University of Kentucky

CLASSify: A Web-based Tool for Machine Learning

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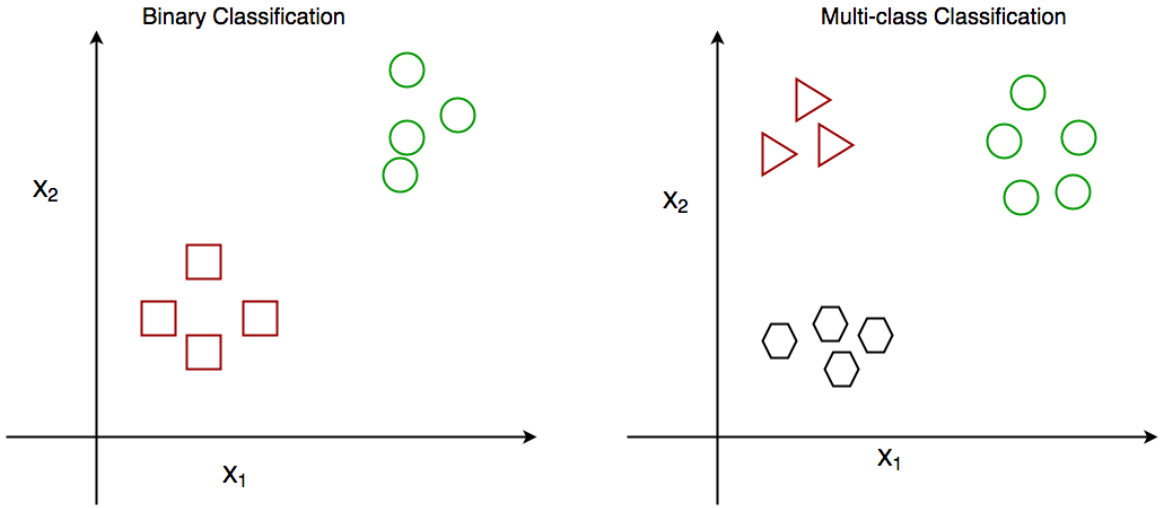
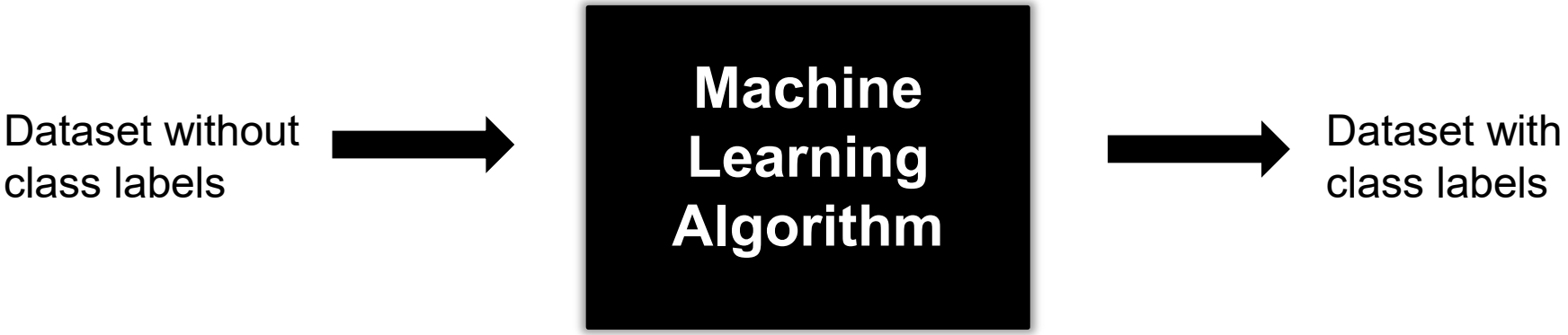
Tabular Classification Problems

- We want to predict/assign a class label for some data point
  - For example, diagnosis or outcome
- Many machine learning methods exist to achieve this



Machine Learning Challenges

- Requires coding knowledge/expertise
- Some models may be computationally expensive
- Class labels can be imbalanced
  - Model will be biased towards majority class
- Little interpretability of results

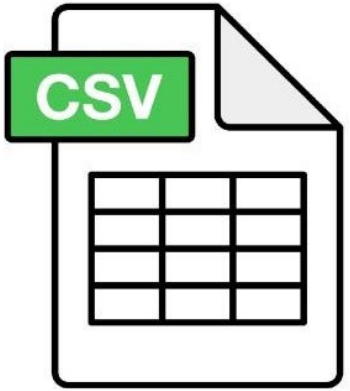


Solution

- CLASSify- a web-based tool for machine learning
  - Easily train and evaluate models with no coding experience
- Class labels can be balanced with synthetically-generated data
- Interpretability provided through SHAP scores
  - Explanations of each feature and their impact on the model's output

CLASSify- Setup

- Built to work with any tabular dataset in a .csv format
- Can be binary or multiclass
- Little preprocessing is required



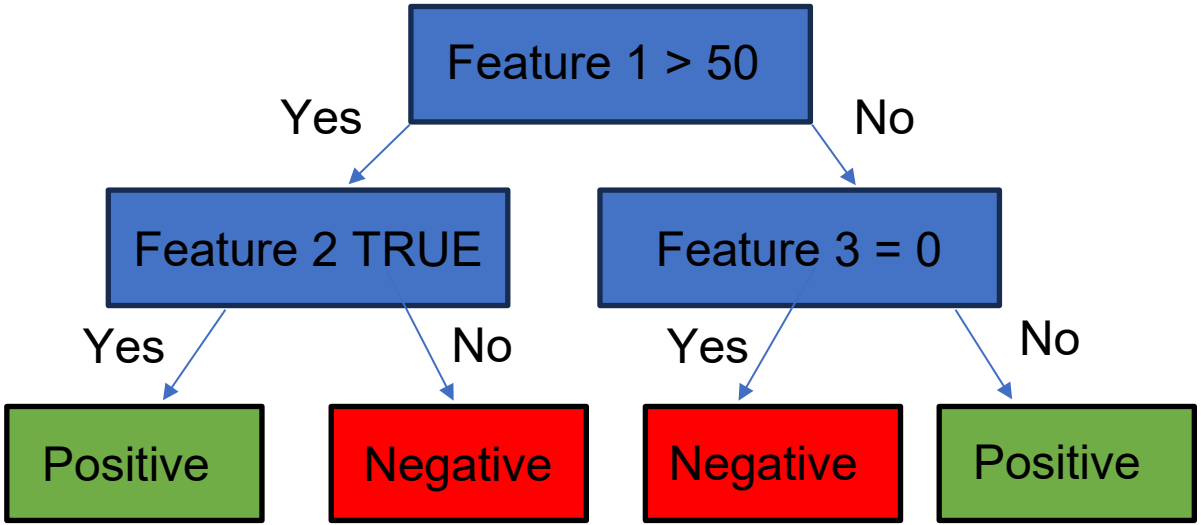
CLASSify- Machine Learning

Ten different classification machine learning models are provided

- Random Forest
- Gradient Boosting
- Histogram-based Gradient Boosting
- XGBoost
- Bagging
- Logistic Regression
- SGD Classifier
- K-Nearest Neighbors
- Multi-layer Perceptron
- TabPFN

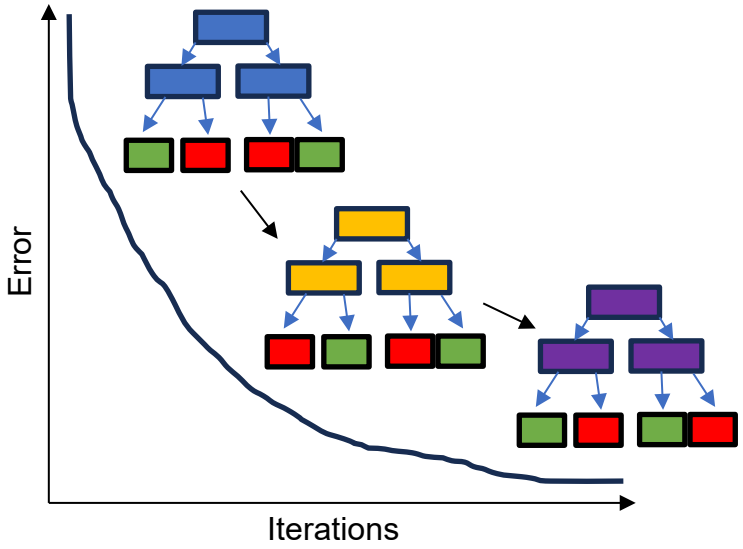
Random Forest

- Common ensemble machine learning algorithm
- Subsets of data are split and used to train separate decision trees
- Each decision tree predicts an output, and the majority class is chosen



Gradient Boosting

- Similar to random forest, but builds trees sequentially rather than in parallel
- Each tree can learn from the errors of the previous tree
- Minimizes loss function for each tree using gradient descent



- **Histogram-based Gradient Boosting-** optimization that bins continuous variables
- **XGBoost** (Extreme Gradient Boosting)- uses regularization and pruning to prevent overfitting

Bagging

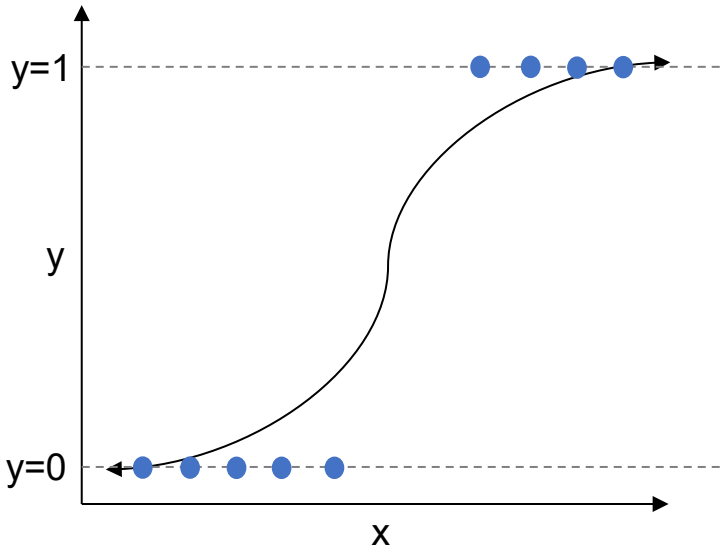
- Uses bootstrapped samples of training data to train many base estimators (frequently decision trees)
- Every tree has access to all features, unlike random forest
- Base estimators can be changed to other simple models

