STAT5243 Project 4: Causal Inference Algorithms Evaluation

Group 2:

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Instruction for using this notebook: You can click Restart & Run ALL to reproduce the full evaluation results. Outputs in each step are only as illustrations of our development workflow.

Introduction ¶

In this project, we studied Causal Inference on two datasets, one high-dimensional and another low-dimensional.

Specifically, we estimated the Average Treatment Effects (ATE) by calculating the Propensity Scores (PS) using the Boosting Stumps algorithms.

The ATEs are then calculated using three models and compared with the true values to estimate accuracy. For each algorithm and method, The performance and computational efficiency were evaluated for each dataset to select the best combination.

Propensity Score Estimation Methods: (Boosting Stumps)

- 1. GBM
- 2. XGboost

We define the *propensity score* in terms of probability as: e(x) = Pr(T = 1 | X = x), where 0 < e(x) < 1

ATE Estimation Methods:

- 1. Stratification
- 2. Regression Adjustment
- 3. Stratification + Regression Adjustment

To aid with propensity score prediction, we also attempted to alleviate the slight imbalance in the data through well known methods such as random oversampling and SMOTE.

Step 0: Import packages

```
In [1]: import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt
        import os
        import time
        from collections import Counter
        import warnings
        warnings.filterwarnings('ignore')
        # Set a random seed for reproduction.
        RANDOM\_STATE = np.random.seed(42)
        # train-test split for propensity score
        from sklearn.model_selection import train_test_split
        # baseline propensity score
        from sklearn.linear model import LogisticRegression
        from sklearn.linear model import LogisticRegressionCV
        # grid search
        from sklearn.model_selection import GridSearchCV
        # propensity score from tree models
        import xgboost as xgb
        from xgboost import XGBClassifier
        from sklearn.ensemble import GradientBoostingClassifier
        # Stratification and Regression Adjustment
        from sklearn.model selection import StratifiedKFold
        from sklearn.linear model import LinearRegression
        # Imbalance techniques
        from imblearn.over_sampling import RandomOverSampler
        from imblearn.combine import SMOTETomek
```

Step 1: Import and explore data

To increase the usability of the notebook, we use generic variable names instead of associating with the datasets used in for the project. To use the notebook with other datasets, simply import with variable name dataset

We have two dataset, High Dimensional Dataset and Low Dimensional Dataset

```
In [2]: # Set up your directory for the datasets
directory = "../"

In [3]: highDim_dataset = pd.read_csv(directory + 'data/highDim_dataset.csv')
    lowDim_dataset = pd.read_csv(directory + 'data/lowDim_dataset.csv')
```

The goal of this project is estimating the ATE of two dataset: high and low dimensional.

```
In [4]: high_true_ATE = -54.8558
low_true_ATE = 2.0901
```

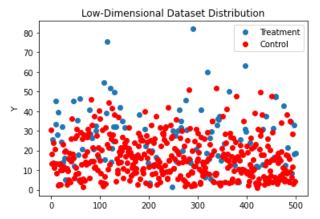
```
In [5]:
        # Choose a development option between highDim dataset and lowDim dataset
        #-----
        dataset = lowDim dataset.copy()
        dataset_name = "Low-Dimensional Dataset"
        true_ATE = low_true_ATE
        #dataset = highDim dataset.copy()
        #dataset name = "High-Dimensional Dataset"
        #true ATE = high true ATE
       dataset.head()
In [6]:
Out[6]:
                                       V5
                                                                                                     V22
                   Α
                       V1
                            V2
                                V3
                                    V4
                                            V6
                                               V7
                                                    V8 ... V13 V14 V15 V16 V17
                                                                               V18
                                                                                    V19
                                                                                         V20
                                                                                             V21
           30.486999
                   0
                      0.00
                          0.00
                               0.00
                                   0.0
                                       0.0
                                          0.00
                                               0.0
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                                                           0.0
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                                                                                0.0
                                                                                    0.00
                                                                                         0.00
                                                                                             9.09
                                                                                                 1.149622
           18.208417
                    0
                      0.00
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                                       0.0
                                          0.00
                                              0.0
                                                  1.40
                                                           0.7
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                                                                                             0.00
                                                                                                 2.887702
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                                                           0.0
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          25.699678 1
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                      2.38
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                                                           0.0
                                                              0.00
                                                                        0.0 2.38
                                                                                0.0
                                                                                    0.00
        4 23.752968 0 0.15 0.15 0.05 0.1 0.0 0.42 0.1 0.95 ...
                                                          0.0 0.36 3.16
                                                                                0.0 0.52 0.31
                                                                                             0.00 1.574639
                                                                        0.0 1.58
        5 rows × 24 columns
```

The high-dimensional dataset has 2000 observations of 187 dimensions, while the low-dimensional dataset has 500 observations of 24 dimensions.

It is convenient to extract only the X portion, which is columns other than Y (treatment result) and A (binary treatment/control group)

```
In [7]:
         data_X = dataset.drop(['Y', 'A'], axis=1).copy()
         data X.head()
In [8]:
Out[8]:
                   V2
                        V3
                            V4
                                 V5
                                      V6
                                          V7
                                               V8
                                                     V9
                                                         V10
                                                                 V13
                                                                      V14
                                                                           V15
                                                                                V16
                                                                                     V17
                                                                                          V18
                                                                                                V19
                                                                                                     V20
                                                                                                                    V22
          0.00
                  0.00 0.00
                                                   0.00
                                                                      0.00
                                                                           0.00
                                                                                     0.00
                                                                                               0.00
                                                                                                               1.149622
                           0.0 0.0
                                    0.00
                                         0.0
                                              0.00
                                                        0.00
                                                                  0.0
                                                                                 0.0
                                                                                           0.0
                                                                                                     0.00
                                                                                                         9.09
             0.00
                  0.00 0.00
                           0.0 0.0
                                    0.00
                                          0.0
                                              1.40
                                                   0.00
                                                        0.00
                                                                  0.7
                                                                      0.00
                                                                           1.40
                                                                                 0.0
                                                                                     1.40
                                                                                           0.0
                                                                                               0.00
                                                                                                     0.00
                                                                                                         0.00
                                                                                                               2.887702
            0.00
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                                          0.0
                                              0.00
                                                   0.00 0.00 ...
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                                                                      0.00
                                                                           3.57
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                                                                                                               0.000000
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                                    0.00
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                                              0.00
                                                                  0.0
                                                                     0.00
                                                                           2.38
                                                                                 0.0
                                                                                     2.38
                                                                                           0.0
                                                                                               0.00
                                                                                                     0.00
                                                                                                         0.00
            0.15  0.15  0.05  0.1  0.0  0.42  0.1  0.95  0.42  0.05  ...
                                                                  0.0 0.36 3.16
                                                                                 0.0
                                                                                     1.58
                                                                                           0.0 0.52 0.31 0.00
         5 rows × 22 columns
In [9]: | def plotComposition(dataset, reset_index=False):
              plt.plot(dataset[dataset.A == 1].Y.reset_index(drop=True)
                        if reset_index
                        else dataset[dataset.A == 1].Y, 'o', label='Treatment')
              plt.plot(dataset[dataset.A == 0].Y.reset_index(drop=True)
                        if reset index
                        else dataset[dataset.A == 0].Y, 'ro', label='Control')
              plt.title(dataset_name + " Distribution")
              plt.ylabel("Y")
              plt.legend()
              plt.show()
```





