# Kaggle Higgs Boson

# Machine Learning Challenge


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NYC Data Science Academy

# Agenda

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- Introduction
- Strategy and Approach
- Exploratory Data Analysis and Feature Engineering
- Training and Cross-Validation
- Results and Findings
- Conclusion

# Introduction

Challenge Definition

Success Metrics

# Challenge and Objectives

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- Apply Machine Language to predict CERN's simulated particle collision events as either a Higgs Boson signal (s) or background (b) noise
- Learn how to strategize, optimize, and fine-tune models, algorithms, and parameters to achieve the best signal prediction possible
- Gain tactical working experience differentiating theory from actual practice
- Develop new skills in model ensembles and stacking techniques

# Success Metrics

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- Achieve the highest Approximate Median Significance (AMS) Score in the Kaggle Private Leaderboard
- Achieve the Top 25% position placement in the Kaggle Private Leaderboard

# Strategy and Approach

Process

Feature Analysis and Engineering

Technology Stack

Models, Ensembles, and Stacking

# Process

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- The machine learns, while we also learn how to learn
  - Agile “chunking” process applied towards machine learning
  - Move fast, fail fast, wash-rinse-repeat = then harvest good results + detailed logs
- Start with the basics to get the patterns and trends
  - Treat data like it’s alive, understand it’s health and heartbeat
  - Get a feel of how the data behaves and reacts to changes
  - Increase complexity as the accuracy improves
- Develop a solid build::create::train::evaluate::predict::score pipeline
  - Make the iterative process fast, repeatable, and reliable
  - Agile “kanban” process applied towards multiple parallel production lines
  - Build in feature analysis and engineering to complement the development process

# Feature Analysis & Engineering

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- Missingness Analysis and Imputation
- Correlation Charts and Multicollinearity
- Principal Component Analysis
- Density Charts
- 5-PHI Fields
- Jet Fields

# Technology Stack

- Python
  - For all modeling and algorithmic related work
  - Numpy, Pandas & Matplotlib.pyplot
- R
  - For all Exploratory Discovery Analysis (EDA) work and plots
- Key Python Libraries
  - Scikit Learn  (Linear_Model.LogisticRegression, svm, DecisionTreeClassifier,  Naive_Bayes.GaussianNB)
  - Scikit Learn Ensemble  (GradientBoostingClassifier, RandomForestClassifier, AdaBoostClassifier)
- Special Libraries
  - XGBoost
  - Neural Network

# Models, Ensembles, Stacking

- Naïve Bayes
- Logistic Regression
- Support Vector Machines
- Decision Tree, Extra Trees, Random Forest
- Gradient Boosting, AdaBoost, XGBoost
- Neural Networking