Original	Bootstrap1	Bootstrap2	Bootstrap3	Bootstrap4
1	1	2	1	1
2	1	3	2	1
3	3	3	3	1
4	3	3	5	4
5	5	4	5	5

Logistic Regression

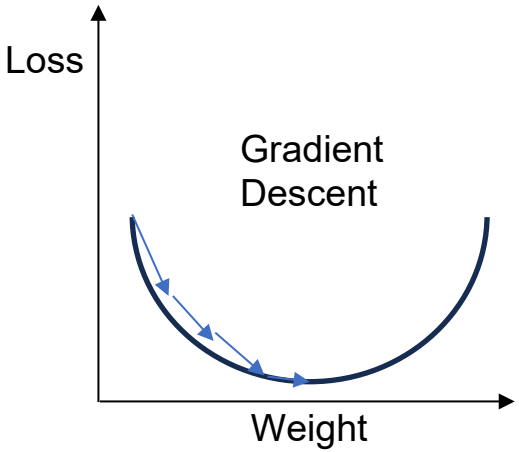
- Statistical method of building linear model
- Use sigmoid function to convert output into probability value

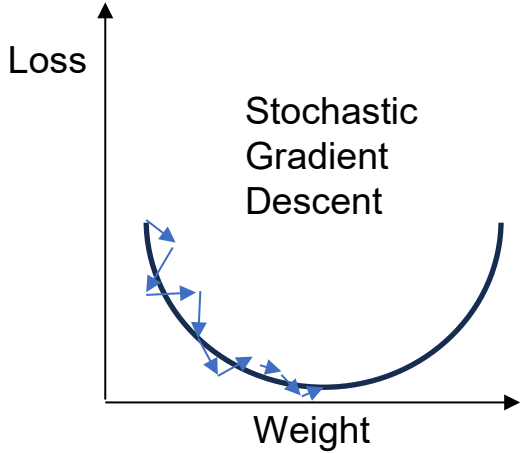
$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots$$



SGD Classifier

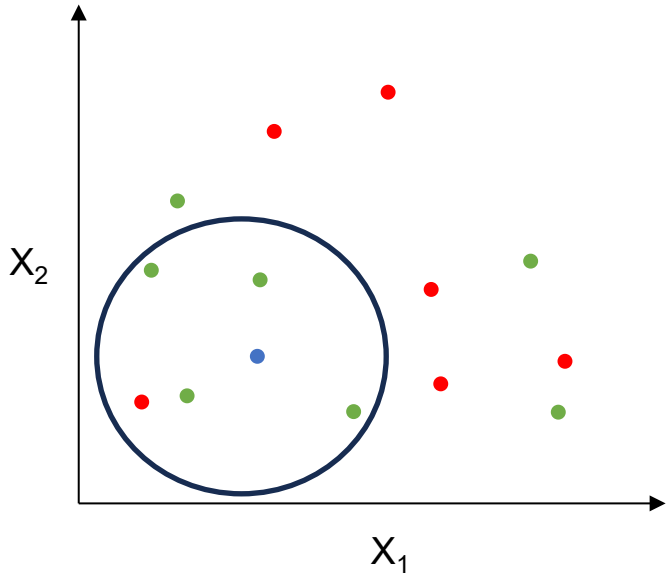
- Uses linear model, such as logistic regression or support vector machine, as base model
- Utilizes stochastic gradient descent to optimize model parameters
  - Gradient descent computes loss gradient using entire dataset
  - SGD computes loss gradient for each individual training example





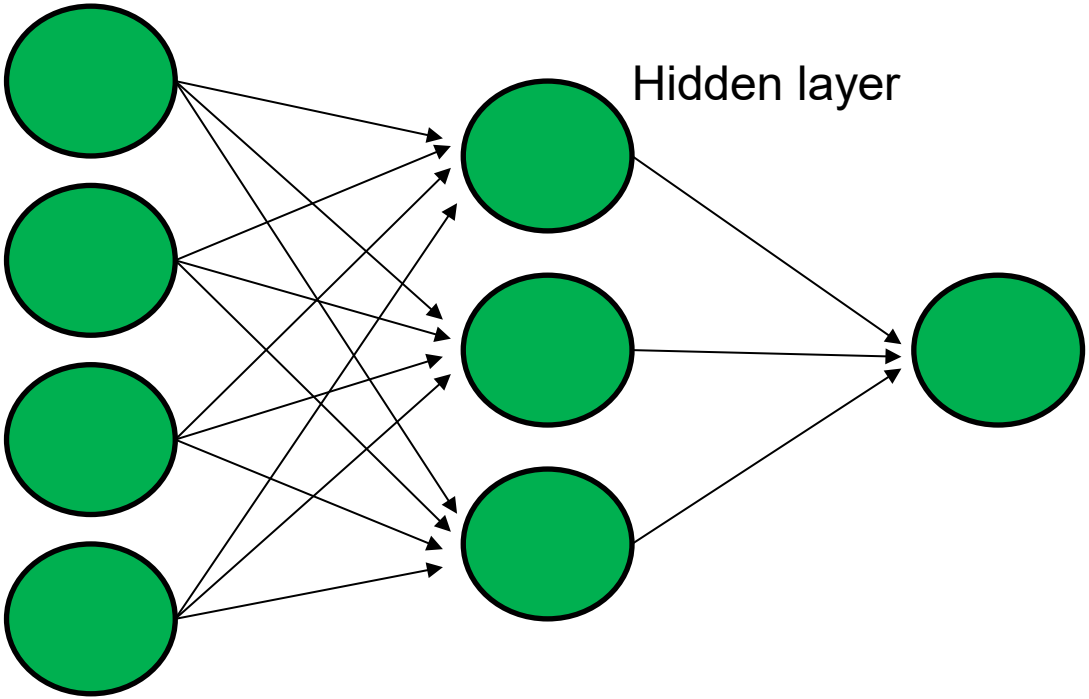
K-Nearest Neighbors

- Compares ‘distance’ between data points to determine what class a point should belong to



Multi-Layer Perceptron

- Neural network designed for classification



TabPFN

- Transformer model for tabular classification
- Transformers: similar to neural networks, with key differences
  - Uses self-attention mechanism to connect different input features
  - Process input in parallel for efficiency

CLASSify- Machine Learning

- Many varied model architectures provided for use and comparison
- Parameter tuning with Optuna
- Job queueing with ClearML
- Storage with Amazon S3 Cloud Storage
- Backend training/evaluation performed on DGX cluster

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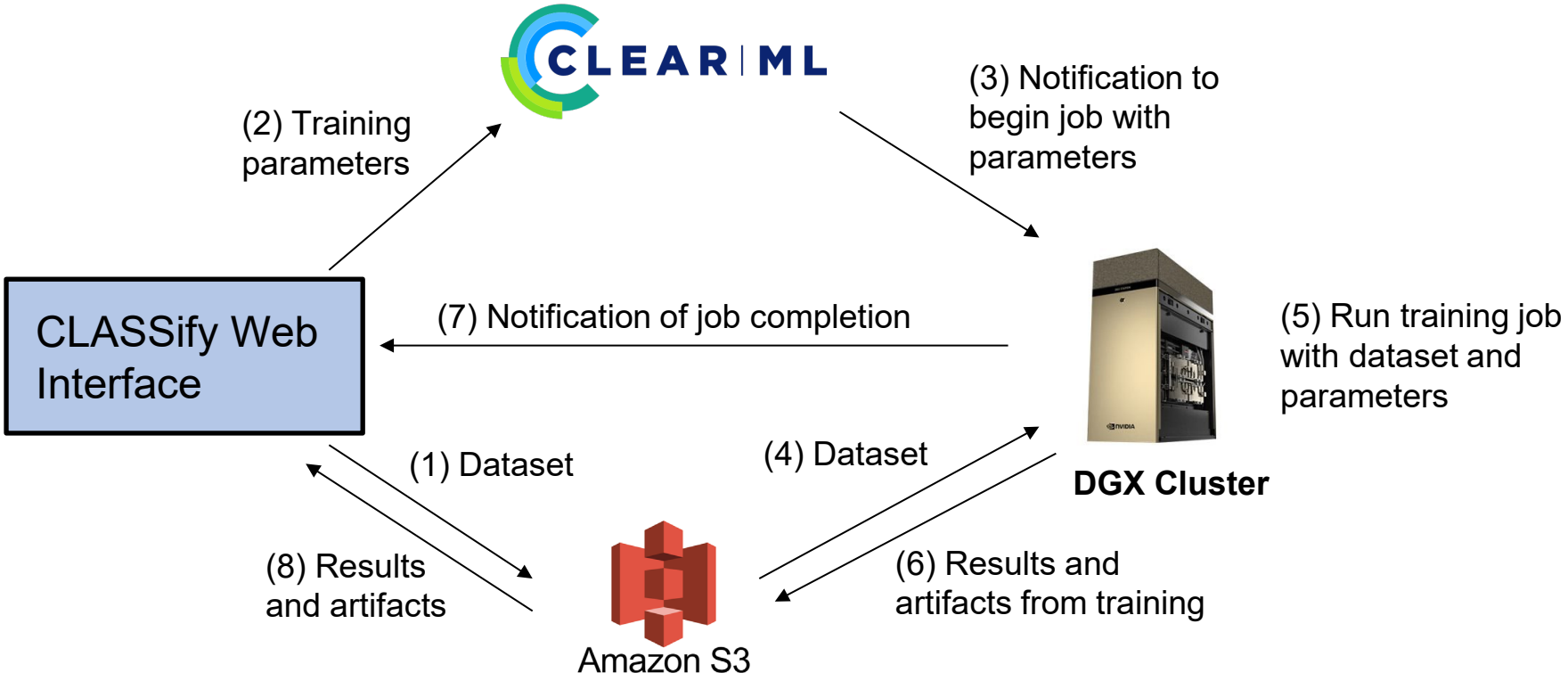
CLASSify- Machine Learning