Are the data sets balanced?

```
In [11]: def checkComposition(dataset):
             print("The dataset contains:\n",len(dataset[dataset.A == 1]), "cases in Treatment group\n",
                    len(dataset[dataset.A == 0]), "cases in Control group.")
             print("Treatment/Control ratio: {}/100".format(round(len(dataset[dataset.A == 1])/len(dataset[dataset.A
         == 0])*100)))
In [12]: | print("High-dimensional")
         checkComposition(highDim_dataset)
         print('-'*20)
         print("Low-dimensional")
         checkComposition(lowDim_dataset)
         High-dimensional
         The dataset contains:
          643 cases in Treatment group
          1357 cases in Control group.
         Treatment/Control ratio: 47/100
         Low-dimensional
         The dataset contains:
          106 cases in Treatment group
          394 cases in Control group.
         Treatment/Control ratio: 27/100
```

In this case, the high-dimensional data is slightly imbalanced, but acceptable. However, the low-dimensional data displays severer imbalance between groups. In any cases, one can use resampling to balance the data, however it may not be beneficial for some ATE estimation algorithms.

Step 2: Naive estimate of ATE

Check the origianl ATE for both high and low dimension data without any steps and algorithms

```
In [13]: def naive_ATE(dataset):
    return np.average(dataset[dataset.A == 1].Y) - np.average(dataset[dataset.A == 0].Y)

In [14]: print("Naive ATE for high-dimensional data:", naive_ATE(highDim_dataset))
    print("Naive ATE for low-dimensional data:", naive_ATE(lowDim_dataset))

Naive ATE for high-dimensional data: -75.17133436876799
    Naive ATE for low-dimensional data: 10.602068661915688
```

Oversampling to deal with the imbalanced data

Resampling data is one of the most commonly preferred approaches to deal with an imbalanced dataset. We used oversampling the minority instead of undersampling the majority since undersampling removes instances from data that may be carrying important information.

1. Random Oversampling:

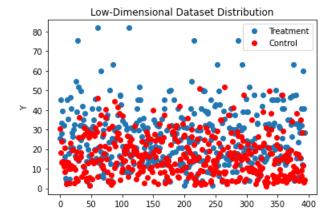
To randomly replicate the small sample to match the size of the larger sample.

1. SMOTE: Synthetic Minority Oversampling Technique

SMOTE generates synthetic samples from the minority class. This algorithm helps to overcome the overfitting problem posed by random oversampling. It focuses on the feature space to generate new instances with the help of interpolation between the positive instances that lie together.

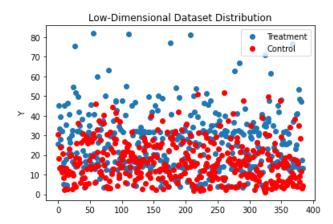
```
In [15]: def Oversample(dataset):
    ovs = RandomOverSampler(random_state = RANDOM_STATE)
    x, y = ovs.fit_resample(dataset.loc[:, dataset.columns != 'A'], dataset.A)
    x.insert(1, 'A', y)
    return x
```

```
The dataset contains:
394 cases in Treatment group
394 cases in Control group.
Treatment/Control ratio: 100/100
```



```
In [17]: def SMOTE(dataset):
    smk = SMOTETomek()
    x, y = smk.fit_resample(dataset.loc[:, dataset.columns != 'A'], dataset.A)
    x.insert(1, 'A', y)
    return x
```

The dataset contains:
384 cases in Treatment group
384 cases in Control group.
Treatment/Control ratio: 100/100



In summary, there are three dataset that can be used: orginial, oversampled, and SMOTE. For testing purpose, change the variable splitted in the beginning of the next section, instead of pasting them all into one notebook.

Step 4: Calculating the propensity scores

The propensity score is estimated by applying machine learning methods on the X variable to fit the label A. For this purpose (and this purpose only) the dataset is splitted into train and test set.

4.1 Split into train and test sets

We split the dataset into train and test with the porpotion of 20:80. We will use the train data to train the model and do the cross validation to avoid overfitting. Then use the test data to check our model

Update dataset name HERE to test the original, oversampled, SMOTE, or any new dataset.

4.2 Propensity Score - Boosted Stumps

In this notebook we use GBM and XGboost. For any choices of learner, it is desirable to perform cross validation and grid search for the best model. We then evaluate the model prediction on the test set.

Gradient Boosting

```
In [21]: | param_grid = {
                        'learning_rate': [0.1, 0.05, 0.01],
                        'max_depth': [2, 3, 5],
                        'min_samples_split': [2, 4],
                        'n_estimators': [5, 10, 15, 20],
                        'min_samples_leaf':[1, 3, 5]
In [22]: def grid search(X:np.array, A:np.array, model, param grid=param grid, cv=10, print step=True, sample weight=
         None):
              Takes a baseline model and does grid search among parameters in the param grid with cross validation.
              Returns the model with best hyparameters after searching
              if sample_weight is None:
                  clf = GridSearchCV(model, param_grid, cv=cv, n_jobs=-1, scoring = 'roc_auc').fit(X, A)
              else:
                  clf = GridSearchCV(model, param grid, cv=cv, n jobs=-1, scoring = 'roc auc').fit(X, A,
                                                                           sample weight = sample weight)
              print("Best accuracy: %0.3f" % (clf.best_score_))
              print()
             print("Best parameters: %r" % clf.best_params_)
              print('-'*30)
              if print_step:
                  means = clf.cv results ['mean test score']
                  stds = clf.cv results ['std test score']
                  for mean, std, params in zip(means, stds, clf.cv_results_['params']):
                      print("%0.3f (+/-%0.03f) for %r" % (mean, std * 2, params))
                  print('-'*30)
              return(model.set_params(**clf.best_params_))
```

Running the cross validation takes a few minutes. Uncomment this cell for developement.