# EDA, Feature Analysis and Engineering

PCA Results

Correlation Results

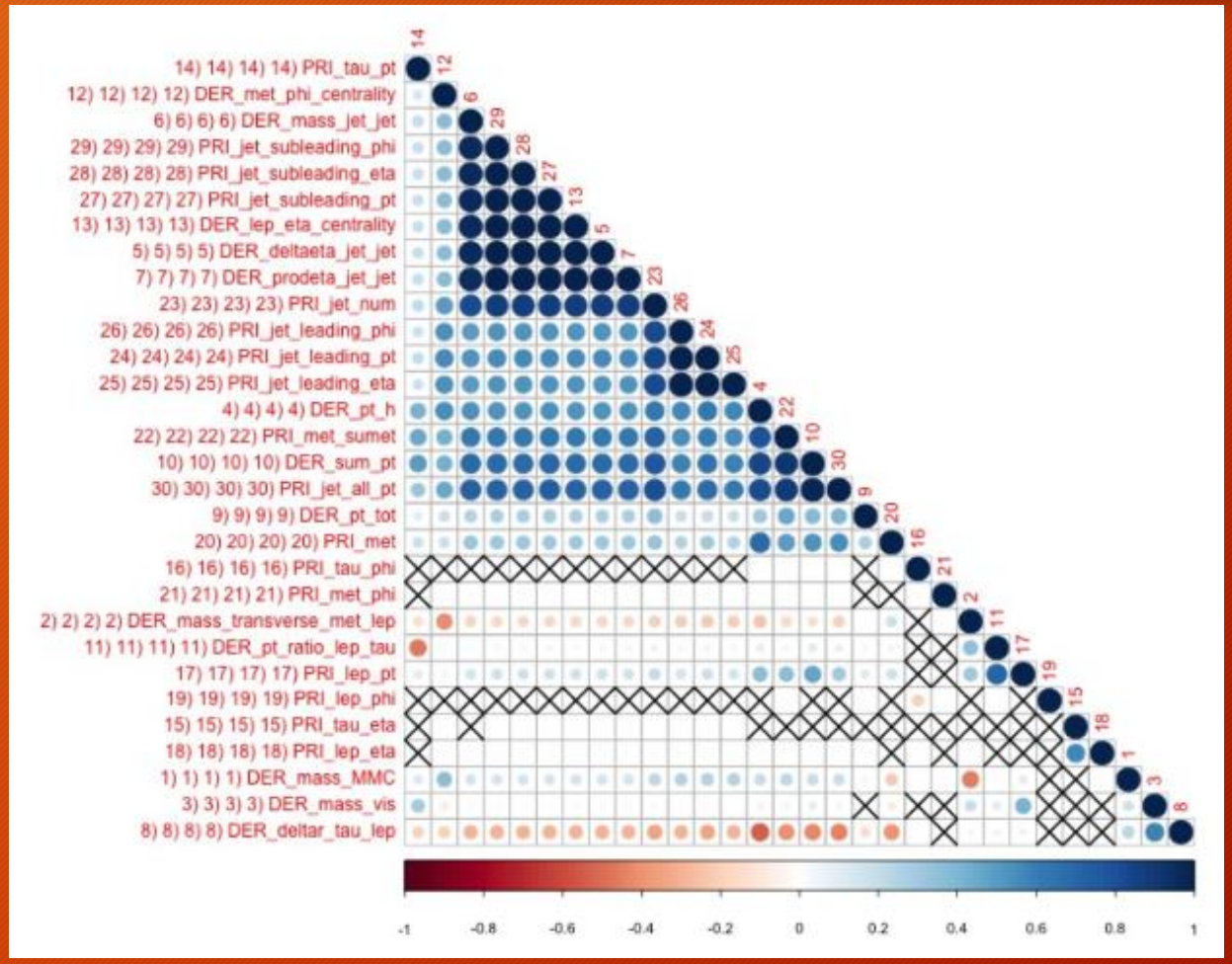
Histograms

Imputation on “Missing” Data

Variable Importance Plot

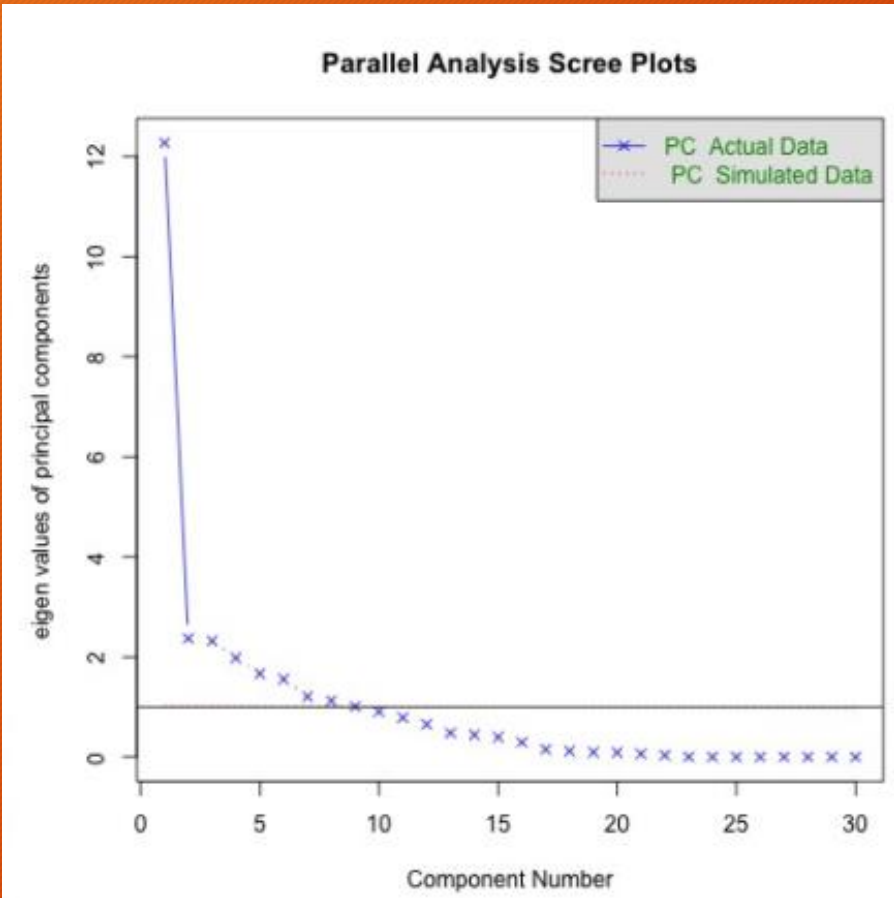
Missing Values Plots

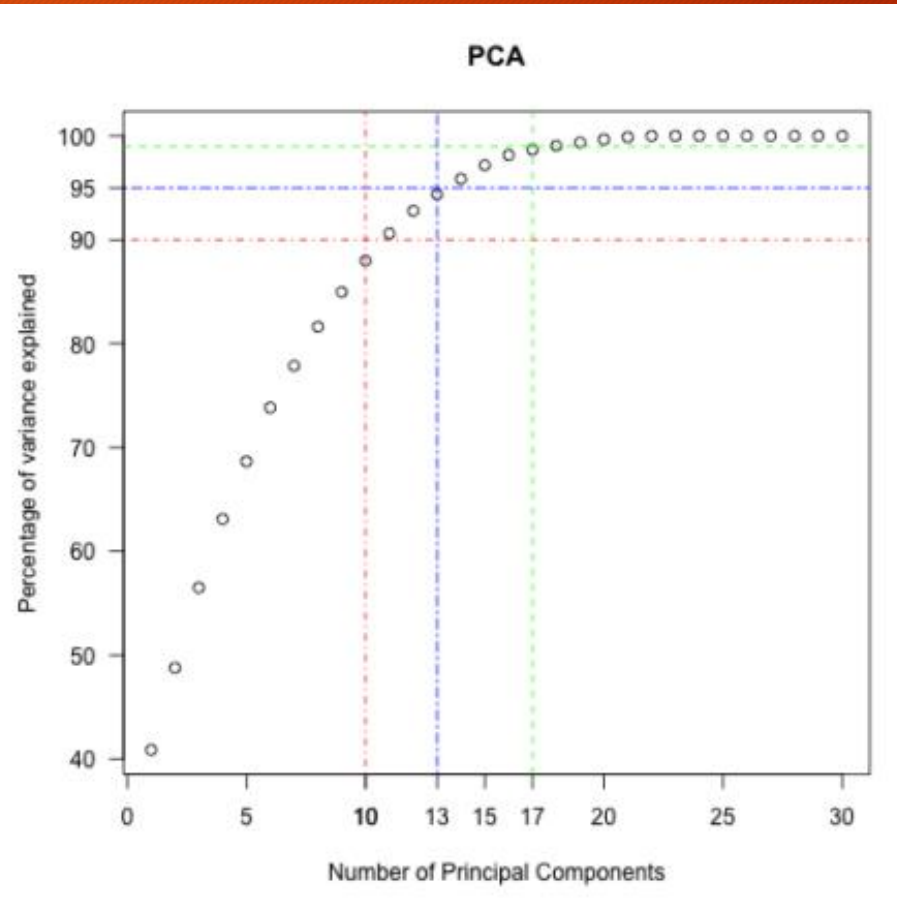
# Features Correlation Plot



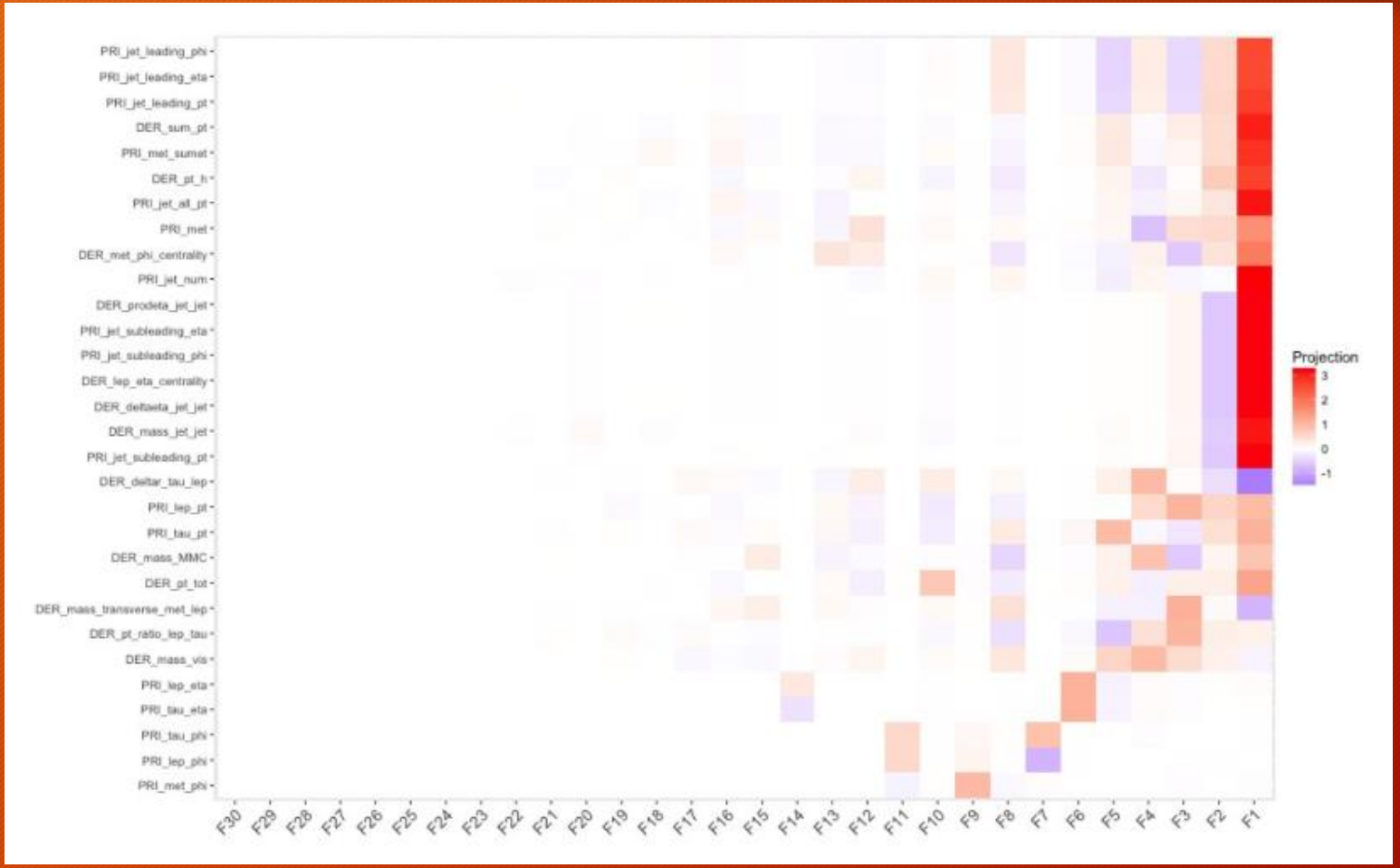
# PCA Plot [1]

