. This is the ideal scenario.

An Asymmetrical Smile: A smile visible only on one side means the new model's advantage is confined to that single class. This is common and often desired when the goal is to improve prediction specifically for a minority class (e.g., a rare disease).

Line Styles & Statistical Significance: A solid line is used to highlight parts of the smile where the difference between the new and reference model is statistically significant (based on a Likelihood Ratio test for each class separately). A dashed line indicates non-significant changes.

5.4. Coefficients & Levels of Analysis

The method provides a hierarchical decomposition of model performance:

Level 1: Point Positions and Sizes (Y and I Values): The raw values for improvement/deterioration (Y) and their frequency (I) for each of the four subgroups.

Level 2: Net Coefficients (Netto): The net prediction improvement calculated separately for the non-event group (Netto_0) and the event group (Netto_1).

Level 3: Overall Coefficient: A single summary statistic of the total net improvement across the entire cohort, combining the contributions from both classes.

6. Troubleshooting

   Error: "Error in model fitting": Ensure your outcome variable is coded as 0/1 and that predictor variables are numeric or properly specified as factors.

   Plot not rendering: Check that the uploaded files are in the correct format and that the required columns are present.

   Unexpected results: Verify that the correct outcome variable has been selected in the sidebar.

7. Support & Contact

   For technical questions, bug reports, or suggestions regarding this Shiny application, please contact:

   Developer: Barbara Więckowska

   Email: bbwieckowska@gmail.com

8. Methodological References

   The U-smile method is based on the following publications:

Kubiak, K. B., Więckowska, B., Jodłowska-Siewert, E., & Guzik, P. (2024). Visualising and quantifying the usefulness of new predictors stratified by outcome class: The U-smile method. PLoS ONE, 19(5), e0303276. https://doi.org/10.1371/journal.pone.0303276

Więckowska, B., Kubiak, K. B., & Guzik, P. (2025). Evaluating the three-level approach of the U-smile method for imbalanced binary classification. PLoS ONE, 20(5), e0321661. https://doi.org/10.1371/journal.pone.0321661

Więckowska, B., & Guzik, P. U-smile Likelihood Evaluation: a threshold-free, explainable framework for binary classification model assessment. [Under Review]