STAT5243 Project 4: Causal Inference Algorithms Evaluation

Group 2:

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```

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** algorithm.

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 Scores: (Boosting Stumps)

1. GBM
2. XGboost

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.

Propensity Score Estimation

We define the propensity score as:

$$e(x) = Pr(T = 1|X = x)$$

The propensity score is given in term of probability

$$0 < e(x) < 1$$

Step 0: Import packages

In [1]:
```python
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

# GBM
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]:
```python
# Set up your directory for the datasets
directory = "../"
```

In [3]:
```python
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]:
```python
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
```

In [6]:
```
dataset.head()
```

Out[6]:

	Y	A	V1	V2	V3	V4	V5	V6	V7	V8	...	V13	V14	V15	V16	V17	V18	V19	V20	V21	V22
0	30.486999	0	0.00	0.00	0.00	0.0	0.0	0.00	0.0	0.00	...	0.0	0.00	0.00	0.0	0.00	0.0	0.00	0.00	9.09	1.149622
1	18.208417	0	0.00	0.00	0.00	0.0	0.0	0.00	0.0	1.40	...	0.7	0.00	1.40	0.0	1.40	0.0	0.00	0.00	0.00	2.887702
2	13.485040	0	0.00	0.00	0.00	0.0	0.0	0.00	0.0	0.00	...	0.0	0.00	3.57	0.0	0.00	0.0	0.00	0.00	0.00	0.000000
3	25.699678	1	2.38	0.00	0.00	0.0	0.0	0.00	0.0	0.00	...	0.0	0.00	2.38	0.0	2.38	0.0	0.00	0.00	0.00	0.405465
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	1.58	0.0	0.52	0.31	0.00	1.574639

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()
```

In [8]:
```
data_X.head()
```

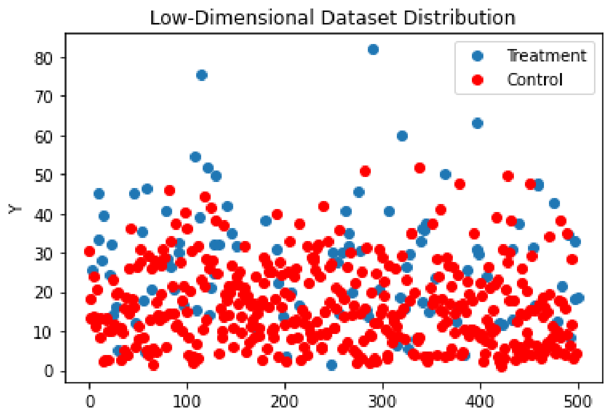
Out[8]:

	V1	V2	V3	V4	V5	V6	V7	V8	V9	V10	...	V13	V14	V15	V16	V17	V18	V19	V20	V21	V22
0	0.00	0.00	0.00	0.0	0.0	0.00	0.0	0.00	0.00	0.00	...	0.0	0.00	0.00	0.0	0.00	0.0	0.00	0.00	9.09	1.149622
1	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
2	0.00	0.00	0.00	0.0	0.0	0.00	0.0	0.00	0.00	0.00	...	0.0	0.00	3.57	0.0	0.00	0.0	0.00	0.00	0.00	0.000000
3	2.38	0.00	0.00	0.0	0.0	0.00	0.0	0.00	0.00	0.00	...	0.0	0.00	2.38	0.0	2.38	0.0	0.00	0.00	0.00	0.405465
4	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	1.574639

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()
```

```
In [10]: plotComposition(dataset)
```



Step 2: Naive estimate of ATE

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

```
In [11]: def naive_ATE(dataset):
             return np.average(dataset[dataset.A == 1].Y) - np.average(dataset[dataset.A == 0].Y)
```

```
In [12]: 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
```

Step 3: Data preprocessing

Are the data sets balanced?

```
In [13]: 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 [14]: 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 oversampling or smote to balance the data, which however may not be beneficial for some ATE estimation algorithms.

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

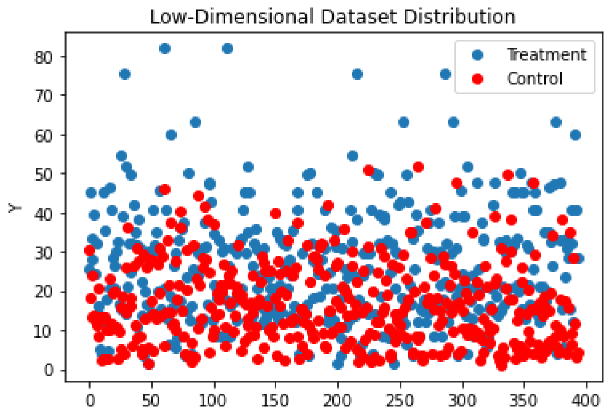
SMOTE generates synthetic samples from the minority class. This algorithm helps to overcome the overfitting problem posed by random oversampling. It focuses on the feature space to generate new instances with the help of interpolation between the positive instances that lie together.

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
```