D

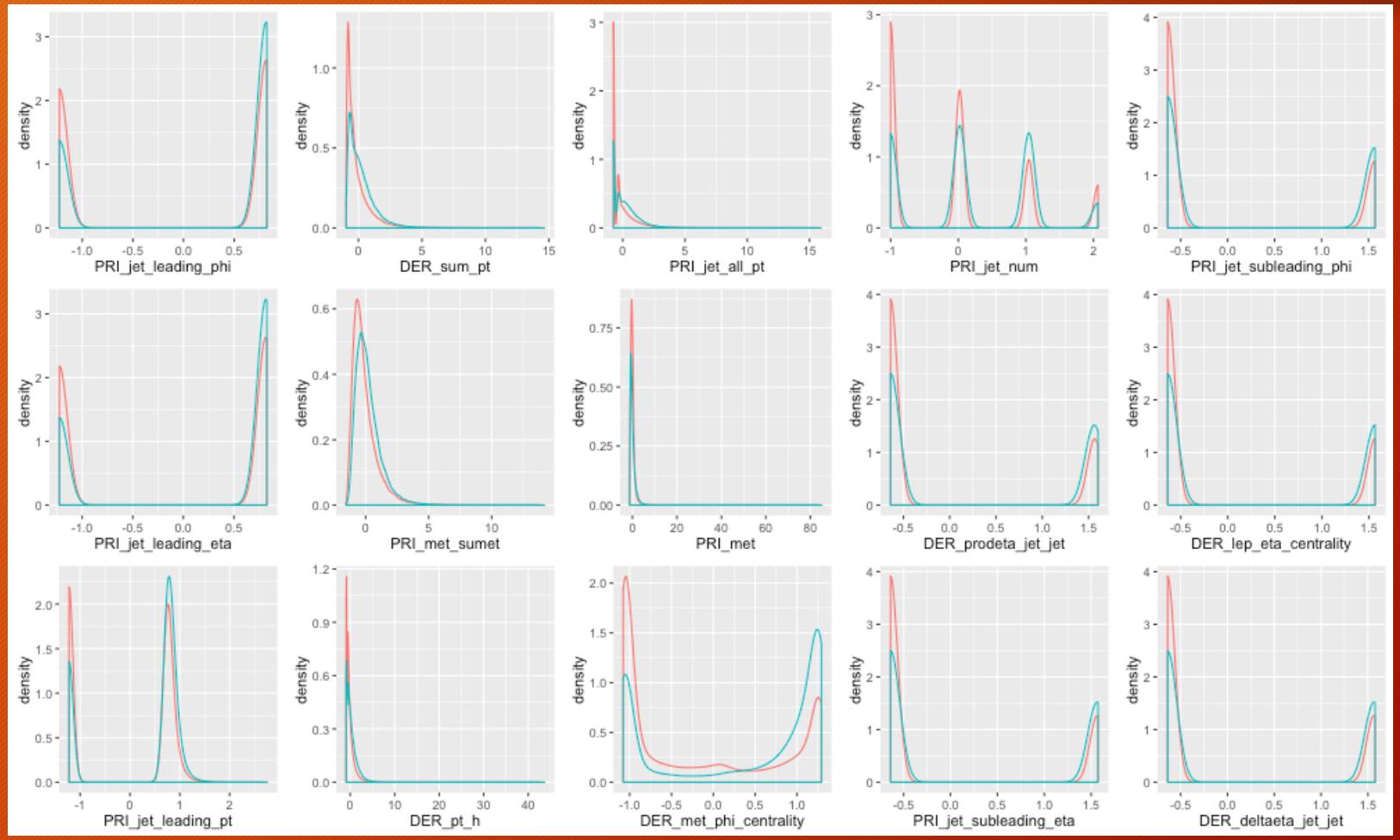

Parallel Analysis Scree Plots
PC Actual Data
PC Simulated Data
eigen values of principal components
0
2
4
6
8
10
12
0
5
10
15
20
25
30
Component Number


PCA
Percentage of variance explained
40
50
60
70
80
90
95
100
0
5
10
13
15
17
20
25
30
Number of Principal Components

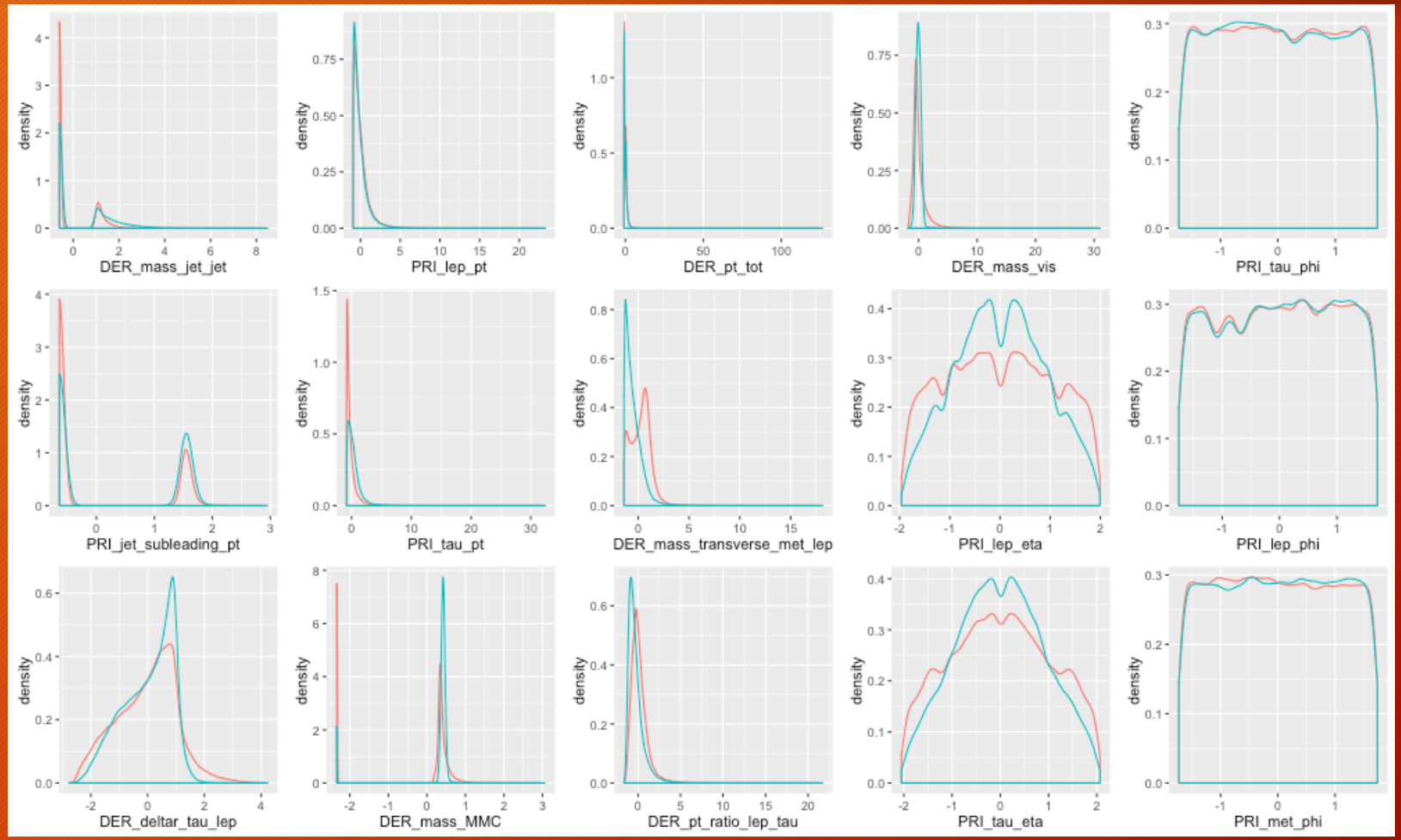
# PCA Plot [2]


PRI_jet_leading_phi
PRI_jet_leading_eta
PRI_jet_leading_pt
DER_sum_pt
PRI_met_sumet
DER_pt_h
PRI_jet_all_pt
PRI_met
DER_met_phi_centrality
PRI_jet_num
DER_prodeta_jet_jet
PRI_jet_subleading_eta
PRI_jet_subleading_phi
DER_lep_eta_centrality
DER_deltaeta_jet_jet
DER_mass_jet_jet
PRI_jet_subleading_pt
DER_deltar_tau_lep
PRI_lep_pt
PRI_tau_pt
DER_mass_MMC
DER_pt_tot
DER_mass_transverse_met_lep
DER_pt_ratio_lep_tau
DER_mass_vis
PRI_lep_eta
PRI_tau_eta
PRI_tau_phi
PRI_lep_phi
PRI_met_phi
F30 F29 F28 F27 F26 F25 F24 F23 F22 F21 F20 F19 F18 F17 F16 F15 F14 F13 F12 F11 F10 F9 F8 F7 F6 F5 F4 F3 F2 F1
Projection
3
2
1
0
-1