A copy of best hyperparameters from grid search

XGBoost

Running the cross validation takes a few minutes. Uncomment this cell for developement.

A copy of best hyperparameters from grid search

To summarize, we have obtained the propensity scores using GBM and XGBoost. These can now be used to calculate the ATE score.

Step 5: Extract relevant data for ATE calculation

It is convenient to attach the newly constructed propensity score with A and Y. For the stratification, this is all required. However for regression method, X is also required to remove further confounding factors.

```
In [33]: def data_preparation_pipeline(dataset:pd.DataFrame, resample=None, label=dataset_name, boost='GBM'):
             Each sampling method results in a different data size, a set of best
             hyperparameters from grid search, and an array of sample weights.
             This pipeline prepares a dataset, with the specified resampling method,
             for the later ATE estimation.
             inputs
             dataset: pd.DataFrame, the dataset used to evaluate algorithms
             resample: str or None, used when resampling methods are applied. Possible values are None, 'over', or 's
         mote'
             label: str, name of the dataset
             boost: str, the boosting method used to predict propensity scores. Possible values are 'GBM', 'XGB'
             outputs
             ps data: pd.DataFrame, contains three columns for propensity scores, group, and outcome variable
             X data: pd.DataFrame, contains X variables
             test_scores = []
             params = []
             weights =[]
             if resample == None:
                 data = dataset
             elif resample == 'over':
                 data = Oversample(dataset)
             elif resample == 'smote':
                 data = SMOTE(dataset)
                 print("Error: Invalid resampling method! Possible options include None, 'over' and 'smote'")
             X_train, X_test, y_train, y_test, A_train, A_test = split_train_test(data)
             if hoost=='GBM':
                 # A copy of the best hyperparameter candidates from grid search:
                 if label == 'Low-Dimensional Dataset':
                     gbm params1 = {'learning rate': 0.05, 'max depth': 2, 'min samples leaf': 3,
                                     'min_samples_split': 2, 'n_estimators': 100}
                     gbm_params2 = {'learning_rate': 0.1, 'max_depth': 5, 'min_samples_leaf': 1,
                                    'min_samples_split': 4,'n_estimators': 100}
                 elif label == "High-Dimensional Dataset":
                     gbm_params1 = {'learning_rate': 0.05, 'max_depth': 2, 'min_samples_leaf': 3,
                                     'min_samples_split': 2, 'n_estimators': 100}
                     gbm params2 = {'learning rate': 0.1, 'max depth': 5, 'min samples leaf': 1,
                                    'min_samples_split': 4, 'n_estimators': 100}
                 else:
                     print("Error: Invalid resampling method! Possible options include None, 'over' and 'smote'")
                 params_list = [gbm_params1, gbm_params2]
                 for i in range(15,22):
                     # high-dimensional weights (the best weights after multiple trials)
                     sample_weights = np.zeros(len(A_train))
                     sample_weights[A_train == 0] = i
                     sample_weights[A_train == 1] = 20
                     for p in params list:
                         gbm = GradientBoostingClassifier().set_params(**p).fit(X_train, A_train,sample_weight=sample
         weights)
                         #print(gbm.score(X_train, A_train), gbm.score(X_test, A_test))
                         test_scores.append(gbm.score(X_test, A_test))
                         params.append(p)
                         weights.append(sample_weights)
                 best_ = params[test_scores.index(max(test_scores))]
                 #print("GBM parameters:", best_)
                 gbm = GradientBoostingClassifier().set_params(**best_).fit(X_train, A_train,
                                          sample_weight=weights[test_scores.index(max(test_scores))])
                 #print("GBM train accuracy: ",gbm.score(X_train, A_train))
                 #print("GBM test accuracy: ", gbm.score(X_test, A_test))
                 propensity_score_gbm = np.exp(gbm.predict_log_proba(data.iloc[:, 2:]))[:, 1]
```

Step 6: Calculating ATE with different algorithms

6.1 ATE Estimate - Stratification

A common approach to estimate ATE using stratification based on propensity scores. The procedure is as follow: : (i) Estimate propensity scores e_i accross all samples; (ii) form K strata according to the sample quantiles of the e_i , such that the treated and control have roughly the same proportion within each strata; (iii) within each stratum, calculate the difference of sample means of the Y_i for each treatment; and (iv) estimate Δ by a weighted sum of the differences of sample means across strata, where weighting is by the proportion of observations falling in each stratum $\frac{\Delta}{S} = \sum_{i=1}^{K} \frac{1}{i} \sum_{i=1}^{K} \frac{1}{i}$

where K is the number of strata, some literature have advocate to use quintiles (K=5). N_{j} is the number of individuals in stratum j. N_{j} is the number of "treated" individuals in stratum j, while N_{j} is the number of "controlled" individuals in stratum j. $Q_{j} = (q_{j-1}, q_{j})$ where Q_{j} is the number of "controlled" individuals in stratum j. $Q_{j} = (q_{j-1}, q_{j})$ where Q_{j} is the jth sample quantile of the estimated propensity scores. (See Lunceford and Davidian (2004))

```
In [35]: def Calculate_ATE_Strat(ps_data:pd.DataFrame, k:int):
    n = ps_data.shape[0]
    data_copy = Stratify(ps_data, k)

# calculate ATE score
ATE = 0
    for k_idx in range(k):

# temporary data frame
    Qj = data_copy[data_copy.bin == k_idx]
    nj = Qj.shape[0]

treat_avg = np.average(Qj[Qj.A==1].Y) if Qj[Qj.A==1].shape[0] != 0 else 0
    control_avg = np.average(Qj[Qj.A==0].Y) if Qj[Qj.A==0].shape[0] != 0 else 0
    ATE += (nj/n) * ( treat_avg - control_avg )
```

6.2 ATE Estimate - Regression Adjustment and Stratification + Regression Adjustment

Regression adjustment can be employed to reduce residual within-stratum confounding. With regression adjustment, data for each bin is further corrected using regression on X, with level variable A.