In [16]:
```
dataset_oversampled = Oversample(dataset)

checkComposition(dataset_oversampled)
plotComposition(dataset_oversampled, reset_index=True)
```

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

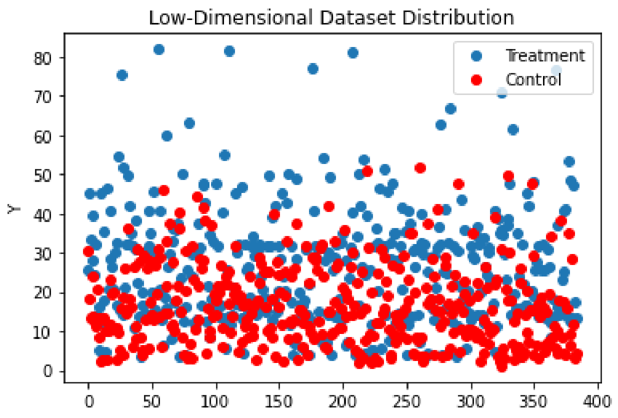


In [17]:
```
def SMOTE(dataset):
    smk = SMOTETomek()
    x, y = smk.fit_resample(dataset.loc[:, dataset.columns != 'A'], dataset.A)
    x.insert(1, 'A', y)
    return x
```

In [18]:
```python
dataset_smote = SMOTE(dataset)

checkComposition(dataset_smote)
plotComposition(dataset_smote, reset_index=True)
```

```
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.

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

In [19]:
```python
def split_train_test(dataset, test_size=0.2):
    X = np.array(dataset.drop(['Y', 'A'], axis=1))
    y = np.array(dataset.Y)
    A = np.array(dataset.A)

    idx_train, idx_test, y_train, y_test = train_test_split(range(X.shape[0]), y,
                                                             test_size=0.2, random_state=RANDOM_STATE)

    X_train = X[idx_train]
    X_test = X[idx_test]
    A_train = A[idx_train]
    A_test = A[idx_test]
    return X_train, X_test, y_train, y_test, A_train, A_test
```

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

In [20]:
```python
#===========================================================================
# Development choices include dataset, dataset_oversampled and dataset_smote
#===========================================================================

X_train, X_test, y_train, y_test, A_train, A_test = split_train_test(dataset)
```

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.

In [23]:
```
# gbm = grid_search(
#     X_train, A_train, model=GradientBoostingClassifier(random_state=RANDOM_STATE),
#     param_grid=param_grid,
#     print_step=True)
```

A copy of best hyperparameters from grid search

In [24]:
```
best_params = {'learning_rate': 0.1, 'max_depth': 5, 'min_samples_leaf': 1, 'min_samples_split': 3,
               'min_samples_split': 4, 'n_estimators': 20}
```

In [25]:
```
gbm = GradientBoostingClassifier(random_state=RANDOM_STATE).set_params(**best_params).fit(X_train, A_train)
```

In [26]:
```
print(gbm.score(X_train, A_train))
print(gbm.score(X_test, A_test))
```

```
0.8975
0.81
```

In [27]:
```
# Predict propensity scores
propensity_score_gbm = np.exp(gbm.predict_log_proba(dataset.iloc[:, 2:]))[:, 1]
```

XGBoost

```
In [28]: param_grid_xgb = {
             'objective':['binary:logistic', 'reg:squarederror'],
             'n_estimators':[5, 10, 15, 20],
             'min_child_weight': [1, 5, 10],
             'gamma': [0.5, 1.0, 1.5],
             'subsample': [0.3, 0.6, 0.8, 1.0],
             'colsample_bytree': [0.6, 0.8],
             'max_depth': [3, 4]
             #'scale_pos_weight':[1, 2, 4]
         }
```

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

```
In [29]: # xgb = grid_search(X_train, A_train,
         #              model=XGBClassifier(n_jobs=-1,random_state=RANDOM_STATE),
         #              param_grid = param_grid_xgb,
         #              print_step=True,
         #              cv=5
         #             )
```

A copy of best hyperparameters from grid search