# Density Plot [1]



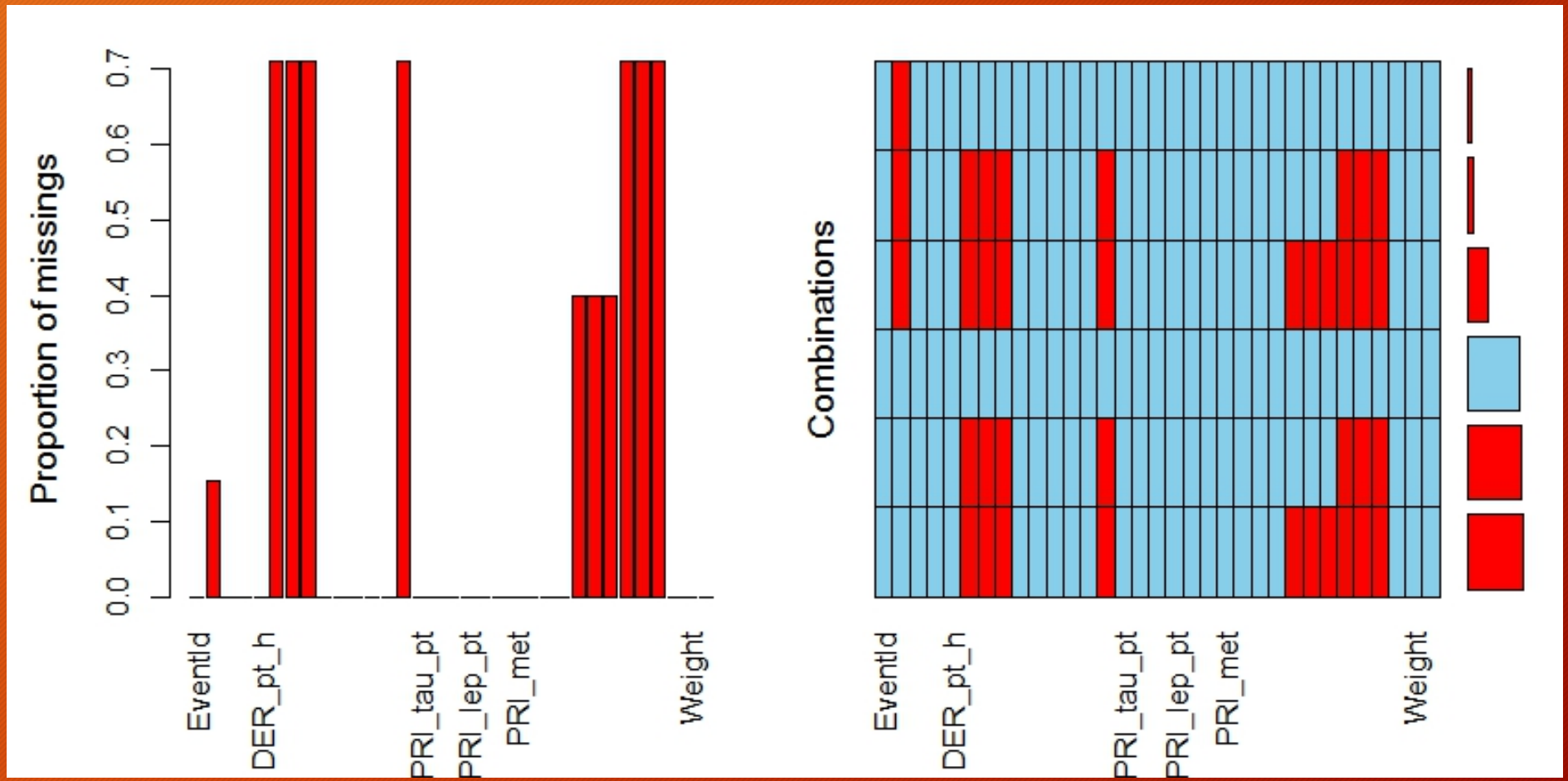
# Density Plot [2]



# Imputation on “Missing” Data

- Zeros
- Mean
- Median
- Most Frequent
- KNN
- Interpolation
- “Do Nothing”

# Missing Values Plots



# Training and Cross Validation

Parameters and Hyper-Parameters

Patterns and Trends

Tuning and Optimization

# Naïve Bayes

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| Algorithm | No. of Features | Threshold | Imputer | Standardized | Whiten | Xval Folds | AMS Score |
|---|---|---|---|---|---|---|---|
| Single Model Algorithms | | | | | | | |
| Naïve Bayes | 30 | 85% | none | False | False | 3 | 0.99202 |
| Naïve Bayes | 30 | 86% | none | False | False | 3 | 0.97608 |
| Naïve Bayes | 30 | 84% | none | False | False | 3 | 1.00702 |
| Naïve Bayes | 30 | 83% | none | False | False | 3 | 1.00969 |
| Naïve Bayes | 30 | 82% | none | False | False | 3 | 1.00280 |
| Naïve Bayes | 30 | 83% | none | False | True | 3 | 0.77996 |
| Naïve Bayes | 30 | 83% | none | True | False | 3 | 1.00983 |
| Naïve Bayes | 30 | 85% | none | True | False | 3 | 0.99227 |
| Naïve Bayes | 30 | 83% | zeros | True | False | 3 | 0.88221 |
| Naïve Bayes | 30 | 83% | mean | True | False | 3 | 0.92456 |
| Naïve Bayes | 30 | 83% | median | True | False | 3 | 0.91496 |
| Naïve Bayes | 30 | 83% | most_frequent | True | False | 3 | 0.88798 |

# Logistic Regression

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| Algorithm | No. of Features | Threshold | Imputer | Standardized | Whiten | Xval Folds | AMS Score |
|---|---|---|---|---|---|---|---|
| Logistic Regression | 30 | 83% | none | True | False | 3 | 1.78299 |
| Logistic Regression | 30 | 83% | none | False | False | 3 | 1.76413 |
| Logistic Regression | 30 | 83% | none | True | True | 3 | 1.55776 |
| Logistic Regression | 30 | 83% | zeros | True | False | 3 | 1.81815 |
| Logistic Regression | 30 | 83% | mean | True | False | 3 | 1.76026 |
| Logistic Regression | 30 | 83% | median | True | False | 3 | 1.78949 |
| Logistic Regression | 30 | 83% | most_frequent | True | False | 3 | 1.81852 |

# Neural Networking Model

| Neural Network | No. of Features | Hidden Layer | Neurons | Standardized | Whiten | Xval Folds | AMS Score | Kaggle Position | Private LB AMS | Top % | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Neural Network | 30 | 1 | 10 | False | False | 10 | 2.066 | | AMS = 2.107 | | Whole Data | |
| Neural Network | 17 | 1 | 10 | False | False | 10 | 1.587 | | AMS = 1.633 | | Removing The DER variables | |
| Neural Network | 17 | 1 | 20 | False | False | 10 | 1.622 | | AMS = 1.627 | | Removing The DER variables | |
| Neural Network | 25 | 1 | 10 | False | False | 10 | 2.306 | | AMS = 2.317 | | Removing The Phi's | |
| Neural Network | 25 | 1 | 20 | False | False | 10 | 2.188 | | AMS = 2.322 | | Removing The Phi's | |
| Neural Network | 25 | 1 | 30 | False | False | 10 | 2.218 | | AMS = 2.327 | | Removing The Phi's | |
| Neural Network | 29 | 1 | 10 | False | False | 10 | 2.552 | | AMS = 2.566 | | Grouping Based On Jet Value | |
| Neural Network | 29 | 1 | 20 | False | False | 10 | 2.309 | | AMS = 2.674 | | Grouping Based On Jet Value | |
| Neural Network | 29 | 1 | 30 | False | False | 10 | 2.698 | Kaggle # 1253 | AMS = 2.745 | Top 70% | Grouping Based On Jet Value | |

# Boosting, Random Forest, SVM

| Algorithm | No. of Features | Threshold | Imputer | Standardized | Whiten | Xval Folds | AMS Score | Kaggle Position | Private LB AMS | Top % |
|---|---|---|---|---|---|---|---|---|---|---|
| Ensemble Models | | | | | | | | | | |
| Gradient Boosting | 30 | 83% | zeros | True | False | 3 | 3.50757 | | | |
| Gradient Boosting | 30 | 83% | zeros | False | False | 3 | 3.50790 | | | |
| Gradient Boosting | 30 | 85% | none | False | False | 3 | 3.53583 | Kaggle # 615 | AMS = 3.58742 | Top 35% |
| Gradient Boosting | 30 | 83% | none | True | True | 3 | 3.25130 | | | |
| Gradient Boosting | 30 | 83% | none | True | False | 3 | 3.52030 | | | |
| Gradient Boosting | 30 | 83% | zeros | True | False | 3 | 3.50760 | | | |
| Gradient Boosting | 30 | 85% | zeros | False | False | 3 | 3.52930 | | | |
| Gradient Boosting | 30 | 83% | none | False | False | 3 | 3.52010 | | | |
| Gradient Boosting | 30 | 85% | mean | False | False | 3 | 3.53420 | | | |
| Gradient Boosting | 30 | 83% | mean | False | False | 3 | 3.49640 | | | |
| Gradient Boosting | 30 | 83% | zeros | False | False | 3 | 3.50790 | | | |
| Gradient Boosting | 30 | 83% | most_frequent | False | False | 3 | 3.52242 | | | |
| Random Forest | 30 | 85% | none | False | False | 10 | 2.82230 | max depth = 7 | | |
| SVM | 30 | 85% | none | False | False | 3 | 2.54300 | | | |