Here, steps (iii) and (iv) above are modified as follows: (iii) within each stratum j = 1,...,K, fit a regression model of the form $m^{(j)}(T, X, \alpha)$ representing the postulated regression relationship E(Y | T, X) within stratum j and, based on the result, estimate treatment effect in stratum j by averaging over X_i in j as

Note that a variation here is using two separate regression for T, which is not considered here.

Finally, setting k = 1 bin is equivalent to performing only regression estimation.

```
In [36]: def Calculate_ATE_StratRegrAdjusted_with_X(data:pd.DataFrame, X_data, k:int):
             n = data.shape[0]
             data adjusted = pd.concat(
                 [Stratify(data, k), X_data.reset_index(drop=True)], axis=1)
             # calculate ATE score
             ATE = 0
             for k idx in range(k):
                 # temporary data frame
                 Qj = data_adjusted[data_adjusted.bin == k_idx]
                 nj = Qj.shape[0]
                 # Regression Adjusted Linearly, then Delta_j = alpha^Z_j
                 X = Qj.drop(['e', 'Y', 'bin'], axis=1)
                 y = Qj.Y
                 reg = LinearRegression().fit(X, y)
                 ATE += reg.coef_[0]
             return ATE / k
```

7.1 Measuring the uncertainty of results

To estimate the accuracy, we used the squared error SE = (\hat{\Delta} - \Delta)^2

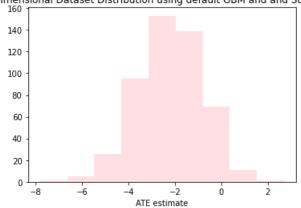
Since the true error is often not known, one can alternatively estimate the uncertainty by random sampling the dataset. To give an example, here is an estimate for the \hat{\Delta}_S using default GBM

```
In [38]: data_for_ATE = combine_data(propensity_score_gbm, dataset.A, dataset.Y)
ATEs = Calculate_ATE_Strat_CV(data_for_ATE, 5)
print("Mean: ", np.nanmean(ATEs), "\n" + "Stdev:", np.nanstd(ATEs))
```

Mean: -2.2035991805034527 Stdev: 1.4114584786952433

```
In [39]: max_bins = 9
    n, bins, patches = plt.hist(ATEs, max_bins, facecolor='pink', alpha=0.5)
    plt.title(dataset_name + " Distribution using default GBM and And Stratification")
    plt.xlabel("ATE estimate")
    plt.show()
```





Thus, for high dimensional dataset, the result can be trusted with uncertainty at around 5 \%, while for low dimensional dataset only give order of magnitude estimate. This may be due the to high dimensional dataset being larger.

7.2 Investigating the effects of different numbers of bins for stratification

```
In [42]: def detailed summary(dataset:pd.DataFrame, max k:int, true ATE=true ATE, title="high", resample=None, boost=
                 This function reads in data and returns best ATE estimation generated from the
                 most appropriate k value for each algorithm. This function is
                inputs
                dataset: pd.DataFrame, the dataset used to evaluate algorithms
                max k: int, the maximum k value used to calculate ATE
                 true ATE: float, the true ATE score used to plot against estimations
                title: str, a string used to label high/low-dimensional datasets in the plot. Possible values are "high"
            or "Low"
                resample: str or None, used when resampling methods are applied. Possible values are None, 'over', or 's
            mote'
                boost: str, the boosting method used to predict propensity scores. Possible values are 'GBM', 'XGB'
                outputs
                 log: pd.DataFrame, chunk of summary table generated from running the experiment
                 data, data X = data preparation pipeline(dataset, resample=resample, label=dataset name, boost=boost)
                 strat results = [Calculate ATE Strat(data, i) for i in range(1, max k+1)]
                 strat reg results = [Calculate ATE StratRegrAdjusted with X(data, data X, i) for i in range(1, max k+1)]
                 error = [abs(strat_results[i] - true_ATE) for i in range(len(strat_results))]
                 best_k_strat = error.index(min(error))+1
                 error = [abs(strat_reg_results[i] - true_ATE) for i in range(len(strat_reg_results))]
                 best k strat reg = error.index(min(error))+1
                 start = time.time()
                 strat = Calculate_ATE_Strat(data, best_k_strat)
                 t_strat = time.time()-start
                 print("Time for calculating ATE with stratification: {}s".format(round(t_strat, 4)))
                 start = time.time()
                 regadj = Calculate_ATE_StratRegrAdjusted_with_X(data, data_X, 1)
                 t_regadj = time.time()-start
                print("Time for calculating ATE with regression adjustment: {}s".format(round(t_regadj, 4)))
                 start = time.time()
                 combined = Calculate_ATE_StratRegrAdjusted_with_X(data, data_X, best_k_strat_reg)
                 t combined = time.time()-start
                print("Time for calculating ATE with stratification + regression adjustment: {}s".format(round(t combine
            d, 4)))
                 print("Estimated ATE by stratification with k = {}: {}".format(best_k_strat, strat))
                 print("Estimated ATE by regression adjustment: {}".format(regadj))
                print("Estimated ATE by stratification + regression adjustment with k = {}: {}".format(best_k_strat_reg,
            combined))
                 # resamping label
                 if resample == 'over':
                     resample_str = '(oversampled)'
                 elif resample == 'smote':
                     resample_str = '(SMOTE)'
                 else: resample str =
                 # Add results to summary
                 summary_cols=["Model", "Data", "PS model", "Estimation time(s)", "Squared error"]
                 log = pd.DataFrame(columns=summary_cols)
                row1= pd.DataFrame([[str('Stratification (K={})'.format(best_k_strat+1)), str(title+'-dim'+resample_str
            ), boost,
                                      t_strat, round((strat-true_ATE)**2,4)]], columns = summary_cols)
                 log = log.append(row1)
                 row2= pd.DataFrame([['Regression Adjustment', str(title+'-dim'+resample_str), boost,
                                      t_regadj, round((regadj - true_ATE)**2,4)]], columns = summary_cols)
                 log = log.append(row2)
                 row3= pd.DataFrame([[str('Strat. + Reg. Adj. (K={})'.format(best_k_strat_reg+1)), str(title+'-dim'+resam
Processing math: 18%le_str), boost,
                                      t_combined, round((combined - true_ATE)**2,4)]], columns = summary_cols)
```

```
log = log.append(row3)
     # Plot:
     plt.figure(figsize=(10,6))
     plt.plot(range(1,max_k+1), strat_results, marker='o',
                    label = 'ATE estimate by stratification')
     plt.plot(range(1,max_k+1), strat_reg_results, marker='o',
                    label = 'ATE estimate by strat + reg_adj')
     plt.scatter(1, regadj, s=150, label='ATE estimate by regression adjustment',alpha=1, marker='o',c='gree
n')
    plt.hlines(true_ATE, 1, max_k, colors='red', linestyles='dashed', label='ATE true')
#plt.hlines(naive_ATE(data), 1, 10, colors='grey', linestyles='dashed', label='ATE Naive')
plt.title("The {}-dimensional dataset {}\nTrue vs. Estimated ATE (PS predicted by {})".format(title, res
ample str,boost))
     plt.xlabel("Number of strata (k)")
     plt.ylabel("ATE")
     plt.legend()
     plt.show()
     return log
```