```
In [30]: best_params_xgb = {'colsample_bytree': 0.8, 'gamma': 0.5, 'max_depth': 4,
                            'min_child_weight': 1, 'n_estimators': 20,
                            'objective': 'reg:squarederror', 'subsample': 1.0}

         xgb = XGBClassifier(n_jobs=-1,random_state=RANDOM_STATE).set_params(**best_params_xgb).fit(X_train, A_train)
```

```
In [31]: print(xgb.score(X_train, A_train))
         print(xgb.score(X_test, A_test))

         0.8775
         0.8
```

```
In [32]: # Predict propensity scores
         propensity_score_xgb = xgb.predict_proba(np.array(dataset.iloc[:, 2:]))[:, 1]
```

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 combine_data(ps, A, y):
             """
             Combines propensity scores with A and y

             Returns a data frame with three columns
             """
             data_combined = pd.DataFrame(
                 np.array([ps, A, y]).T,
                 columns=['e', 'A', 'Y']
             )
             return data_combined
```

We summarized the selected models in the following pipeline:

```
In [34]: 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)
    else:
        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)

    # ================================== Predict PS with GBM ==================================
    if boost=='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]
        ps_data = combine_data(propensity_score_gbm, data.A, data.Y)

    # =================================== Predict PS with XGB ===================================
    elif boost=='XGB':
        best_params_xgb = {'colsample_bytree': 0.8, 'gamma': 0.5, 'max_depth': 4,
                     'min_child_weight': 1, 'n_estimators': 20,
                     'objective': 'reg:squarederror', 'subsample': 1.0}

        xgb = XGBClassifier(n_jobs=-1,random_state=RANDOM_STATE).set_params(**best_params_xgb).fit(X_train,
A_train)
        print("XGboost train accuracy: ",xgb.score(X_train, A_train))
        print("XGboost test accuracy: ", xgb.score(X_test, A_test))
        propensity_score_xgb = xgb.predict_proba(np.array(data.iloc[:, 2:]))[:, 1]
        ps_data = combine_data(propensity_score_xgb, data.A, data.Y)

    else:
        print("Error: Wrong boosting methods! Possible options include 'GBM' and 'XGB'")

    X_data = data.drop(['Y', 'A'], axis=1)
    return ps_data, X_data
```

Step 6: Calculating ATE with different algorithms

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

$$\hat{\Delta}_S = \sum_{j=1}^{k}(N_j/N)\{N_{1j}^{-1}\sum_{i=1}^{N}T_i * Y_i * I(e_i \in Q_j) - N_{0j}^{-1} * \sum_{i=1}^{N}(1-T_i)Y_i * I(e_i \in Q_j)$$

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_{1j} is the number of “treated” individuals in stratum `j` , while N_{0j} 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 Stratify(ps_data:pd.DataFrame, k:int):

             data_copy = ps_data.copy()

             # rank to resolve duplicate edge cases
             data_copy['bin'] = pd.qcut(
                 data_copy.e.rank(method='first'), k, labels=False
             )

             return data_copy
```

In [36]:
```python
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 )

    return ATE
```

ATE Estimate - Regression 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 $j = 1, \dots, K$, fit a regression model of the form $m^{(j)}(T, X, \alpha(j))$ 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

$$\hat{\Delta}^{(j)} = n_j^{-1} \sum_{i=1}^{n} I(e_i \in Q_j)(m^{(j)}(1, X, \alpha^{(j)}) - m^{(j)}(0, X, \alpha^{(j)}))$$

and (iv) estimate Δ by the averaging

$$\hat{\Delta}_{SR} = \frac{1}{K} \sum_{j=1}^{K} \Delta^{(j)}$$

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 [37]:
```python
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
```

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

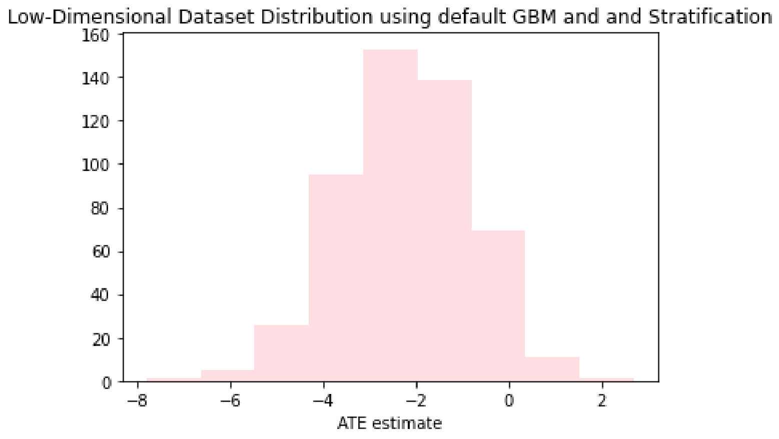
In [38]:
```
def Calculate_ATE_Strat_CV(
    data_for_ATE:pd.DataFrame, k:int, frac=0.9, n=500
):
    ATEs = []
    m = data_for_ATE.shape[0]
    for i in range(n):
        temp = data_for_ATE.sample(frac=frac, replace=True)
        ATEs.append( Calculate_ATE_Strat(temp, k) )