# XGBoost

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| Algorithm | No. of Features | Threshold | Imputer | Standardized | Whiten | Xval Folds | AMS Score | Kaggle Position | Private LB AMS | Top % |
|---|---|---|---|---|---|---|---|---|---|---|
| XGBoost | 30 | 85% | none | False | False | 3 | 3.60760 | Kaggle # 474 | AMS = 3.64051 | Top 27% |
| XGBoost | 30 | 83% | none | False | False | 3 | 3.58665 | | | |
| XGBoost | 30 | 85% | mean | False | False | 3 | 3.55439 | | | |
| XGBoost | 30 | 85% | median | False | False | 3 | 3.58718 | | | |
| XGBoost | 30 | 85% | zeros | False | False | 3 | 3.59191 | | | |
| XGBoost | 30 | 85% | most_frequent | False | False | 3 | 3.55665 | | | |
| XGBoost | 30 | 85% | none | True | False | 3 | 3.58810 | | | |
| XGBoost | 30 | 85% | none | True | True | 3 | 3.35131 | | | |
| XGBoost | 30 | 85% | none | False | True | 3 | 3.42500 | | | |
| XGBoost | 30 | 85% | none | False | False | 5 | 3.58605 | | | |
| XGBoost | 30 | 85% | none | False | False | 10 | 3.64842 | Overfitted | Same AMS | |
| XGBoost | 30 | 85% | none | False | False | 15 | 3.64190 | | | |
| XGBoost | 30 | 85% | none | False | False | 20 | 3.64129 | | | |
| XGBoost | 30 | 85% | none | False | False | 30 | 3.65412 | Overfitted | Same AMS | |

# Drop the 5-phi Features

| Algorithm | No. of Features | Threshold | Imputer | Standardized | Whiten | Xval Folds | AMS Score | Kaggle Position | Private LB AMS | Top % |
|---|---|---|---|---|---|---|---|---|---|---|
| Feature Engineering - Remove 5 PHI based variables | | | | | | | | | | |
| XGBoost | 25 | 85% | none | False | False | 10 | 3.64040 | | | |
| SVM | 13 | 85% | none | False | False | 3 | 0.67110 | - 12 DER vars | | |

# Drop Features with >70% Missing Data

| Algorithm | No. of Features | Threshold | Imputer | Standardized | Whiten | Xval Folds | AMS Score |
|---|---|---|---|---|---|---|---|
| Feature Drops - Remove 7 Features Based on NA > 70% --- "DER_mass_transverse_met_lep", "DER_mass_vis","DER_pt_h","DER_ | | | | | | | |
| XGBoost | 23 | 85% | none | False | False | 3 | 3.38995 |
| XGBoost | 23 | 83% | none | False | False | 3 | 3.33877 |
| XGBoost | 23 | 85% | none | True | False | 3 | 3.41482 |
| XGBoost | 23 | 85% | none | True | True | 3 | 3.28738 |
| XGBoost | 23 | 85% | none | False | True | 3 | 3.28994 |
| XGBoost | 23 | 85% | zeros | False | False | 3 | 3.39736 |
| XGBoost | 23 | 85% | mean | False | False | 3 | 3.38502 |
| XGBoost | 23 | 85% | median | False | False | 3 | 3.36454 |
| XGBoost | 23 | 85% | most_frequent | False | False | 3 | 3.40686 |

# Polynomial Features

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| Algorithm | No. of Features | Threshold | Imputer | Standardized | Whiten | Xval Folds | AMS Score | Kaggle Position | Private LB AMS | Top % |
|---|---|---|---|---|---|---|---|---|---|---|
| Feature Engineering - Created Polynomial Params on multicollinear pairs features - tested with source features included | | | | | | | | | | |
| XGBoost | 78 | 85% | none | False | False | 3 | 3.57455 | Kaggle # 453 | AMS = 3.64580 | Top 25% |
| XGBoost | 78 | 85% | none | True | False | 3 | 3.59784 | Kaggle # 462 | AMS = 3.64441 | Top 26% |
| XGBoost | 78 | 85% | none | True | False | 30 | 3.63050 | Overfitted | Same AMS | |
| XGBoost | 23 | 85% | none | False | False | 3 | 3.38995 | | | |

```
# ------------------------------------------------------------------
# Fields with high multicollinearity
# ------------------------------------------------------------------

- C01   # 25, 5   PRI_jet_leading_pt    DER_pt_h
- C02   # 23, 5   PRI_met_sumet         DER_pt_h
- C03   # 11, 5   DER_sum_pt            DER_pt_h
- C04   # 31, 5   PRI_jet_all_pt        DER_pt_h
- C05   # 23, 28  PRI_met_sumet         PRI_jet_subleading_pt
- C06   # 11, 28  DER_sum_pt            PRI_jet_subleading_pt
- C07   # 31, 28  PRI_jet_all_pt        PRI_jet_subleading_pt
- C08   # 23, 25  PRI_met_sumet         PRI_jet_leading_pt
- C09   # 11, 25  DER_sum_pt            PRI_jet_leading_pt
- C10   # 31, 25  PRI_jet_all_pt        PRI_jet_leading_pt
- C11   # 11, 23  DER_sum_pt            PRI_met_sumet
- C12   # 31, 23  PRI_jet_all_pt        PRI_met_sumet
- C13   # 31, 11  PRI_jet_all_pt        DER_sum_pt
- C14   # 4, 2    DER_mass_vis          DER_mass_MMC
- C15   # 18, 12  PRI_lep_pt            DER_pt_ratio_lep_tau
- C16   # 24, 10  PRI_jet_num           DER_pt_tot
```

# XGBoost Hyper-Parm Tuning

B

| Algorithm | No. of Features | Threshold | Imputer | Standardized | Whiten | Xval Folds | AMS Score | Kaggle Position | Private LB AMS | Top % | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| XGBoost Hyper-Parameters Optimization and Finetuning | | | | | | | | | | | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.60760 | objective = **binary:logitraw** / binary:logistic / reg:logistic | | | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.49675 | objective = reg:linear | | | |
| XGBoost | 30 | 85% | none | False | False | 3 | 1.08533 | objective = count:poisson | | | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.45721 | objective = rank:pairwise | | | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.06477 | eta = 0.01 | | | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.45622 | eta = 0.04 | | | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.58646 | Kaggle # 275 | AMS = 3.65857 | Top 15% | eta = 0.12 / max depth = 7 |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.54356 | eta = 0.16 | max depth = 7 | | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.48748 | eta = 0.12 | max depth = 9 | | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.54902 | eta = 0.08 | max depth = 9 | | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.54930 | eta = 0.12 | max depth = 7 | subsample = 0.9 | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.58646 | eta = 0.12 | max depth = 7 | eval metric overfitted | |
| XGBoost | 30 | 85% | none | False | False | 3 | 3.58646 | eta = 0.12 | max depth = 7 | eval metric overfitted | |
| XGBoost | 78 | 85% | none | False | False | 3 | 3.56471 | eta = 0.12 | max depth = 7 | 78 polynomial features | |
| XGBoost | 78 | 85% | none | False | False | 5 | 3.60254 | eta = 0.12 | max depth = 7 | 78 polynomial features | |
| XGBoost | 25 | 85% | none | False | False | 3 | 3.57257 | Kaggle # 144 | AMS = 3.68305 | Top 8% | eta = 0.12 / max depth = 7 / Drop 5 phi features |
| XGBoost | 25 | 85% | none | False | False | 3 | 3.59074 | eta = 0.08 | max depth = 7 | Drop 5 phi features | |