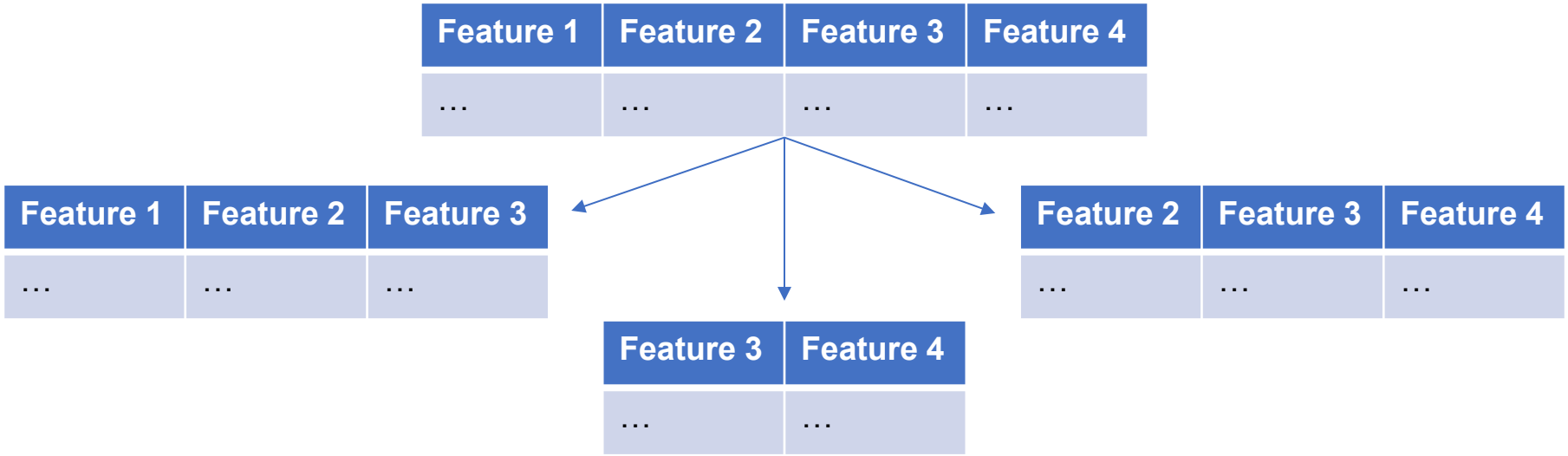


CLASSify- Additional Features

- Feature Effectiveness Evaluation
- Synthetic Data Generation
- SHAP Explainability Scores
- Explanatory Visualizations

CLASSify- Feature Evaluation

- Train many different models on different combinations of features
- By comparing results, can determine which features improve or worsen performance



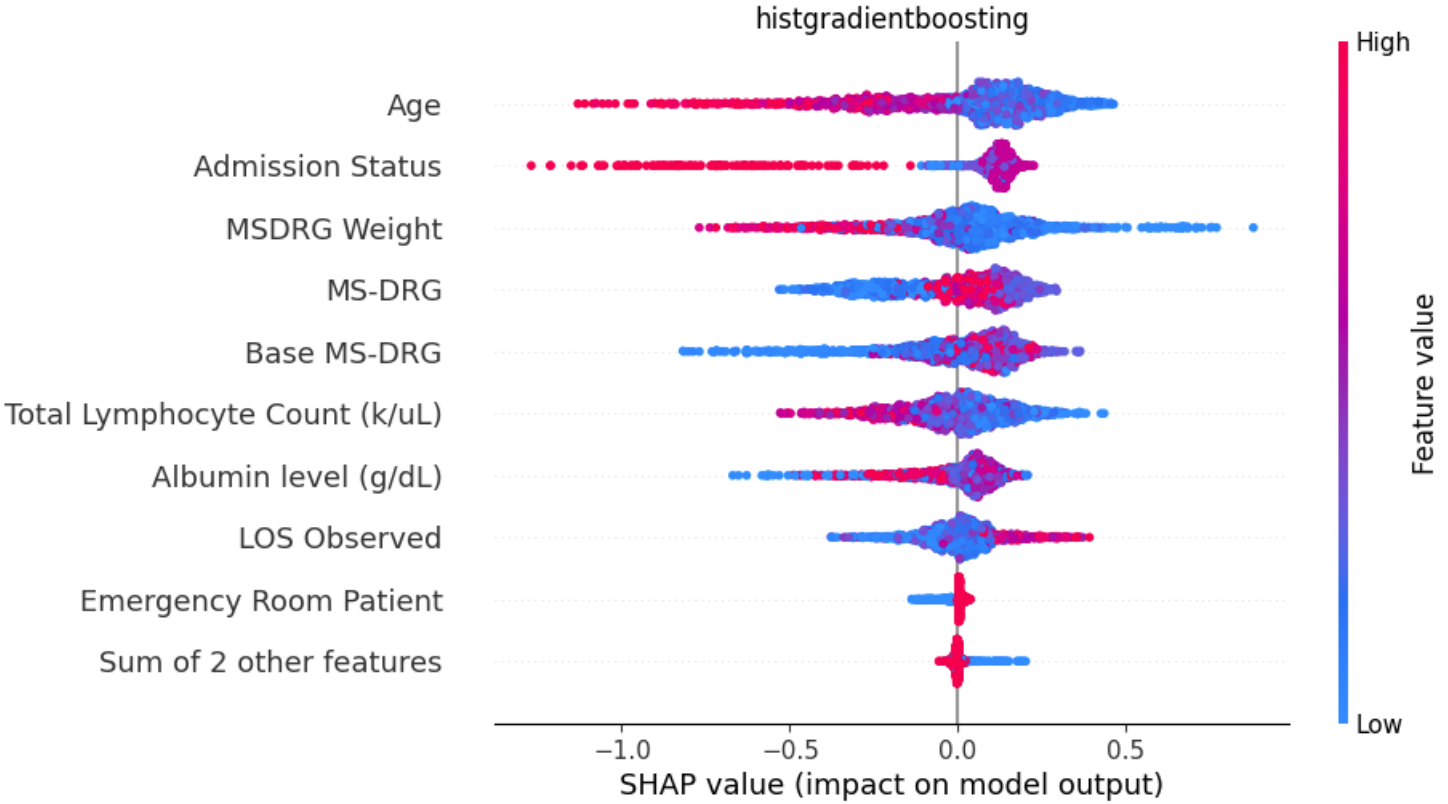
CLASSify- Synthetic Data Generation

- Synthetic data can be helpful if:

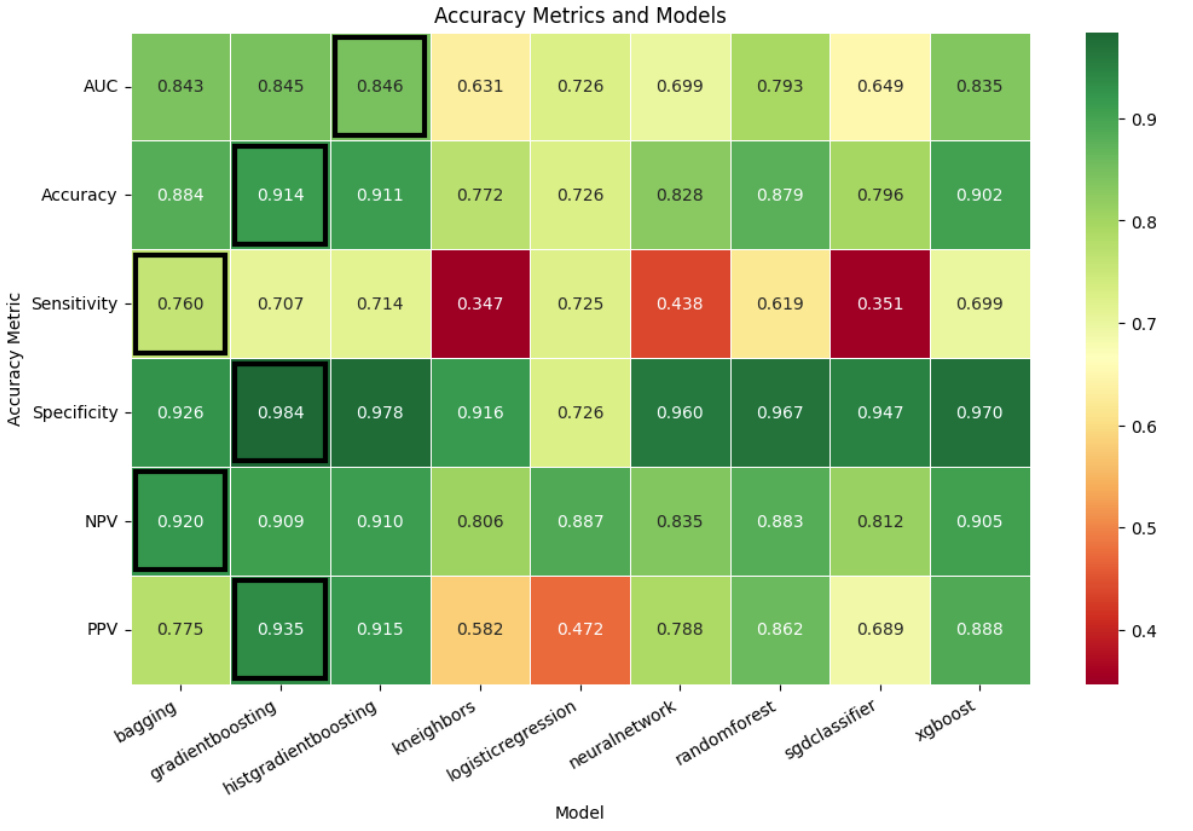
SDV
The Synthetic Data Vault

Class labels are significantly imbalanced	→	Can generate minority class labels to balance dataset
Original data is protected	→	Can create entirely new datasets
Many missing values throughout data	→	Can fill missing values with imputing methods