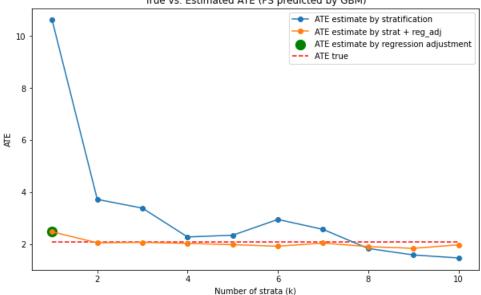
```
In [43]: # To visualize the stability of stratification and strat + reg.adj. for different K values:
    # Development choice: use the lowDim dataset
    dataset = lowDim_dataset.copy()
    dataset_name = "Low-Dimensional Dataset"
    true_ATE = low_true_ATE

#dataset = highDim_dataset.copy()
#dataset_name = "High-Dimensional Dataset"
#true_ATE = high_true_ATE

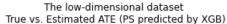
for r in [None,'over','smote']:
    for b in ['GBM','XGB']:
        log = detailed_summary(dataset, max_k=10, true_ATE=true_ATE, title="low", resample=r, boost=b)
```

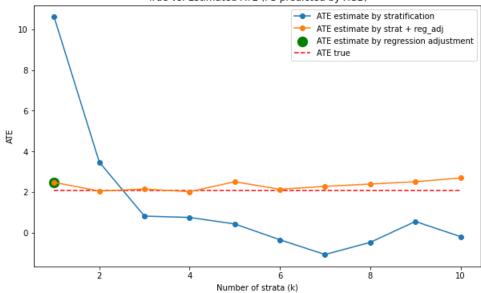
Time for calculating ATE with stratification: 0.0089sTime for calculating ATE with regression adjustment: 0.005sTime for calculating ATE with stratification + regression adjustment: 0.012sEstimated ATE by stratification with k = 4: 2.275243121990381Estimated ATE by regression adjustment: 2.472655707042314Estimated ATE by stratification + regression adjustment with k = 3: 2.0685854818779466

The low-dimensional dataset True vs. Estimated ATE (PS predicted by GBM)



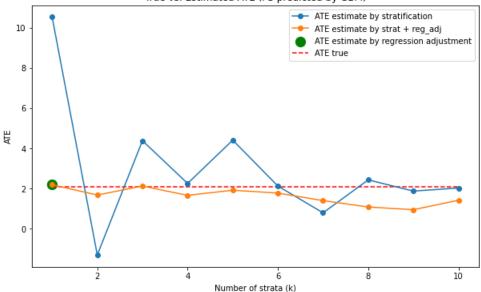
Time for calculating ATE with stratification: 0.009sTime for calculating ATE with regression adjustment: 0.004sTime for calculating ATE with stratification + regression adjustment: 0.006sEstimated ATE by stratification with k=3: 0.8137233699590745Estimated ATE by regression adjustment: 2.472655707042314Estimated ATE by stratification + regression adjustment with k=2: 2.048101012119834



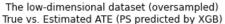


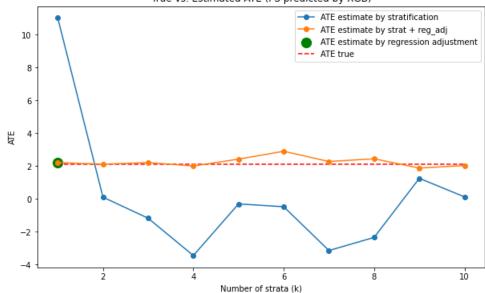
Time for calculating ATE with stratification: 0.013s Time for calculating ATE with regression adjustment: 0.004s Time for calculating ATE with stratification + regression adjustment: 0.009s Estimated ATE by stratification with k=6: 2.1227408863742427 Estimated ATE by regression adjustment: 2.1878718993061588 Estimated ATE by stratification + regression adjustment with k=3: 2.123898789019409

The low-dimensional dataset (oversampled) True vs. Estimated ATE (PS predicted by GBM)



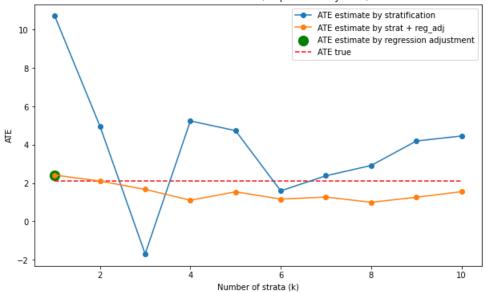
Time for calculating ATE with stratification: 0.02s Time for calculating ATE with regression adjustment: 0.005s Time for calculating ATE with stratification + regression adjustment: 0.007s Estimated ATE by stratification with k=9: 1.2514904189364446 Estimated ATE by regression adjustment: 2.209937764279153 Estimated ATE by stratification + regression adjustment with k=2: 2.1134031438048693



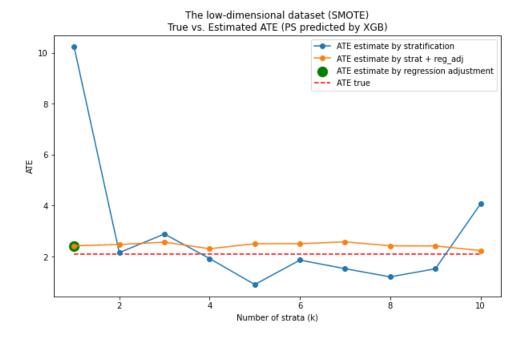


Time for calculating ATE with stratification: 0.013s Time for calculating ATE with regression adjustment: 0.005s Time for calculating ATE with stratification + regression adjustment: 0.007s Estimated ATE by stratification with k=7: 2.3816122055896414 Estimated ATE by regression adjustment: 2.416625281591553 Estimated ATE by stratification + regression adjustment with k=2: 2.1046535420727404

The low-dimensional dataset (SMOTE) True vs. Estimated ATE (PS predicted by GBM)



```
Time for calculating ATE with stratification: 0.005s
Time for calculating ATE with regression adjustment: 0.005s
Time for calculating ATE with stratification + regression adjustment: 0.025s
Estimated ATE by stratification with k = 2: 2.1534495482142892
Estimated ATE by regression adjustment: 2.4205426104457826
Estimated ATE by stratification + regression adjustment with k = 10: 2.2341187270718974
```



Note: When using the highDim_dataset, the ATE estimates would become far off for larger numbers of strata (K>8), so here consider reasonable K values in development with the highDim_dataset.