# Model Ensemble Stacking Tuning

| Algorithm | No. of Features | Threshold | Imputer | Standardized | Whiten | Xval Folds | AMS Score | Kaggle Position | Private LB AMS | Top % | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Model Ensemble Stacking | | | | | | | | | | | |
| Model Stacking | 30 | 85% | none | False | False | 3 | 0.58160 | 3% of training data | | | boost + xgboost -> logistic |
| Model Stacking | 30 | 85% | none | False | False | 3 | 2.01150 | 30% of training data | | | boost + xgboost -> logistic |
| Model Stacking | 30 | 85% | none | False | False | 3 | 3.65192 | Kaggle # 127 | AMS = 3.68787 | Top 7% | boost + xgboost -> logistic |
| Model Stacking | 30 | 85% | none | False | False | 5 | 3.68160 | Kaggle # 118 | AMS = 3.69373 | Top 7% | boost + xgboost -> logistic |
| Model Stacking | 25 | 85% | none | False | False | 5 | 3.67733 | Kaggle # 107 | AMS = 3.69600 | Top 6% | boost + xgboost -> logistic / drop 5 PHI features / eta=0.08 |
| Model Stacking | 25 | 85% | none | False | False | 5 | 3.68163 | Kaggle # 99 | AMS = 3.69919 | Top 6% | boost + xgboost -> logistic / drop 5 PHI features / eta=0.08 / depth = 10 |
| Model Stacking | 25 | 85% | none | False | False | 5 | 3.65121 | Kaggle # 90 | AMS = 3.70123 | Top 5% | forest + adaboost + boost + xgboost -> logistic / drop 5 PHI features / eta=0.08 / depth = 10 |
| Model Stacking | 25 | 85% | none | False | False | 5 | 3.68000 | Kaggle # 45 | AMS = 3.71929 | Top 3% | boost + xgboost -> logistic / drop 5 PHI features / eta=0.08 / boost depth = 9 |
| Model Stacking | 25 | 85% | none | False | False | 5 | 3.68989 | Kaggle # 34 | AMS = 3.72250 | Top 2% | boost + xgboost -> logistic / drop 5 PHI features / eta=0.08 / boost depth = 9 / xgb depth = 7 |
| Model Stacking | 25 | 85% | none | False | False | 5 | 3.68743 | Kaggle # 34 | AMS = 3.72254 | Top 2% | adaboost + boost + xgboost -> logistic / drop 5 PHI features / eta=0.08 / boost depth = 9 / xgb depth = 7 |

# Results and Findings

Interpretation

Discovery and Insights

# Feature Analysis

D

- Some variables are meaningless or cannot be computed; value is –999.0, which is outside the normal range of all variables
  - Another reason to not impute -999.0
  - Imputation is a bad idea and wrong because –999.0 is not missing at all
  - -999.0 indicates nothing is meant to be there
- Split training and test data into 6 categories according to level of undefined features
- PRI_jet_num is a categorical variable telling which of 4 {jets(1,2,3) and no (0) jet} event happened
- 7 variables are missing more than 70 % of data in training set
- Last variables in PCA feature plots have least influence in their current form
- Weights and Labels are dependent on each other from chisquare test of dependence
- Signal events have low weights and Background events have high weights
- Signal events weight range is exclusively separated from background event weight range
- Signal seems to have only three weights Looks like they are looking for three channels of Higgs Boson
- Not worth spending time coming up with the formula It's already done for us

# Findings

- The Variable Importance plot as well as PCA showed that the 5 angle ('phi') variables seemed to be the least important of the 30 predictors. Although removal of the above variables did not result in a significant improvement of the AMS score using a single model, it did help increase the score quite a bit for the Ensemble model
- Ensemble models performed better than single models and stacking the Ensemble models provided the best result in achieving the final AMS score
- The final Stacking model consisted of AdaBoost, Gradient Boost, XGBoost as Level 0 classifiers followed by Logistic Regression as Level 1 classifier
- Stacking several models in the base layer does not always enhance the final result (AMS score). In our testing, three base classifiers (AdaBoost, Gradient Boost and XGBoost) provided almost equivalent results compared to two base classifiers
- Cross Validation plays a key role in testing the model. Based on our testing, the optimal number of folds for cross validation was determined as 5 since 3 folds seemed to underfit the model while 10 folds seemed to overfit the model

# Lessons Learned

NB

- An increase in the local AMS score based on the training data does not always translate to an increase in the private Kaggle Leaderboard score due to potential overfitting of the model
- Methodical Tuning of the parameters is critical during testing (focusing on one parameter at a time). Random tuning of the parameters would make it difficult to keep track of the changes and may result in over-tuning that would end up decreasing the Kaggle score
- SVM is highly computation intensive and the features and parameters need to be carefully selected before the execution of the algorithm. The algorithm runs for several hours even with reduced features and data
- The maximum number of trees used need not be the same for all the models in a stacked classifier. Increasing the number of trees helped in improving the AMS score only up to a certain threshold. Any further increase in the trees resulted in decreasing the overall AMS score due to potential overfitting

# Insights

B

- Feature engineering (creating new features) did not really work that well – it was not the worth effort
- Ensembles and stacking clearly demonstrated significant improvements
- Hyper-parameters fine-tuning and optimization are very difficult and time consuming
  - Each little change in hyper-parameters could decrease or increase accuracy significantly
  - A fine line exists balancing across effort vs computing time vs complexity vs accuracy
- No clear strategy to deal with missing data except to just leave it alone
- Managing theoretical feature significance to improve prediction accuracy was very challenging in actual practice
- Prediction accuracy would have been even more challenging during a real competition due to the absence of the private leaderboard

# What We Would Have Liked to Do

- Find new or better techniques to automatically generate new features to increase prediction accuracy
  - Explore SVM in depth and try various options for tuning parameters and analyze the effects on final score
  - Blending machine learning and physics (or business) models have a big potential for increased accuracy
- Build out our expertise in ensembles and stacking strategies
- Invest more time and effort to optimize our neural network frameworks
  - Enhance the current Ensemble model by including the Neural Network algorithm (Deep Learning) and test the predictive accuracy
- Use a Bayesian Optimizer tool to automate pipeline iterations to find best combination of hyper-parameters (given its complexity)
  - Use GridSearch to determine the best combination of parameters for the Tree based Boosting models

# Conclusion

Summary and Synopsis

Final Thoughts

# Summary

B

- We have met our objectives in this Machine Learning Challenge, being able to apply various models, algorithms, and strategies to achieve relatively good predictions
- We have obtained the final private leaderboard score of **3.72254**, the 34$^{th}$ position
- We have a renewed sense of appreciation of what machine learning can do, and also the power behind the complexity
- We have learned and developed a lot of new skills from the project, but also realize how much more we still don't know

# Final Thoughts

"Being great at Data Science is more than just depending on an individual's smarts and skills

Knowing how to form a great team that works well together is a huge factor"

# Final Private LB AMS Score

| | | | | | |
|---|---|---|---|---|---|
| 30 | ↑59 | all your HADRON are belong to us | 3.72654 | 65 | Mon, 15 Sep 2014 15:14:34 |
| 31 | ↑33 | mymo | 3.72594 | 73 | Sun, 14 Sep 2014 20:32:19 (-2.4d) |
| 32 | ↓13 | BlackMagic | 3.72491 | 33 | Sat, 23 Aug 2014 20:53:47 (-74.4d) |
| 33 | ↑45 | Alayne | 3.72403 | 101 | Mon, 08 Sep 2014 13:04:55 (-38.2d) |
| - | | **Team Demibots (Bernard-Nanda-Venkat-Deepak)** | **3.72254** | - | **Sat, 27 Aug 2016 03:32:40** **Post-Deadline** |

Top 2%

**Post-Deadline Entry**
If you would have submitted this entry during the competition, you would have been around here on the leaderboard.

| | | | | | |
|---|---|---|---|---|---|
| 34 | ↑49 | Wei Wu | 3.72235 | 45 | Mon, 15 Sep 2014 14:35:18 (-0h) |
| 35 | ↑201 | Phil Culliton | 3.72224 | 91 | Mon, 15 Sep 2014 21:24:55 |
| 36 | ↓8 | cherrybarry | 3.72204 | 144 | Mon, 15 Sep 2014 23:53:31 (-0.1h) |
| 37 | ↑21 | Carlos Fernandez | 3.72180 | 108 | Mon, 15 Sep 2014 16:20:02 (-0.2h) |

# Appendix

More Details :