CLASSify- SHAP Explainability Scores



CLASSify- Explanatory Visualizations



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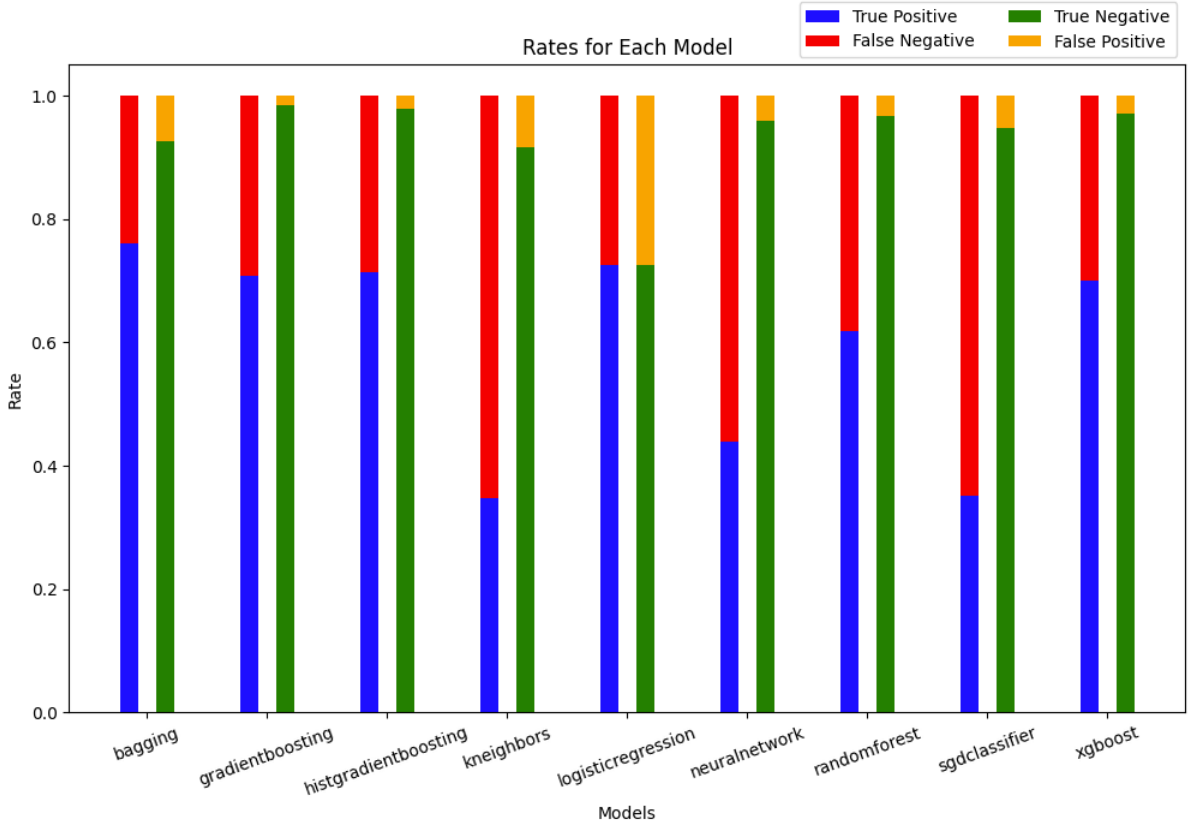
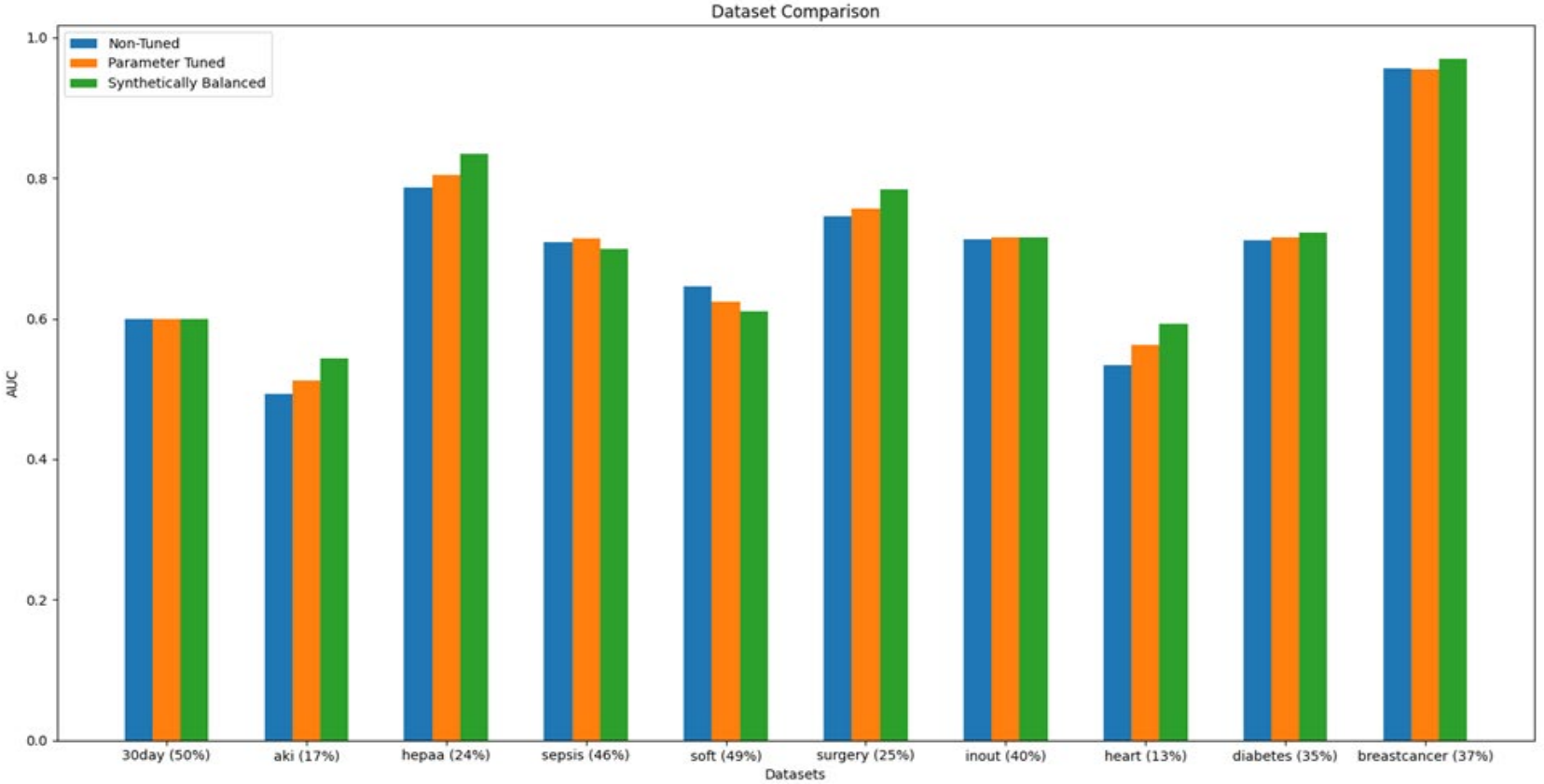


CLASSify- Example Results



CLASSify- Future Plans

- Incorporate new tabular transformer models
  - GANDALF, Tabular Transformer…
- HIPAA Compliance
- Interface with REDCap
- Build similar tool for time series data
  - Perform forecasting with variety of models

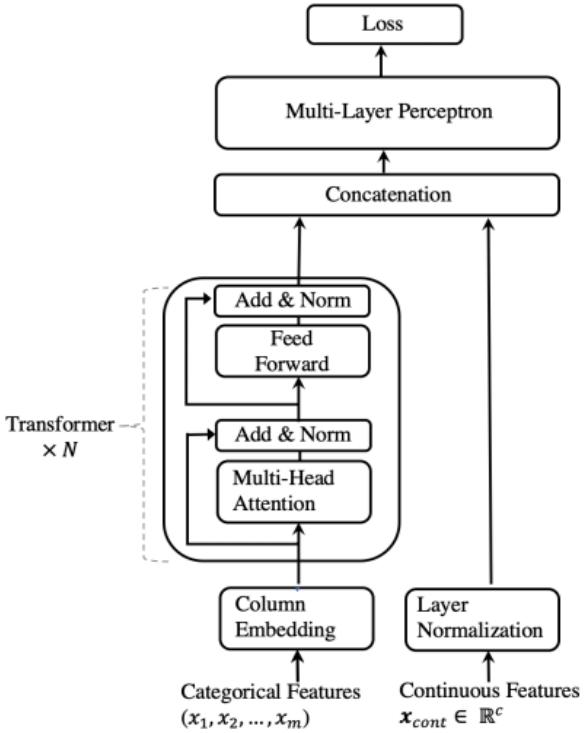


Figure 1: The architecture of TabTransformer.