7.3 Evaluation summary

```
In [44]: summary_cols=["Model", "Data", "PS model", "Estimation time(s)", "Squared error"]
summary = pd.DataFrame(columns=summary_cols)
```

```
In [45]: def estimation summary(dataset:pd.DataFrame, k:int, true ATE=true ATE, title="high", resample=None, boost='G
         BM'):
             This function reads in data and returns best ATE estimation generated from each algorithm.
             dataset: pd.DataFrame, the dataset used to evaluate algorithms
             k: int, the k value used in stratification to calculate ATE
             true ATE: float, the true ATE score used to plot against estimations
             title: str, a string used to label high/low-dimensional datasets in the plot. Possible values are "high"
         or "Low"
             resample: str or None, used when resampling methods are applied. Possible values are None, 'over', or 's
         mote'
             boost: str, the boosting method used to predict propensity scores. Possible values are 'GBM', 'XGB'
             outputs
             log: pd.DataFrame, chunk of summary table generated from running the experiment
             data, data_X = data_preparation_pipeline(dataset, resample=resample, label=dataset_name, boost=boost)
             start = time.time()
             strat = Calculate ATE Strat(data, k)
             t_strat = time.time()-start
             print("Time for calculating ATE with stratification: {}s".format(round(t_strat, 4)))
             print("Estimated ATE by stratification with k = {}: {}".format(k, strat))
             start = time.time()
             regadj = Calculate ATE StratRegrAdjusted with X(data, data X, 1)
             t regadj = time.time()-start
             print("Time for calculating ATE with regression adjustment: {}s".format(round(t regadj, 4)))
             print("Estimated ATE by regression adjustment: {}".format(regadj))
             start = time.time()
             combined = Calculate ATE StratRegrAdjusted with X(data, data X, k)
             t combined = time.time()-start
             print("Time for calculating ATE with stratification + regression adjustment: {}s".format(round(t combine
             print("Estimated ATE by stratification + regression adjustment with k = {}: {}".format(k, combined))
             print('-'*30)
             # resamping label
             if resample == 'over':
                 resample_str = '(oversampled)'
             elif resample == 'smote':
                 resample_str = '(SMOTE)'
             else: resample_str = '
             # Add results to summary
             log = pd.DataFrame(columns=summary_cols)
             row1= pd.DataFrame([[str('Stratification (K={})'.format(k)), str(title+'-dim'+resample_str), boost,
                                   t_strat, round((strat-true_ATE)**2,4)]], columns = summary_cols)
             log = log.append(row1)
             row2= pd.DataFrame([['Regression Adjustment', str(title+'-dim'+resample_str), boost,
                                   t_regadj, round((regadj - true_ATE)**2,4)]], columns = summary_cols)
             log = log.append(row2)
             row3= pd.DataFrame([[str('Strat. + Reg. Adj. (K={})'.format(k)), str(title+'-dim'+resample_str), boost,
                                   t_combined, round((combined - true_ATE)**2,4)]], columns = summary_cols)
             log = log.append(row3)
             return log
```

High dimensional dataset

Note: We picked the number of strata k = 5 for evaluation. A higher number of bins creates imbalance between strata.

```
In [46]: dataset = highDim_dataset.copy()
         dataset name = "High-Dimensional Dataset"
         true ATE = high_true ATE
         for r in [None, 'over', 'smote']:
             for b in ['GBM','XGB']:
                 log = estimation_summary(dataset, k=5, true_ATE=true_ATE, title="high", resample=r, boost=b)
                 summary = summary.append(log)
         Time for calculating ATE with stratification: 0.012s
         Estimated ATE by stratification with k = 5: -53.45272334704037
         Time for calculating ATE with regression adjustment: 0.03s
         Estimated ATE by regression adjustment: -59.365443691851674
         Time for calculating ATE with stratification + regression adjustment: 0.048s
         Estimated ATE by stratification + regression adjustment with k = 5: -51.643415457975365
         -----
         Time for calculating ATE with stratification: 0.018s
         Estimated ATE by stratification with k = 5: -58.14981696800761
         Time for calculating ATE with regression adjustment: 0.037s
         Estimated ATE by regression adjustment: -59.365443691851674
         Time for calculating ATE with stratification + regression adjustment: 0.082s
         Estimated ATE by stratification + regression adjustment with k = 5: -55.1992213301049
         _____
         Time for calculating ATE with stratification: 0.01s
         Estimated ATE by stratification with k = 5: -50.37279967991793
         Time for calculating ATE with regression adjustment: 0.026s
         Estimated ATE by regression adjustment: -59.08961831414915
         Time for calculating ATE with stratification + regression adjustment: 0.054s
         Estimated ATE by stratification + regression adjustment with k = 5: -53.644298126768945
         -----
         Time for calculating ATE with stratification: 0.018s
         Estimated ATE by stratification with k = 5: -48.83608210608958
         Time for calculating ATE with regression adjustment: 0.04s
         Estimated ATE by regression adjustment: -58.98479290009399
         Time for calculating ATE with stratification + regression adjustment: 0.063s
         Estimated ATE by stratification + regression adjustment with k = 5: -53.580515953955
         Time for calculating ATE with stratification: 0.011s
         Estimated ATE by stratification with k = 5: -52.89962862216692
         Time for calculating ATE with regression adjustment: 0.028s
         Estimated ATE by regression adjustment: -57.93632651309089
         Time for calculating ATE with stratification + regression adjustment: 0.07s
         Estimated ATE by stratification + regression adjustment with k = 5: -42.245941627462074
         -----
         Time for calculating ATE with stratification: 0.018s
         Estimated ATE by stratification with k = 5: -49.09588017474781
         Time for calculating ATE with regression adjustment: 0.042s
         Estimated ATE by regression adjustment: -57.60714720976665
         Time for calculating ATE with stratification + regression adjustment: 0.068s
```