XGBoost Details

More EDA Plots

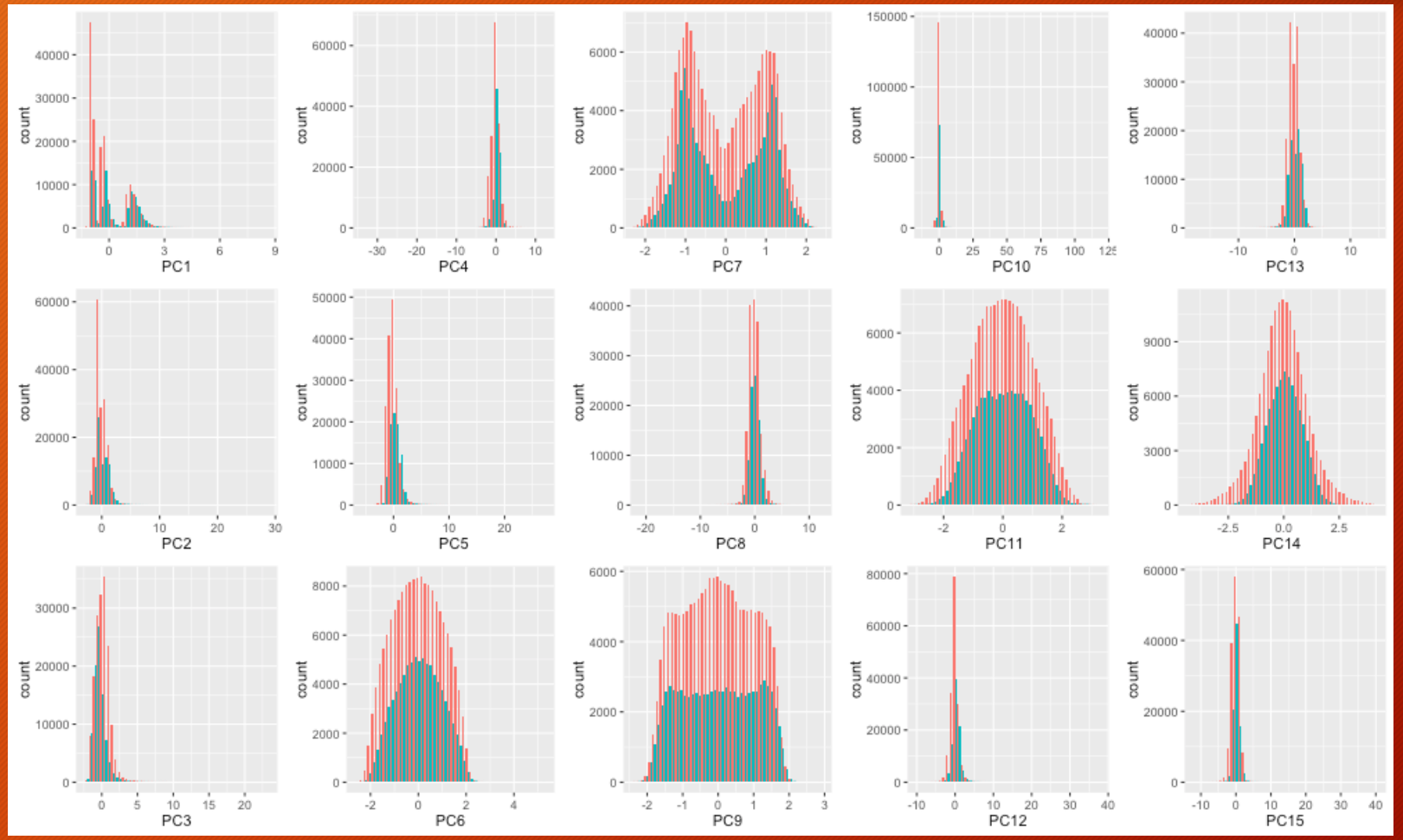
# Benefits of XGBoost

- **Regularization & Parallel Processing**
  - XGBoost implements regularization that helps in reducing overfitting. It also implements parallel processing that significantly expedites the model fitting process compared to GBM.
  - XGBoost utilizes OpenMP which can parallelize the code on a multithreaded CPU automatically. XGBoost has defined a data structure DMatrix to store the data matrix. This data structure will perform some preprocessing work on the data so that the latter iterations run faster.
- **High Flexibility**
  - XGBoost allow users to define custom optimization objectives and evaluation criteria. This adds a whole new dimension to the model and significantly enhances the flexibility
- **Handling Missing Values**
  - XGBoost has an in-built routine to handle missing values.
  - User is required to supply a different value than other observations and pass that as a parameter. XGBoost tries different things as it encounters a missing value on each node and learns which path to take for missing values in future.
- **Tree Pruning**
  - A GBM would stop splitting a node when it encounters a negative loss in the split. Thus it is more of a greedy algorithm.
  - XGBoost on the other hand makes the splits up to the max_depth specified and then start pruning the tree backwards and remove splits beyond which there is no positive gain.
  - Another advantage is that sometimes a split of negative loss say -2 may be followed by a split of positive loss +10. GBM would stop as it encounters -2. But XGBoost will go deeper and it will see a combined effect of +8 of the split and keep both.