Questions?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Example Dataset

- Surgery dataset
  - Publicly available, deidentified data collected from Cleveland hospital
  - Contains demographic, time, and medical recordings
  - Class label indicates whether complications arose during surgery
  - Number of records = 14,635
  - Class Balance: 75% negative, 25% positive

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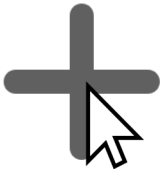
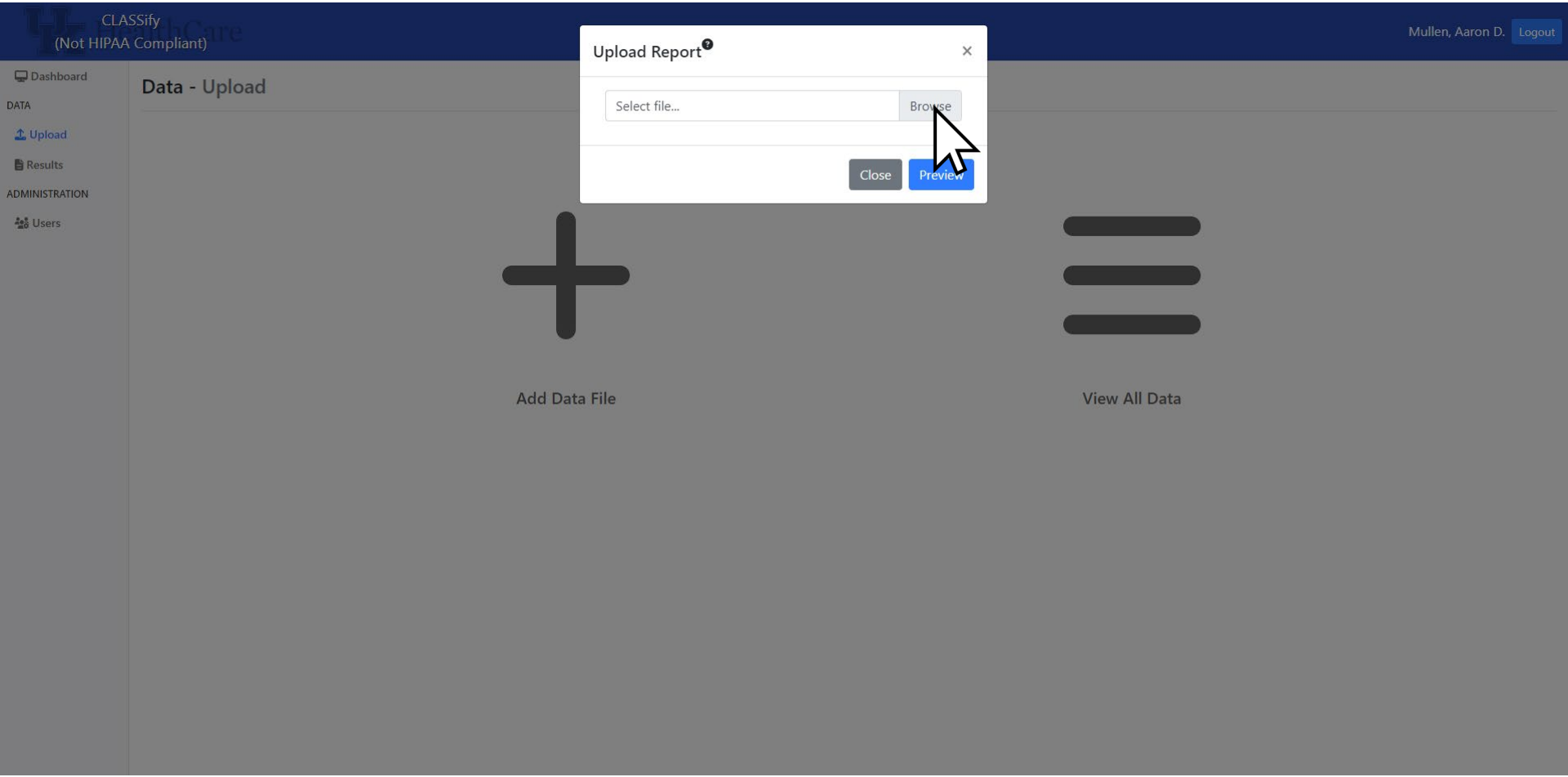


Add Data File

View All Data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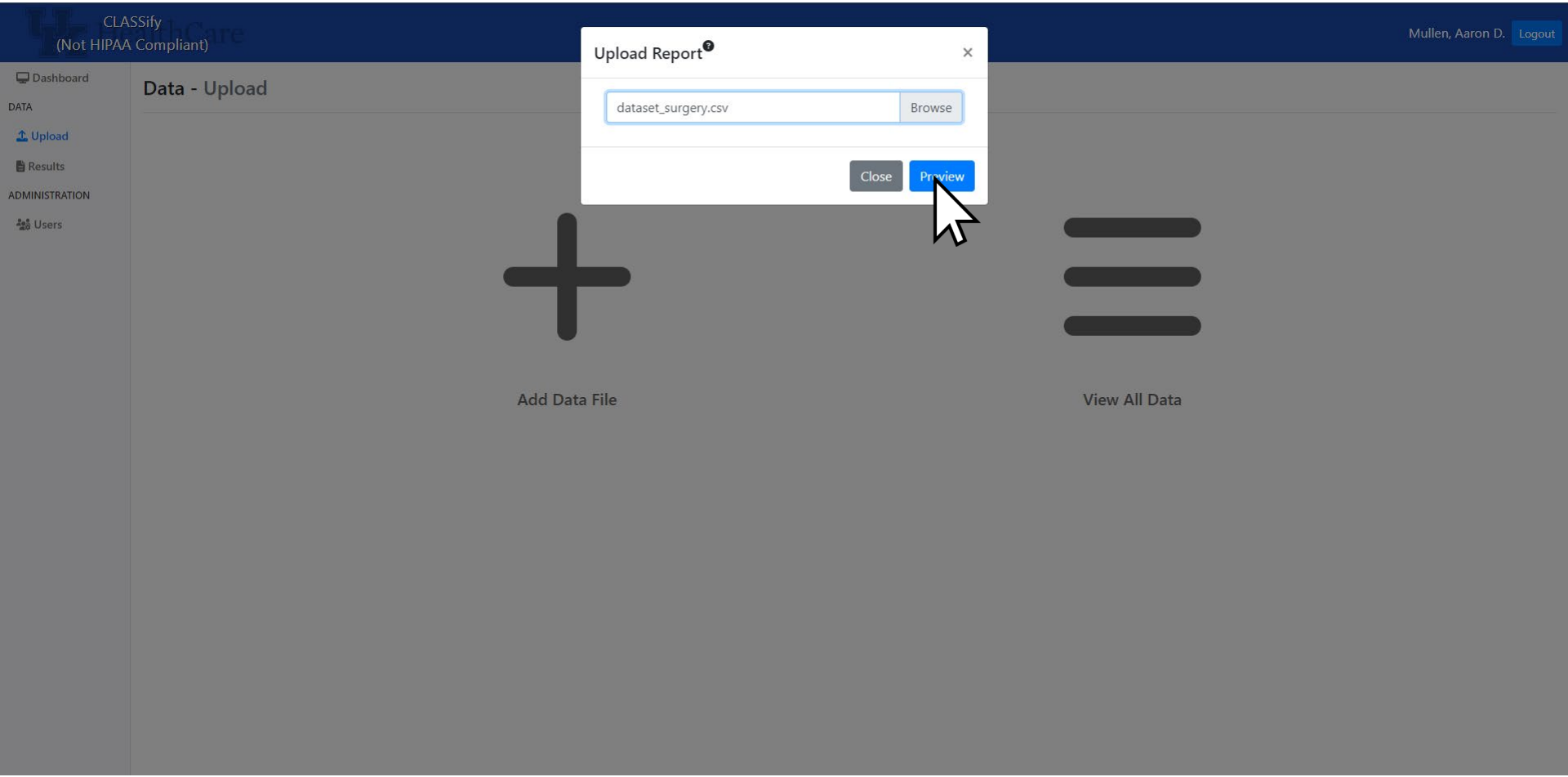
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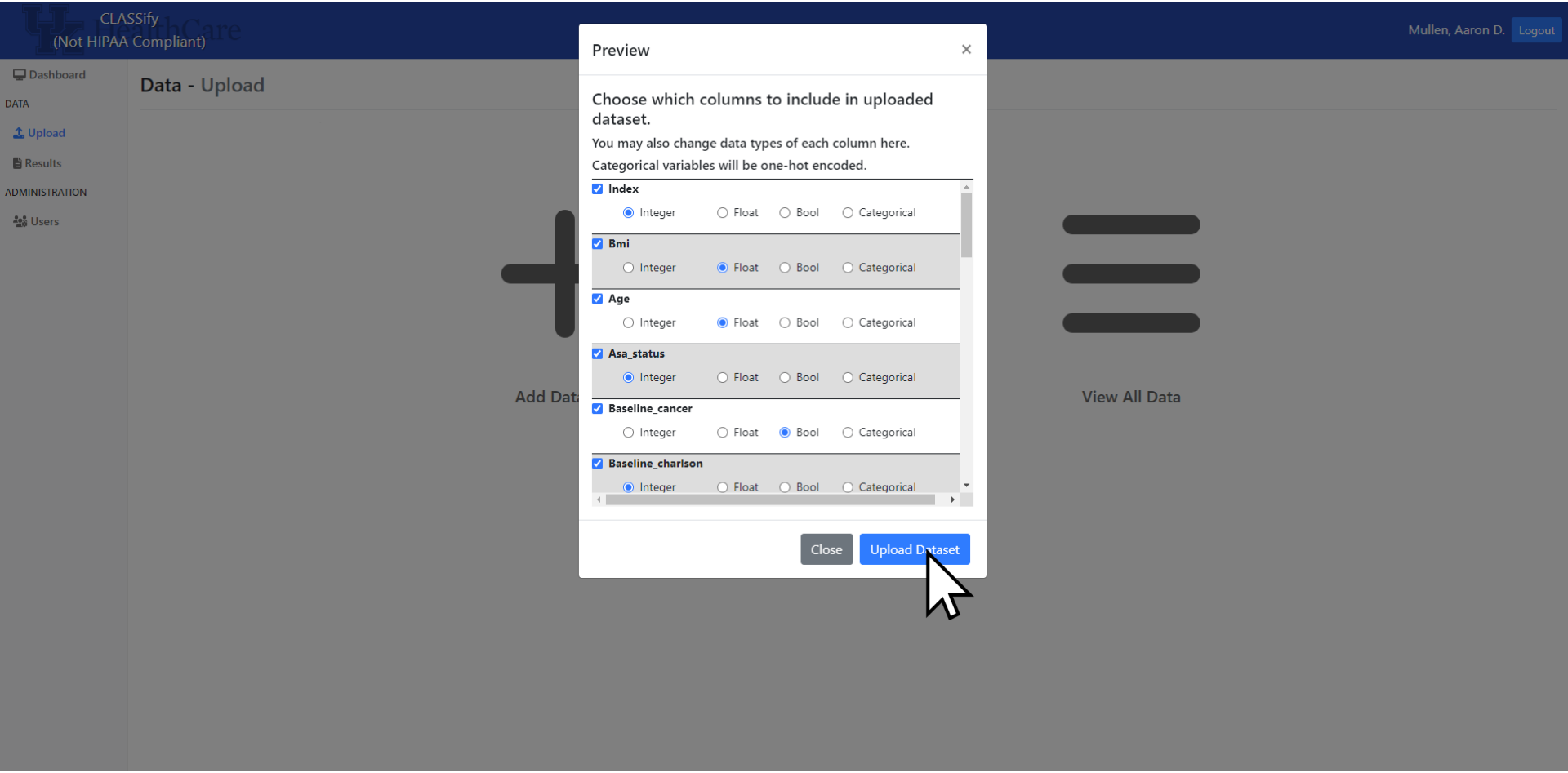
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Preview
Choose which columns to include in uploaded dataset.
You may also change data types of each column here.
Categorical variables will be one-hot encoded.
Index
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Float
Bool
Categorical
Bmi
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Float
Bool
Categorical
Age
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Show 10 rows | Column visibility