Estimated ATE by stratification + regression adjustment with k = 5: -54.02062656235639

Low dimensional dataset

```
In [47]: dataset = lowDim_dataset.copy()
         dataset name = "Low-Dimensional Dataset"
         true ATE = low true ATE
         for r in [None, 'over', 'smote']:
             for b in ['GBM','XGB']:
                 log = estimation_summary(dataset, k=5, true_ATE=true_ATE, title="low", resample=r, boost=b)
                 summary = summary.append(log)
         Time for calculating ATE with stratification: 0.01s
         Estimated ATE by stratification with k = 5: 0.5946656023361272
         Time for calculating ATE with regression adjustment: 0.005s
         Estimated ATE by regression adjustment: 2.472655707042314
         Time for calculating ATE with stratification + regression adjustment: 0.012s
         Estimated ATE by stratification + regression adjustment with k = 5: 1.9889652385564751
         -----
         Time for calculating ATE with stratification: 0.014s
         Estimated ATE by stratification with k = 5: -1.1683831998426197
         Time for calculating ATE with regression adjustment: 0.006s
         Estimated ATE by regression adjustment: 2.472655707042314
         Time for calculating ATE with stratification + regression adjustment: 0.018s
         Estimated ATE by stratification + regression adjustment with k = 5: 2.080286761006241
         -----
         Time for calculating ATE with stratification: 0.011s
         Estimated ATE by stratification with k = 5: 2.538474601920444
         Time for calculating ATE with regression adjustment: 0.004s
         Estimated ATE by regression adjustment: 2.490376700872916
         Time for calculating ATE with stratification + regression adjustment: 0.014s
         Estimated ATE by stratification + regression adjustment with k = 5: 1.1338481701889067
         _____
         Time for calculating ATE with stratification: 0.014s
         Estimated ATE by stratification with k = 5: -4.358936571634633
         Time for calculating ATE with regression adjustment: 0.006s
         Estimated ATE by regression adjustment: 2.3079780079892878
         Time for calculating ATE with stratification + regression adjustment: 0.019s
         Estimated ATE by stratification + regression adjustment with k = 5: 2.6500341867421953
         Time for calculating ATE with stratification: 0.01s
         Estimated ATE by stratification with k = 5: -1.1513158385698077
         Time for calculating ATE with regression adjustment: 0.005s
         Estimated ATE by regression adjustment: 2.2406901934792067
         Time for calculating ATE with stratification + regression adjustment: 0.015s
         Estimated ATE by stratification + regression adjustment with k = 5: 2.0419299440946577
         Time for calculating ATE with stratification: 0.015s
         Estimated ATE by stratification with k = 5: -1.1256143349630436
         Time for calculating ATE with regression adjustment: 0.006s
         Estimated ATE by regression adjustment: 2.2960375479972446
         Time for calculating ATE with stratification + regression adjustment: 0.019s
         Estimated ATE by stratification + regression adjustment with k = 5: 2.0064262389267475
```

In [48]: summary = summary.reset index().drop(['index'], axis=1)

summary.to_csv('../output/evaluations.csv', index=False)

Conclusion and recommendations

Among three algorithms, **regression** is the simplest, while **stratification with regression adjustment** is the most complicated model. The regression precedure makes use of the covariate variable X to account for the confounding factor, while the **stratification** makes use of the assumption that the treatment exposure is unrelated to the counterfactuals for individual sharing the propensity score (X and T independent within strata). Theoretically, the **stratification with regression adjustment**, which was shown to offer an unbiased estimate, offers a **double robustness** even when the regression models are incorrect, thus should be the most accurate.

On the estimation accuracy, for the low-dimensional dataset, **stratification with regression adjustment** has the most accurate estimate. On the high-dimensional dataset, **stratification** achieves the best ATE estimate closest to the true ATE with k = 5. Interestingly, the **regression** gives a smaller estimate, while **regression adjustment to stratification** gives higher estimate. This reduction of accuracy may be due to esimation for the propensity score being overfitted. A shallower tree stump model (with only 10 estimator) indicates the reverse: **stratification adjustment** actually offers an improvement over **stratification** and gives the best result.

With the true ATEs provided, we were able to also experiment on different numbers of bins k. For some higher number of k, it was observed that some bins contain no T = 1 datapoint. By plotting ATE estimates against different k values, we can tell that **stratification with regression adjustment** is more stable and robust that it does not depend much on the choice of k to achieve accurate ATE estimates, whereas **stratification** needs more careful attention on the choice of k since a bad k can lead to very off estimates

On time complexity, **stratification with regression adjustment** is generally the lowest when estimating ATE. **Regression adjustment** works the fastest when the dataset has low dimensions, but when the dataset increases in its dimensionality, **Regression adjustment** slows down and **stratification** becomes faster.

We also discussed the effects of resampling on the model performance. Since the dataset was not too imbalanced and GBM model is quite robust dealing with data imbalance, the resampling methods didn't bring much improvement.

In summary, both **stratification** and **stratification with regression adjustment** are flexible which enable us to choose a specified k that fits the dataset better, whereas **regression adjustment** procedure is mostly set and offers less adjustibility. To check the **stratification**, it is recommended that one makes sure the bins are balanced between the treatment/control group. Finally, the propensity score should not be overfitted, as this will skew the confound factor extracted from the covariate variable X.

```
In [49]: evaluation = pd.read_csv('../output/evaluations.csv')
# Sort by estimation accuracy
evaluation.sort_values(by=['Squared error', 'Estimation time(s)'])
```

Out[49]:

	Model	Data	PS model	Estimation time(s)	Squared error
23	Strat. + Reg. Adj. (K=5)	low-dim	XGB	0.018001	0.0001
32	Strat. + Reg. Adj. (K=5)	low-dim(SMOTE)	GBM	0.015001	0.0023
35	Strat. + Reg. Adj. (K=5)	low-dim(SMOTE)	XGB	0.019000	0.0070
20	Strat. + Reg. Adj. (K=5)	low-dim	GBM	0.011988	0.0102
31	Regression Adjustment	low-dim(SMOTE)	GBM	0.004959	0.0227
34	Regression Adjustment	low-dim(SMOTE)	XGB	0.006002	0.0424
28	Regression Adjustment	low-dim(oversampled)	XGB	0.005998	0.0475
5	Strat. + Reg. Adj. (K=5)	high-dim	XGB	0.082000	0.1179
19	Regression Adjustment	low-dim	GBM	0.004997	0.1463
22	Regression Adjustment	low-dim	XGB	0.005999	0.1463
25	Regression Adjustment	low-dim(oversampled)	GBM	0.004000	0.1602
24	Stratification (K=5)	low-dim(oversampled)	GBM	0.011001	0.2010
29	Strat. + Reg. Adj. (K=5)	low-dim(oversampled)	XGB	0.019000	0.3135
17	Strat. + Reg. Adj. (K=5)	high-dim(SMOTE)	XGB	0.068000	0.6975
26	Strat. + Reg. Adj. (K=5)	low-dim(oversampled)	GBM	0.013998	0.9144
8	Strat. + Reg. Adj. (K=5)	high-dim(oversampled)	GBM	0.054001	1.4677
11	Strat. + Reg. Adj. (K=5)	high-dim(oversampled)	XGB	0.063002	1.6263
0	Stratification (K=5)	high-dim	GBM	0.012034	1.9686
18	Stratification (K=5)	low-dim	GBM	0.010006	2.2363
12	Stratification (K=5)	high-dim(SMOTE)	GBM	0.011000	3.8266
16	Regression Adjustment	high-dim(SMOTE)	XGB	0.042001	7.5699
13	Regression Adjustment	high-dim(SMOTE)	GBM	0.028000	9.4896
2	Strat. + Reg. Adj. (K=5)	high-dim	GBM	0.048000	10.3194
33	Stratification (K=5)	low-dim(SMOTE)	XGB	0.015000	10.3408
30	Stratification (K=5)	low-dim(SMOTE)	GBM	0.010005	10.5068
21	Stratification (K=5)	low-dim	XGB	0.014002	10.6177
3	Stratification (K=5)	high-dim	XGB	0.018000	10.8505
10	Regression Adjustment	high-dim(oversampled)	XGB	0.039998	17.0486
7	Regression Adjustment	high-dim(oversampled)	GBM	0.025967	17.9252
6	Stratification (K=5)	high-dim(oversampled)	GBM	0.009966	20.0973
1	Regression Adjustment	high-dim	GBM	0.029966	20.3369
4	Regression Adjustment	high-dim	XGB	0.037000	20.3369
15	Stratification (K=5)	high-dim(SMOTE)	XGB	0.018000	33.1767
9	Stratification (K=5)	high-dim(oversampled)	XGB	0.018000	36.2370
27	Stratification (K=5)	low-dim(oversampled)	XGB	0.014000	41.5901
14	Strat. + Reg. Adj. (K=5)	high-dim(SMOTE)	GBM	0.070000	159.0085

Out[50]:

	Model	Data	PS model	Estimation time(s)	Squared error
25	Regression Adjustment	low-dim(oversampled)	GBM	0.004000	0.1602
31	Regression Adjustment	low-dim(SMOTE)	GBM	0.004959	0.0227
19	Regression Adjustment	low-dim	GBM	0.004997	0.1463
28	Regression Adjustment	low-dim(oversampled)	XGB	0.005998	0.0475
22	Regression Adjustment	low-dim	XGB	0.005999	0.1463
34	Regression Adjustment	low-dim(SMOTE)	XGB	0.006002	0.0424
6	Stratification (K=5)	high-dim(oversampled)	GBM	0.009966	20.0973
30	Stratification (K=5)	low-dim(SMOTE)	GBM	0.010005	10.5068
18	Stratification (K=5)	low-dim	GBM	0.010006	2.2363
12	Stratification (K=5)	high-dim(SMOTE)	GBM	0.011000	3.8266
24	Stratification (K=5)	low-dim(oversampled)	GBM	0.011001	0.2010
20	Strat. + Reg. Adj. (K=5)	low-dim	GBM	0.011988	0.0102
0	Stratification (K=5)	high-dim	GBM	0.012034	1.9686
26	Strat. + Reg. Adj. (K=5)	low-dim(oversampled)	GBM	0.013998	0.9144
27	Stratification (K=5)	low-dim(oversampled)	XGB	0.014000	41.5901
21	Stratification (K=5)	low-dim	XGB	0.014002	10.6177
33	Stratification (K=5)	low-dim(SMOTE)	XGB	0.015000	10.3408
32	Strat. + Reg. Adj. (K=5)	low-dim(SMOTE)	GBM	0.015001	0.0023
9	Stratification (K=5)	high-dim(oversampled)	XGB	0.018000	36.2370
15	Stratification (K=5)	high-dim(SMOTE)	XGB	0.018000	33.1767
3	Stratification (K=5)	high-dim	XGB	0.018000	10.8505
23	Strat. + Reg. Adj. (K=5)	low-dim	XGB	0.018001	0.0001
29	Strat. + Reg. Adj. (K=5)	low-dim(oversampled)	XGB	0.019000	0.3135
35	Strat. + Reg. Adj. (K=5)	low-dim(SMOTE)	XGB	0.019000	0.0070
7	Regression Adjustment	high-dim(oversampled)	GBM	0.025967	17.9252
13	Regression Adjustment	high-dim(SMOTE)	GBM	0.028000	9.4896
1	Regression Adjustment	high-dim	GBM	0.029966	20.3369
4	Regression Adjustment	high-dim	XGB	0.037000	20.3369
10	Regression Adjustment	high-dim(oversampled)	XGB	0.039998	17.0486
16	Regression Adjustment	high-dim(SMOTE)	XGB	0.042001	7.5699
2	Strat. + Reg. Adj. (K=5)	high-dim	GBM	0.048000	10.3194
8	Strat. + Reg. Adj. (K=5)	high-dim(oversampled)	GBM	0.054001	1.4677
11	Strat. + Reg. Adj. (K=5)	high-dim(oversampled)	XGB	0.063002	1.6263
17	Strat. + Reg. Adj. (K=5)	high-dim(SMOTE)	XGB	0.068000	0.6975
14	Strat. + Reg. Adj. (K=5)	high-dim(SMOTE)	GBM	0.070000	159.0085
5	Strat. + Reg. Adj. (K=5)	high-dim	XGB	0.082000	0.1179

References

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