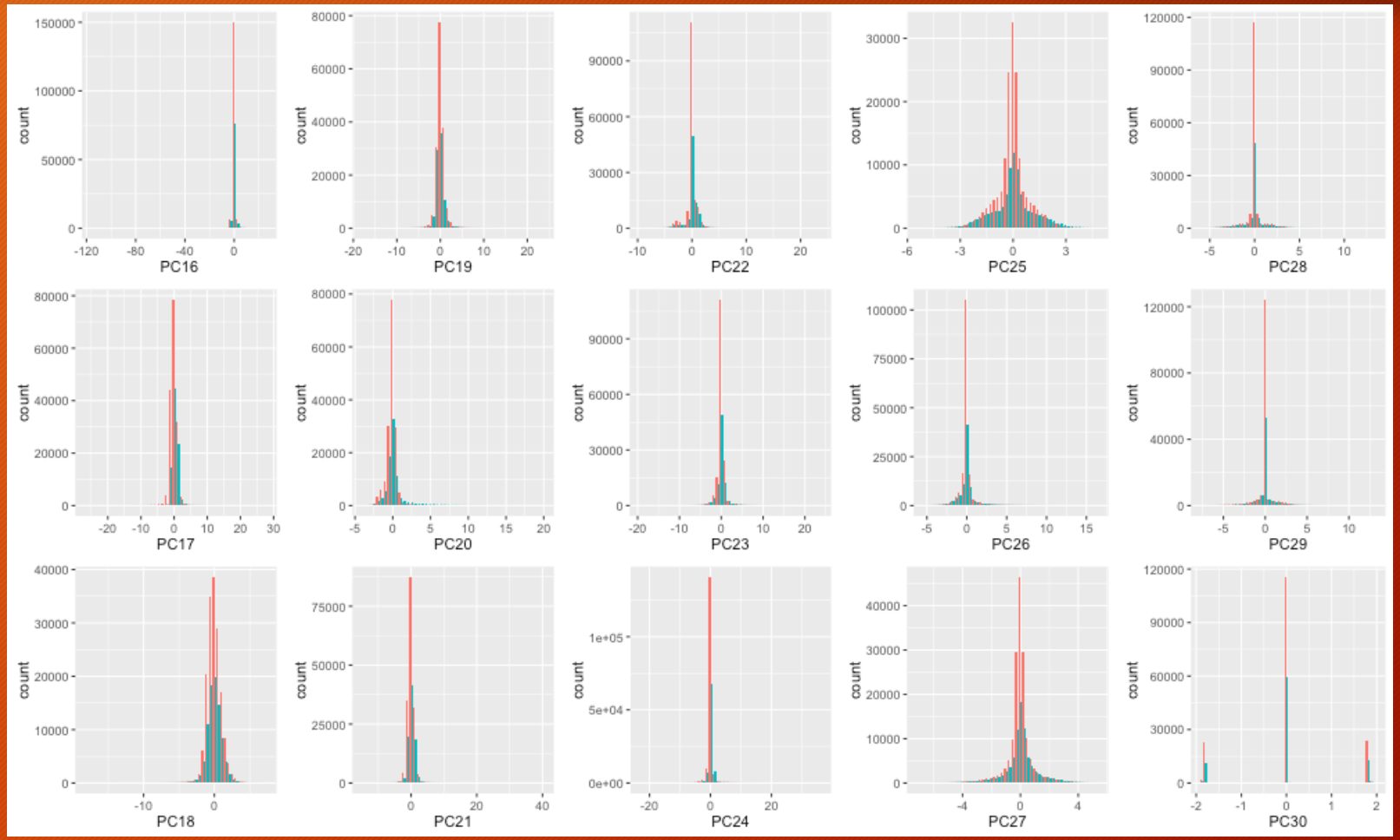
# XGBoost Hyper-Parameters

- General Parameters
  - booster [default=gbtree]: The type of booster to be used. This value can be gbtree, gblinear or dart. gbtree and dart use tree based model while gblinear uses linear function.
  - silent [default=0]: 0 means printing running messages, 1 means silent mode.
  - nthread [default to maximum number of threads available if not set]: number of parallel threads used to run xgboost
  - num_pbuffer [set automatically by xgboost, no need to be set by user]: size of prediction buffer, normally set to number of training instances. The buffers are used to save the prediction results of last boosting step.
  - num_feature [set automatically by xgboost, no need to be set by user]: feature dimension used in boosting, set to maximum dimension of the feature
- Tree Booster Parameters
  - eta [default=0.3] :  step size shrinkage used in update to prevents overfitting. After each boosting step, we can directly get the weights of new features. and eta actually shrinks the feature weights to make the boosting process more conservative.
  - max_depth [default=6] : maximum depth of a tree, increase this value will make model more complex / likely to be overfitting.
  - scale_pos_weight [default=0]: Control the balance of positive and negative weights, useful for unbalanced classes. A typical value to consider: sum(negative cases) / sum(positive cases)
  - subsample [default=1] : subsample ratio of the training instance. Setting it to 0.5 means that XGBoost randomly collected half of the data instances to grow trees and this will prevent overfitting.
- Learning Task Parameters
  - objective [ default=reg:linear ] Used "binary:logitraw"  for this scenario. Logistic regression for binary classification that outputs score before logistic transformation
  - eval_metric : evaluation metrics for validation data, a default metric will be assigned according to objective( RMSE for regression, and error for classification, mean average precision for ranking )

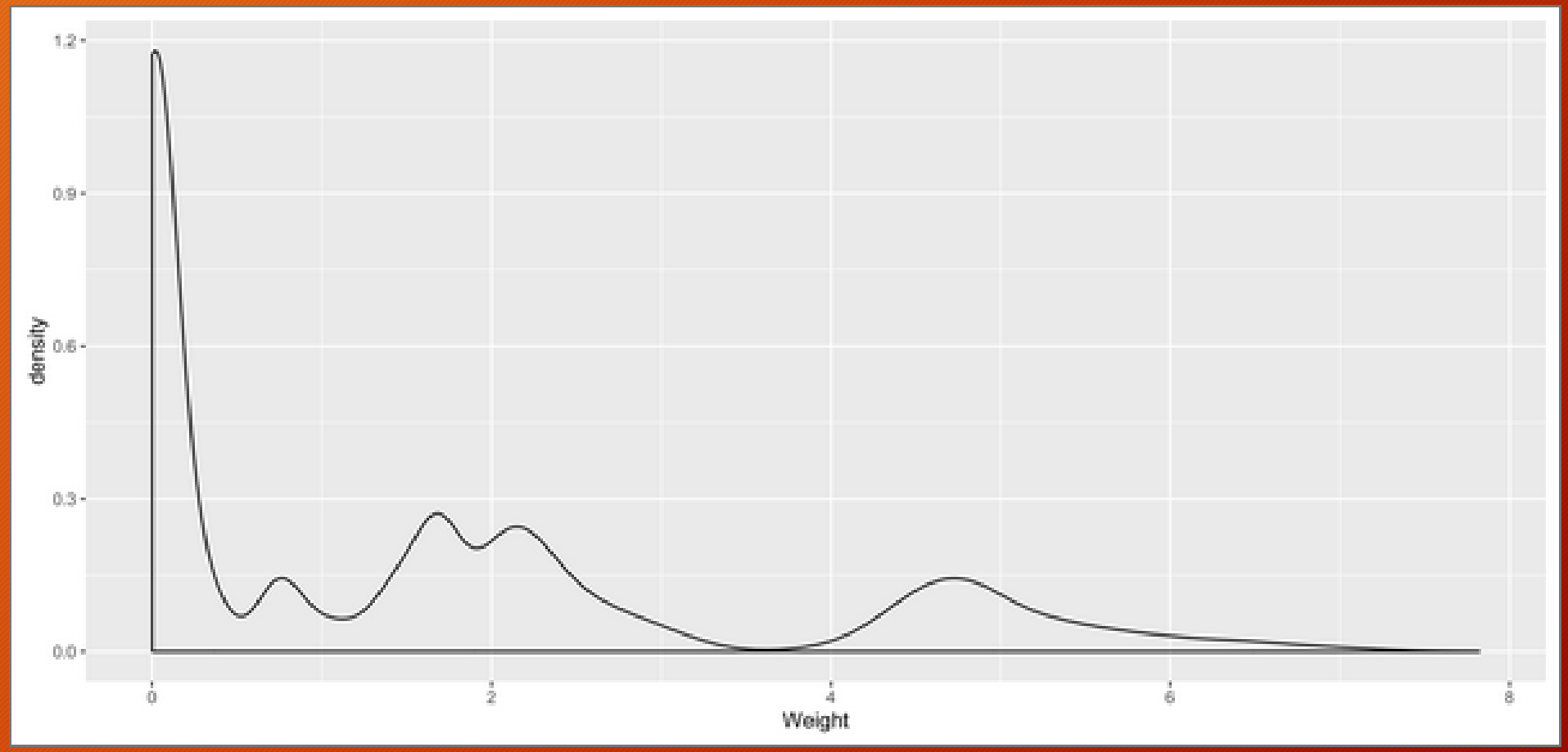
# Histograms [1]



# Histograms [2]



# s & b Weight Density Plot



# Variance Inflation Factors

| VIF | Status of predictors |
|---|---|
| VIF = 1 | Not correlated |
| 1 < VIF < 5 | Moderately correlated |
| VIF > 5 to 10 | Highly correlated |

| | Variables | VIF |
|---|---|---|
| 1 | EventId | 1.008405e+00 |
| 22 | PRI_met_phi | 1.030121e+00 |
| 17 | PRI_tau_phi | 1.087984e+00 |
| 20 | PRI_lep_phi | 1.099111e+00 |
| 16 | PRI_tau_eta | 1.405905e+00 |
| 19 | PRI_lep_eta | 1.416351e+00 |
| 10 | DER_pt_tot | 1.790023e+00 |
| 2 | DER_mass_MMC | 1.948378e+00 |
| 13 | DER_met_phi_centrality | 2.038035e+00 |
| 3 | DER_mass_transverse_met_lep | 2.782868e+00 |
| 32 | Weight | 2.808043e+00 |
| 4 | DER_mass_vis | 3.810547e+00 |
| 9 | DER_deltar_tau_lep | 4.156143e+00 |
| 21 | PRI_met | 4.399020e+00 |
| 12 | DER_pt_ratio_lep_tau | 6.172214e+00 |
| 23 | PRI_met_sumet | 6.217087e+00 |
| 5 | DER_pt_h | 1.313237e+01 |
| 7 | DER_mass_jet_jet | 3.899132e+01 |
| 24 | PRI_jet_num | 3.981534e+01 |
| 25 | PRI_jet_leading_pt | 3.135464e+03 |
| 28 | PRI_jet_subleading_pt | 4.729789e+03 |
| 26 | PRI_jet_leading_eta | 7.179173e+04 |
| 27 | PRI_jet_leading_phi | 7.235446e+04 |
| 8 | DER_prodeta_jet_jet | 1.589050e+05 |
| 29 | PRI_jet_subleading_eta | 1.797135e+05 |
| 30 | PRI_jet_subleading_phi | 2.218772e+05 |
| 6 | DER_deltaeta_jet_jet | 1.365005e+06 |
| 14 | DER_lep_eta_centrality | 2.235745e+06 |
| 15 | PRI_tau_pt | 1.433504e+09 |
| 18 | PRI_lep_pt | 1.558959e+09 |
| 31 | PRI_jet_all_pt | 2.853603e+10 |
| 11 | DER_sum_pt | 3.968489e+10 |
| 33 | Label | NA |

# Variable Importance Plots