Search:

Filename	Date Added	Status	Actions
dataset_surgery.csv	2024-09-20 17:16:50+00	Uploaded	Prepare Dataset, Delete Dataset
osteopathy_multiclass_dropped_2.csv	2024-09-12 17:20:43+00	Processed	View Results, Re-Run Data, Delete Results
osteopathy_binary_dropped.csv	2024-09-12 16:42:21+00	Processed	View Results, Re-Run Data, Delete Results
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embeddings.csv	2024-05-30 11:01:56+00	Processed	View Results, Re-Run Data, Delete Results
Filename	**Date Added**	**Status**	**Actions**

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Reset to Defaults | Submit for Training

- [ ] Multiclass
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- [x] Parameter Tune
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- [ ] Standard Scaler
- [ ] Separate Testset
- [ ] Synthesize Original
- [ ] Synthesize New
- [ ] Synthesize Missing
- [ ] Evaluate Features

Train Group: randomforest, neuralnetw

General Parameters

Test Size	0.2	Verbose	0
N Iter	100	Train Sample Type	0
Random State	42	Shap Sample Size	10
Folds	5	Repeats	1
Starting Feature Num	3	Synthesize Model	tabular
Ending Feature Num	5	Parameter Goal	f1_macro
N Features Loop	10		

Model Parameters

N Estimators Start	10	C Start	0.1
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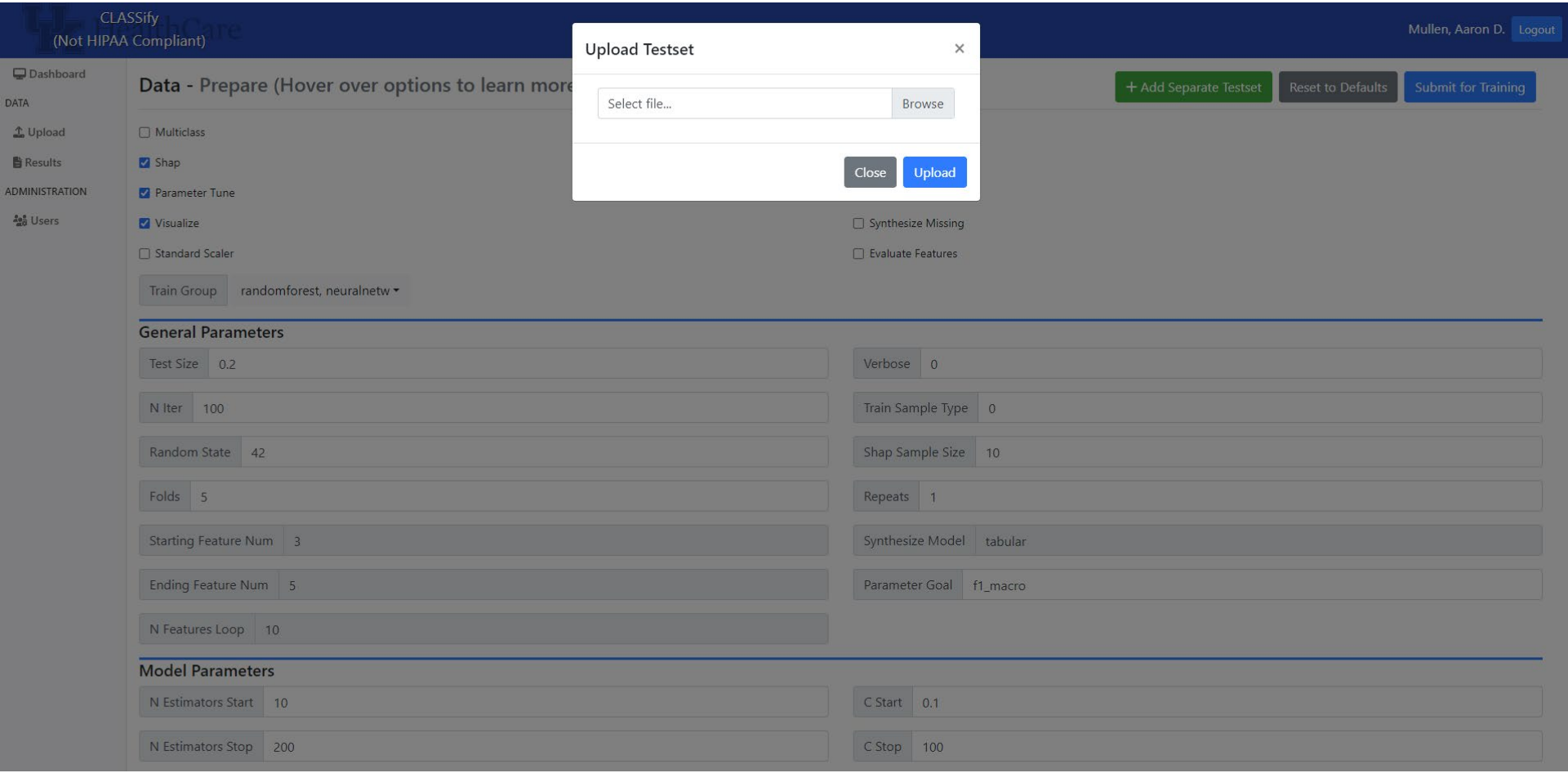
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- [ ] Standard Scaler
- [ ] Separate Testset
- [x] Synthesize Original
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- [ ] Evaluate Features

Train Group: randomforest, neuralnetw

General Parameters

Test Size	0.2	Verbose	0
N Iter	100	Train Sample Type	0
Random State	42	Shap Sample Size	10
Folds	5	Repeats	1
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Train Group: randomforest, neuralnetw

Select All | Deselect All

- [x] randomforest
- [x] neuralnetwork
- [x] tabpfn
- [x] xgboost
- [x] gradientboosting
- [x] histgradientboosting
- [x] bagging
- [x] sgdclassifier
- [x] logisticregression
- [x] kneighbors

General Para

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Train Group: neuralnetwork

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Model Parameters

N Estimators Start	10	C Start	0.1
N Estimators Stop	200	C Stop	100

N Estimators Step	10	C Step	0.1
Max Depth Start	5	Max Features Start	0.02
Max Depth Stop	500	Max Features Stop	1
Max Depth Step	10	Max Features Step	0.02
Subsample Start	0.1	Validation Fraction Start	0.01
Subsample Stop	1	Validation Fraction Stop	0.5
Subsample Step	0.1	Validation Fraction Step	0.01
N Iter No Change Start	5	Learning Rate Start	0.01
N Iter No Change Stop	50	Learning Rate Stop	1
N Iter No Change Step	5	Learning Rate Step	0.01
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Nn Hidden Layer Sizes Stop	1000	Nn Hidden Layer Depth Stop	2
Nn Hidden Layer Sizes Step	10	Nn Hidden Layer Depth Step	1
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Nn Learning Rate Stop	0.01	Alpha Stop	0.001
Nn Learning Rate Step	0.001	Alpha Step	0.00001

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osteopathy_binary.csv	2024-09-12 15:05:01+00	Processed	View Results, Re-Run Data, Delete Results
osteopathy_multiclass.csv	2024-09-12 14:33:31+00	Processed	View Results, Re-Run Data, Delete Results
test_embeddings_smaller_binary.csv	2024-08-26 18:20:51+00	Processed	View Results, Re-Run Data, Delete Results
test_embeddings.csv	2024-06-05 14:33:25+00	Processed	View Results, Re-Run Data, Delete Results
embeddings.csv	2024-05-30 11:01:56+00	Processed	View Results, Re-Run Data, Delete Results
Filename	**Date Added**	**Status**	**Actions**

Showing 1 to 8 of 8 entries

First Previous 1 Next Last

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Show 10 rows | Column visibility

Search:

Filename	Date Added	Status	Actions
dataset_surgery.csv	2024-09-22 14:52:00+00	Processed	View Results / Re-Run Data / Delete Results
osteopathy_multiclass_dropped_2.csv	2024-09-12 17:20:43+00	Processed	View Results / Re-Run Data / Delete Results
osteopathy_binary_dropped.csv	2024-09-12 16:42:21+00	Processed	View Results / Re-Run Data / Delete Results
osteopathy_binary.csv	2024-09-12 15:05:01+00	Processed	View Results / Re-Run Data / Delete Results
osteopathy_multiclass.csv	2024-09-12 14:33:31+00	Processed	View Results / Re-Run Data / Delete Results
test_embeddings_smaller_binary.csv	2024-08-26 18:20:51+00	Processed	View Results / Re-Run Data / Delete Results
test_embeddings.csv	2024-06-05 14:33:25+00	Processed	View Results / Re-Run Data / Delete Results
embeddings.csv	2024-05-30 11:01:56+00	Processed	View Results / Re-Run Data / Delete Results
Filename	**Date Added**	**Status**	**Actions**