    return ATEs
```

In [39]:
```
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 [40]:
```
num_bins = 9
n, bins, patches = plt.hist(ATEs, num_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.

Result summary

In [41]:
```
summary_cols=["Model", "Data", "PS model", "Estimation time(s)","Squared error"]
summary = pd.DataFrame(columns=summary_cols)
```

```
In [42]: def estimation_summary(dataset:pd.DataFrame, max_k:int, true_ATE=true_ATE, title="high", resample=None, boos
         t='GBM'):
             """
             This function reads in data and returns best ATE estimation generated from the
             most appropriate k value for each algorithm.

             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
             #best_ATE_strat = strat_results[best_k_strat]

             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
             #best_ATE_strat_reg = strat_reg_results[best_k_strat_reg]

             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
             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
         ple_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
```

High dimensional dataset

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, max_k=8, true_ATE=true_ATE, title="high", resample=r, boost=b) summary = summary.append(log)

Note: The ATE estimates become more inaccurate for larger numbers of strata (K>8), so here we only plot reasonable K values.

Low dimensional dataset

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, max_k=10, true_ATE=true_ATE, title="low", resample=r, boost=b) summary = summary.append(log)summary = summary.reset_index().drop(['index'], axis=1) summary.to_csv('../output/summary.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 by setting $k = 5$. 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.

The number of strata k was optimized at 5 bins, as higher number of bins creates imbalance between strata. For some higher number of k, it was observed that some bins contain no $T = 1$ datapoint.

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 [43]:
```python
summary = pd.read_csv('../output/summary.csv')
# Sort by estimation accuracy
summary.sort_values(by=['Squared error', 'Estimation time(s)'])
```

Out[43]:

	Model	Data	PS model	Estimation time(s)	Squared error
35	Strat. + Reg. Adj. (K=3)	low-dim(SMOTE)	XGB	0.008985	0.0000
20	Strat. + Reg. Adj. (K=4)	low-dim	GBM	0.012000	0.0001
29	Strat. + Reg. Adj. (K=2)	low-dim(oversampled)	XGB	0.004999	0.0013
28	Regression Adjustment	low-dim(oversampled)	XGB	0.006000	0.0013
21	Stratification (K=4)	low-dim	XGB	0.009000	0.0085
12	Stratification (K=3)	high-dim(SMOTE)	GBM	0.006997	0.0107
32	Strat. + Reg. Adj. (K=3)	low-dim(SMOTE)	GBM	0.008001	0.0107
23	Strat. + Reg. Adj. (K=6)	low-dim	XGB	0.016045	0.0119
8	Strat. + Reg. Adj. (K=3)	high-dim(oversampled)	GBM	0.034001	0.0216
34	Regression Adjustment	low-dim(SMOTE)	XGB	0.006001	0.0386
26	Strat. + Reg. Adj. (K=2)	low-dim(oversampled)	GBM	0.004999	0.0461
25	Regression Adjustment	low-dim(oversampled)	GBM	0.005999	0.0461
31	Regression Adjustment	low-dim(SMOTE)	GBM	0.004998	0.0506
5	Strat. + Reg. Adj. (K=9)	high-dim	XGB	0.071036	0.0664
33	Stratification (K=3)	low-dim(SMOTE)	XGB	0.007000	0.1217
22	Regression Adjustment	low-dim	XGB	0.005000	0.1463
19	Regression Adjustment	low-dim	GBM	0.005000	0.1463
3	Stratification (K=5)	high-dim	XGB	0.011001	0.1792
18	Stratification (K=3)	low-dim	GBM	0.006000	0.1842