Showing 1 to 8 of 8 entries

First | Previous | 1 | Next | Last

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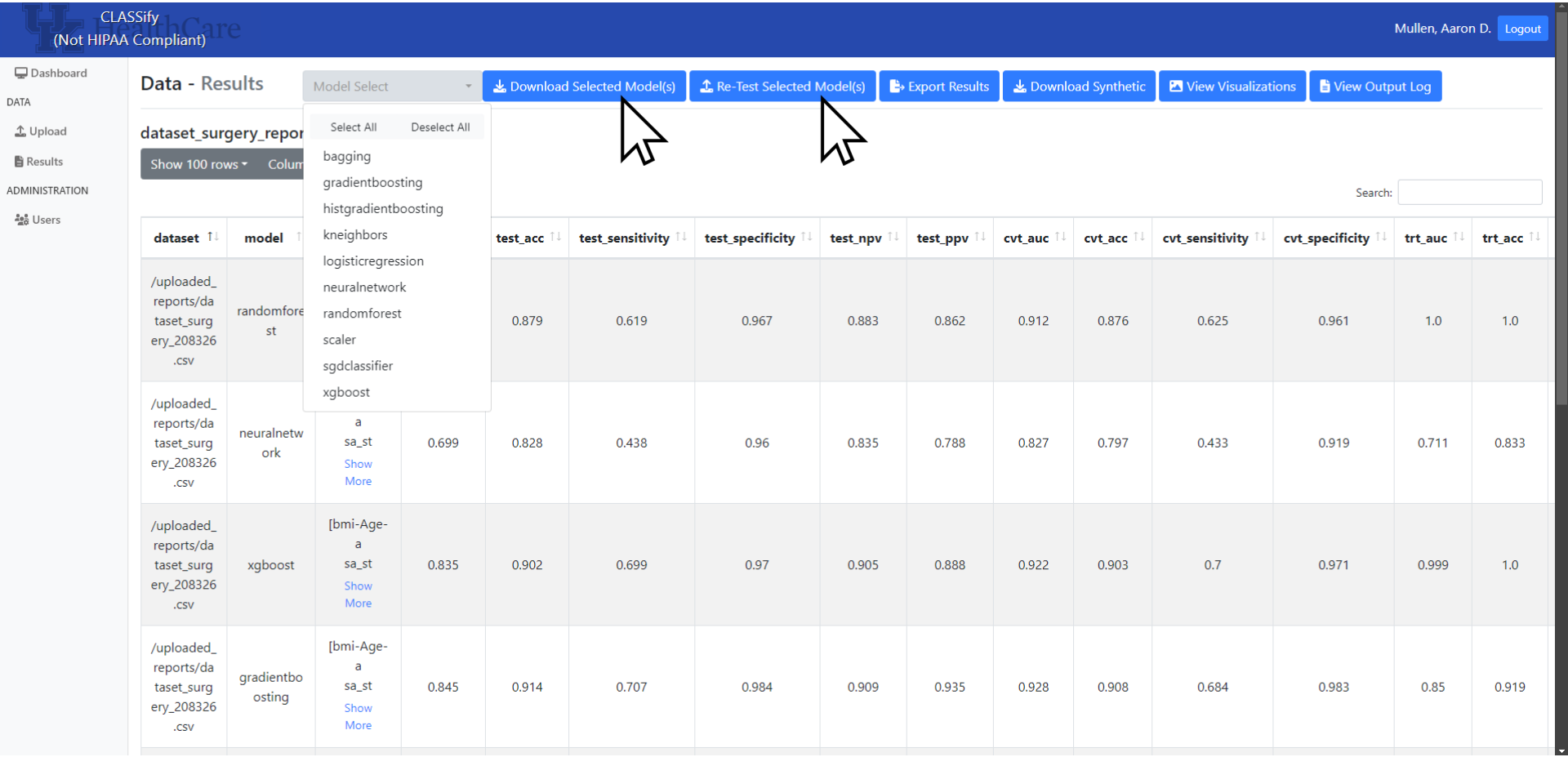
Model Select | Download Selected Model(s) | Re-Test Selected Model(s) | Export Results | Download Synthetic | View Visualizations | View Output Log

dataset_surgery_report.csv

Show 100 rows | Column visibility

Search:

dataset	model	features	test_auc	test_acc	test_sensitivity	test_specificity	test_npv	test_ppv	cvt_auc	cvt_acc	cvt_sensitivity	cvt_specificity	trt_auc	trt_acc
/uploaded_reports/dataset_surgery_208326.csv	randomforest	[bmi-Age-asa_st Show More	0.793	0.879	0.619	0.967	0.883	0.862	0.912	0.876	0.625	0.961	1.0	1.0
/uploaded_reports/dataset_surgery_208326.csv	neuralnetwork	[bmi-Age-asa_st Show More	0.699	0.828	0.438	0.96	0.835	0.788	0.827	0.797	0.433	0.919	0.711	0.833
/uploaded_reports/dataset_surgery_208326.csv	xgboost	[bmi-Age-asa_st Show More	0.835	0.902	0.699	0.97	0.905	0.888	0.922	0.903	0.7	0.971	0.999	1.0
/uploaded_reports/dataset_surgery_208326.csv	gradientboosting	[bmi-Age-asa_st Show More	0.845	0.914	0.707	0.984	0.909	0.935	0.928	0.908	0.684	0.983	0.85	0.919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Model Select
Download Selected Model(s)
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histgradientboosting
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xgboost
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test_sensitivity
test_specificity
test_npv
test_ppv
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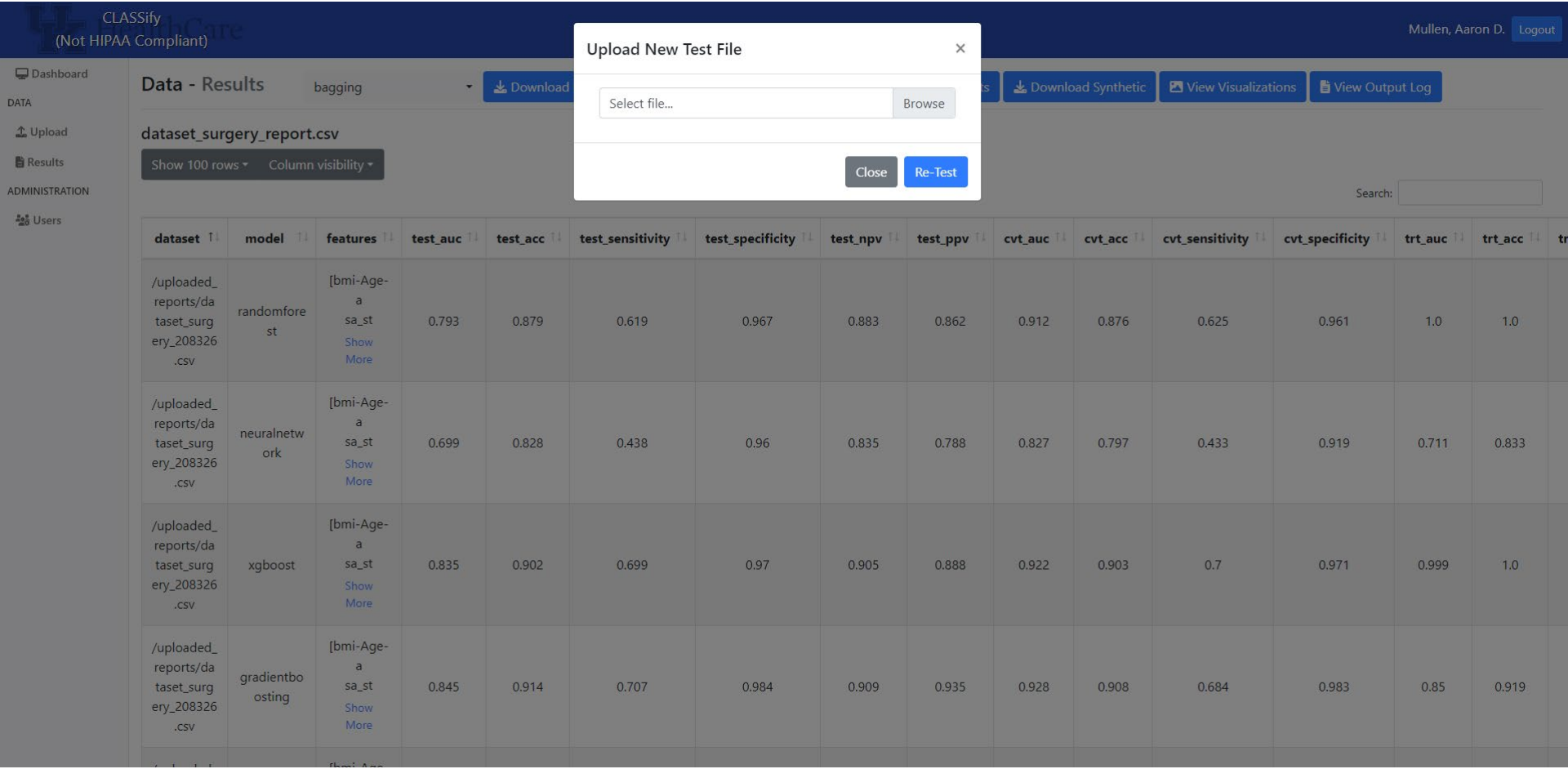
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Download Synthetic
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Select file...
Browse
Close
Re-Test
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test_acc
test_sensitivity
test_specificity
test_npv
test_ppv
cvt_auc
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dataset_surgery_report.csv

Show 100 rows | Column visibility

Search:

dataset	model	features	test_auc	test_acc	test_sensitivity	test_specificity	test_npv	test_ppv	cvt_auc	cvt_acc	cvt_sensitivity	cvt_specificity	trt_auc	trt_acc
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/uploaded_reports/dataset_surgery_208326.csv	gradientboosting	[bmi-Age-asa_st Show More	0.845	0.914	0.707	0.984	0.909	0.935	0.928	0.908	0.684	0.983	0.85	0.919

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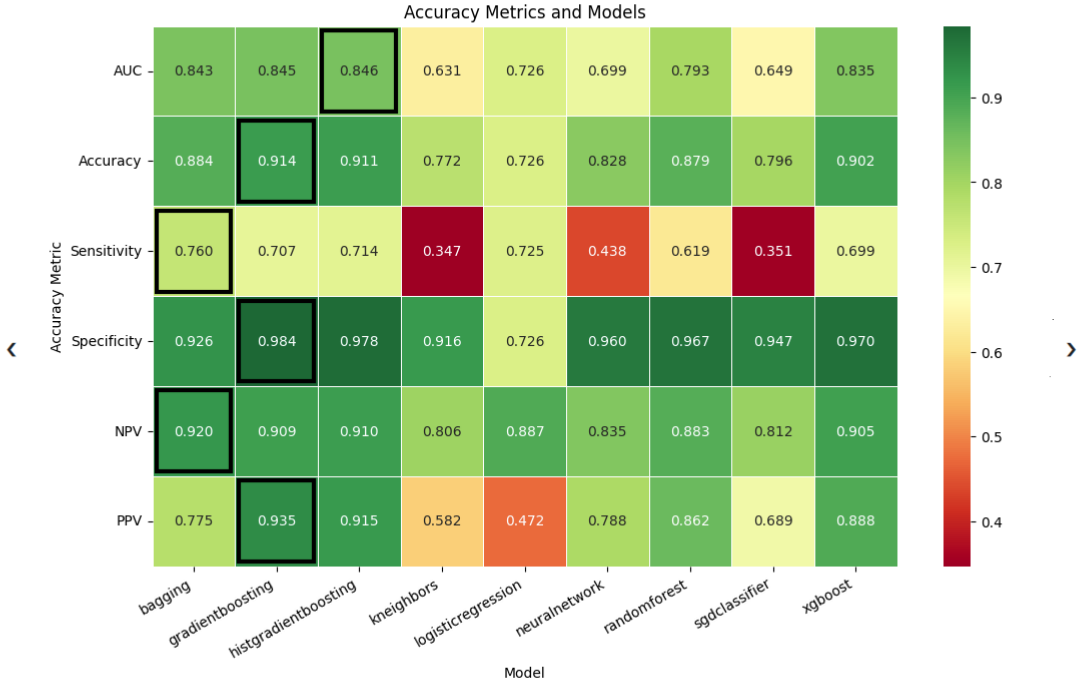

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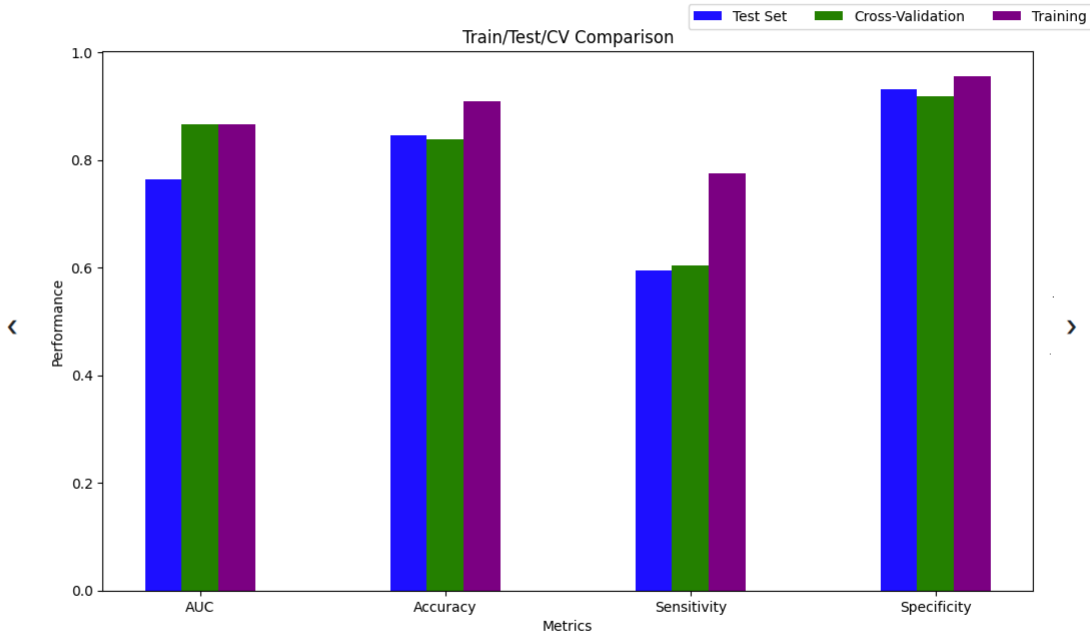

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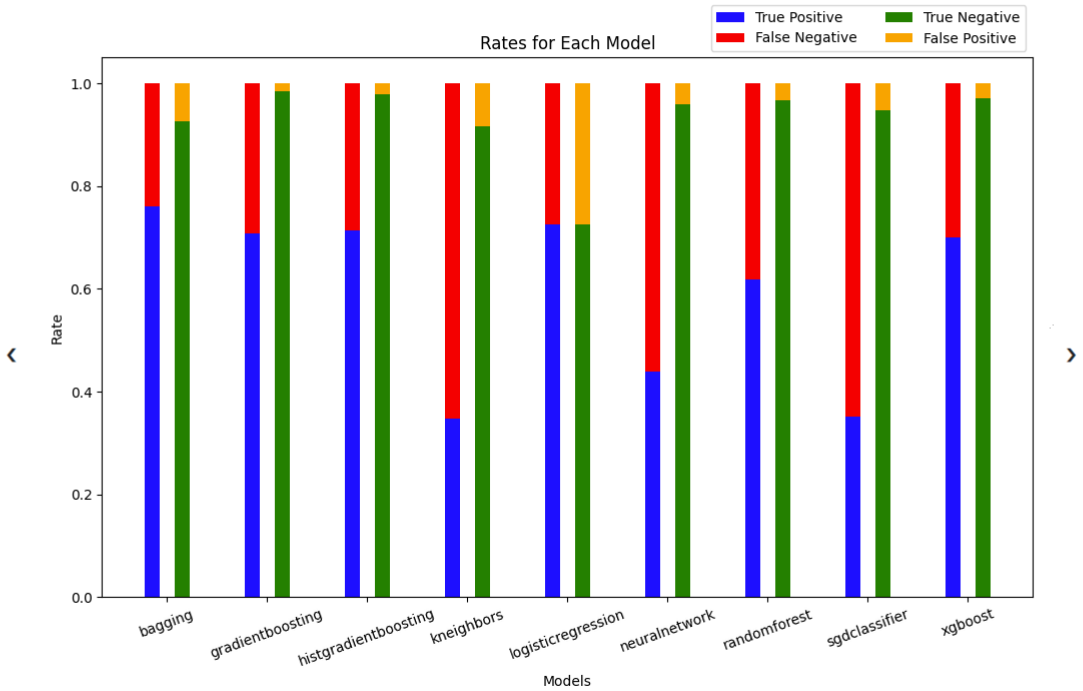

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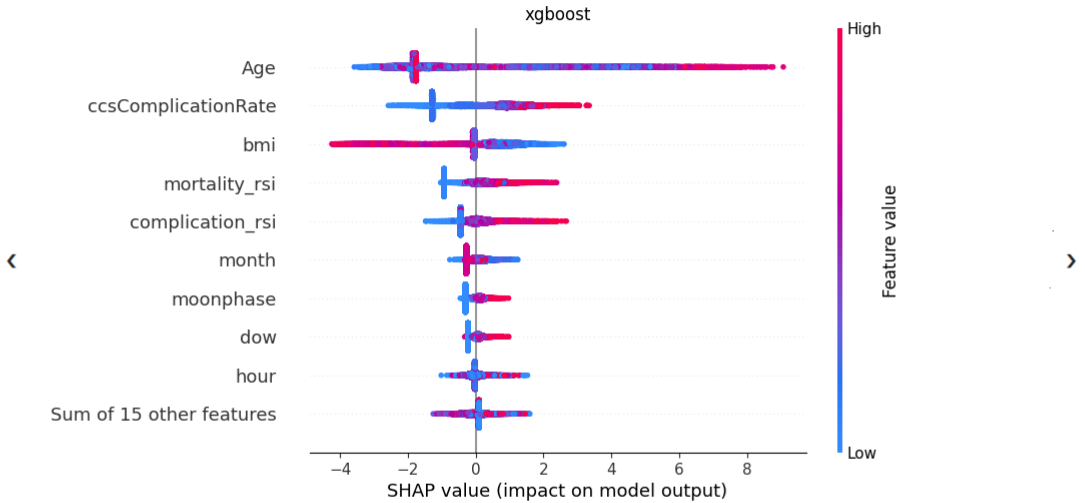

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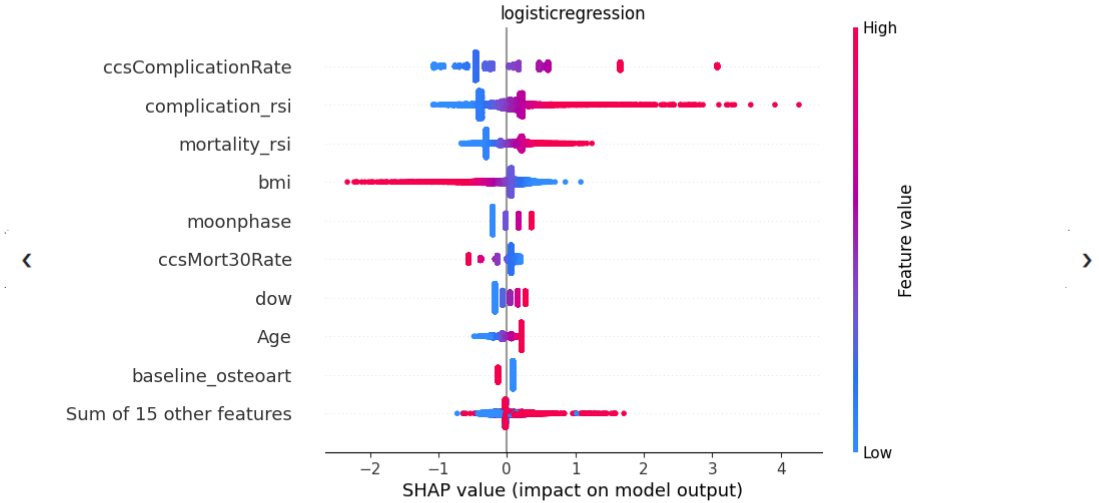

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