0	Stratification (K=5)	high-dim	GBM	0.010005	0.2212
11	Strat. + Reg. Adj. (K=3)	high-dim(oversampled)	XGB	0.036969	0.3432
2	Strat. + Reg. Adj. (K=3)	high-dim	GBM	0.048999	0.4916
17	Strat. + Reg. Adj. (K=9)	high-dim(SMOTE)	XGB	0.091000	1.5513
30	Stratification (K=7)	low-dim(SMOTE)	GBM	0.017998	2.1691
24	Stratification (K=6)	low-dim(oversampled)	GBM	0.011000	2.9614
14	Strat. + Reg. Adj. (K=3)	high-dim(SMOTE)	GBM	0.044999	3.9503
9	Stratification (K=4)	high-dim(oversampled)	XGB	0.007999	7.7027
16	Regression Adjustment	high-dim(SMOTE)	XGB	0.033000	8.5698
13	Regression Adjustment	high-dim(SMOTE)	GBM	0.033001	10.4772
6	Stratification (K=5)	high-dim(oversampled)	GBM	0.011001	11.0950
15	Stratification (K=8)	high-dim(SMOTE)	XGB	0.018985	13.6025
27	Stratification (K=3)	low-dim(oversampled)	XGB	0.007000	13.9054
7	Regression Adjustment	high-dim(oversampled)	GBM	0.030999	17.4686
10	Regression Adjustment	high-dim(oversampled)	XGB	0.028033	19.6681
1	Regression Adjustment	high-dim	GBM	0.028006	20.3369
4	Regression Adjustment	high-dim	XGB	0.028999	20.3369

In [44]:
```
# Sort by time complexity
summary.sort_values(by=['Estimation time(s)'])
```

Out[44]:

	Model	Data	PS model	Estimation time(s)	Squared error
31	Regression Adjustment	low-dim(SMOTE)	GBM	0.004998	0.0506
29	Strat. + Reg. Adj. (K=2)	low-dim(oversampled)	XGB	0.004999	0.0013
26	Strat. + Reg. Adj. (K=2)	low-dim(oversampled)	GBM	0.004999	0.0461
22	Regression Adjustment	low-dim	XGB	0.005000	0.1463
19	Regression Adjustment	low-dim	GBM	0.005000	0.1463
25	Regression Adjustment	low-dim(oversampled)	GBM	0.005999	0.0461
18	Stratification (K=3)	low-dim	GBM	0.006000	0.1842
28	Regression Adjustment	low-dim(oversampled)	XGB	0.006000	0.0013
34	Regression Adjustment	low-dim(SMOTE)	XGB	0.006001	0.0386
12	Stratification (K=3)	high-dim(SMOTE)	GBM	0.006997	0.0107
27	Stratification (K=3)	low-dim(oversampled)	XGB	0.007000	13.9054
33	Stratification (K=3)	low-dim(SMOTE)	XGB	0.007000	0.1217
9	Stratification (K=4)	high-dim(oversampled)	XGB	0.007999	7.7027
32	Strat. + Reg. Adj. (K=3)	low-dim(SMOTE)	GBM	0.008001	0.0107
35	Strat. + Reg. Adj. (K=3)	low-dim(SMOTE)	XGB	0.008985	0.0000
21	Stratification (K=4)	low-dim	XGB	0.009000	0.0085
0	Stratification (K=5)	high-dim	GBM	0.010005	0.2212
24	Stratification (K=6)	low-dim(oversampled)	GBM	0.011000	2.9614
3	Stratification (K=5)	high-dim	XGB	0.011001	0.1792
6	Stratification (K=5)	high-dim(oversampled)	GBM	0.011001	11.0950
20	Strat. + Reg. Adj. (K=4)	low-dim	GBM	0.012000	0.0001
23	Strat. + Reg. Adj. (K=6)	low-dim	XGB	0.016045	0.0119
30	Stratification (K=7)	low-dim(SMOTE)	GBM	0.017998	2.1691
15	Stratification (K=8)	high-dim(SMOTE)	XGB	0.018985	13.6025
1	Regression Adjustment	high-dim	GBM	0.028006	20.3369
10	Regression Adjustment	high-dim(oversampled)	XGB	0.028033	19.6681
4	Regression Adjustment	high-dim	XGB	0.028999	20.3369
7	Regression Adjustment	high-dim(oversampled)	GBM	0.030999	17.4686
16	Regression Adjustment	high-dim(SMOTE)	XGB	0.033000	8.5698
13	Regression Adjustment	high-dim(SMOTE)	GBM	0.033001	10.4772
8	Strat. + Reg. Adj. (K=3)	high-dim(oversampled)	GBM	0.034001	0.0216
11	Strat. + Reg. Adj. (K=3)	high-dim(oversampled)	XGB	0.036969	0.3432
14	Strat. + Reg. Adj. (K=3)	high-dim(SMOTE)	GBM	0.044999	3.9503
2	Strat. + Reg. Adj. (K=3)	high-dim	GBM	0.048999	0.4916
5	Strat. + Reg. Adj. (K=9)	high-dim	XGB	0.071036	0.0664
17	Strat. + Reg. Adj. (K=9)	high-dim(SMOTE)	XGB	0.091000	1.5513

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