Elo Model Building and Training This notebook focuses on building different regression models for the Elo Merchant Category Recommendation problem. We analyze the performance of different models and choose the best model for our final prediction. In [1]: import numpy as np import pandas as pd import warnings warnings.filterwarnings('ignore') import pickle from prettytable import PrettyTable from sklearn.model selection import StratifiedKFold from sklearn.metrics import mean squared error from sklearn.model selection import GridSearchCV from sklearn.linear model import Ridge from sklearn.neighbors import KNeighborsRegressor import lightgbm as lgb import xgboost as xgb import optuna Function to reduce the memory usage by any pandas dataframe variable #https://www.kaggle.com/c/champs-scalar-coupling/discussion/96655 def reduce mem usage(df, verbose=True): numerics = ['int16', 'int32', 'int64', 'float16', 'float32', 'float64'] start mem = df.memory usage().sum() / 1024**2for col in df.columns: col type = df[col].dtypes if col type in numerics: c min = df[col].min() c max = df[col].max()if str(col type)[:3] == 'int': if c min > np.iinfo(np.int8).min and c max < np.iinfo(np.int8).max:</pre> df[col] = df[col].astype(np.int8) elif c min > np.iinfo(np.int16).min and c max < np.iinfo(np.int16).max:</pre> df[col] = df[col].astype(np.int16) elif c min > np.iinfo(np.int32).min and c max < np.iinfo(np.int32).max:</pre> df[col] = df[col].astype(np.int32)elif c min > np.iinfo(np.int64).min and c max < np.iinfo(np.int64).max:</pre> df[col] = df[col].astype(np.int64) else: if c min > np.finfo(np.float16).min and c max < np.finfo(np.float16).max:</pre> df[col] = df[col].astype(np.float16) elif c min > np.finfo(np.float32).min and c max < np.finfo(np.float32).max:</pre> df[col] = df[col].astype(np.float32) else: df[col] = df[col].astype(np.float64) end mem = df.memory usage().sum() / 1024**2if verbose: print('Mem. usage decreased to {:5.2f} Mb ({:.1f}% reduction)'.format(end mem, 100 * (start mem - end mem) / s return df Loading featurized train and test dataset In [3]: train = pd.read_csv('data/featurized train.csv') test = pd.read csv('data/featurized test.csv') In [4]: train = reduce_mem_usage(train) test = reduce_mem_usage(test) Mem. usage decreased to 176.00 Mb (67.3% reduction) Mem. usage decreased to 113.53 Mb (65.3% reduction) We will use the target column in train set as Y train and outlier column as Outlier array to stratify while splitting data. Then we will drop the card id, target and outlier from train and card id from test. In [5]: Y_train = train['target'] Outlier = train['outlier'] X_train = train.drop(columns = ['card_id', 'target', 'outlier']) X_test = test.drop(columns = ['card id']) **Model Training** We will be training different models for our problem and analyze which model performs better. There is large variation in values of different features since the values are not normalized, so we will be using non-linear regression models for our problem. **Baseline Model** The Baseline model will predict the mean of the target values of train as target for all test points. The RSME score of the Baseline model will provide us with benchmark from where we have to increase our model performance. Each of our model should have RMSE score less than the RSME score of the Baseline model. In [6]: Y_train_mean = pd.DataFrame(Y_train, columns = ['target']) Y_train_mean['target'] = Y_train.astype('float').mean() rsme_baseline = np.sqrt(mean_squared_error(Y_train, Y_train_mean)) print("RSME score for Baseline Model: ", rsme baseline) RSME score for Baseline Model: 3.850440680607971 KNNRegressor Model First non-linear model we will use is KNN Regressor which is the simplest of the regression models. We will use Grid Search to find the optimum value of number of neighbors and then train the final model with that number of neighbors. In [7]: knn_model = KNeighborsRegressor(algorithm = 'kd tree') parameters = {"n neighbors" : [1, 2, 5, 10, 50, 100, 200]} knn folds = StratifiedKFold(n splits = 4, random state = 9, shuffle = True).split(X train, Outlier.values) regressor KNN = GridSearchCV(knn model, parameters, cv = knn folds, scoring = 'neg mean squared error', n jobs regressor_KNN.fit(X_train, Y_train) In [8]: GridSearchCV(cv=<generator object _BaseKFold.split at 0x000001CEBC88E3B0>, Out[8]: estimator=KNeighborsRegressor(algorithm='kd tree'), n jobs=-1, param_grid={'n_neighbors': [1, 2, 5, 10, 50, 100, 200]}, scoring='neg_mean_squared_error') In [9]: best_params = regressor_KNN.best_params print("RSME :", np.sqrt(abs(regressor_KNN.best_score_))) print("Best Hyperparameters") print('-' * 20) for hyperparameter, value in best params.items(): print(hyperparameter, ' : ', value) RSME : 3.8250306371322047 Best Hyperparameters n neighbors : 200 We will now use the best parameters for KNN Regressor obtained from grid search to train the KNN Regressor Model and check its performance using RMSE score. In [7]: Y_train_pred = np.zeros(len(X train)) knn_folds = StratifiedKFold(n_splits = 4, shuffle = True, random_state = 9) for fold, (train_idx, val_idx) in enumerate(knn_folds.split(X_train, Outlier.values)): print("Training for fold {}........".format(fold + 1)) regressor_KNN = KNeighborsRegressor(n_neighbors = 200) regressor_KNN.fit(X_train.iloc[train_idx], Y_train.iloc[train_idx]) Y train pred[val idx] = regressor KNN.predict(X train.iloc[val idx]) Training for fold 1..... Training for fold 2..... Training for fold 3..... Training for fold 4..... In [8]: rsme knn = np.sqrt(mean squared error(Y train, Y train pred)) print("RSME score for KNN Regressor model: ", rsme knn) RSME score for KNN Regressor model: 3.824844001316022 The KNNRegressor model with RMSE score of 3.8248 shows a small improvement over the Baseline model. We will now build some complex models for our problem. XGBoost Model Now we will build a XGBoost model for our problem. But before we build the final XGBoost model we will use Optuna for finding the optimum hyperparameters for the model. In [7]: def objective(trial): parameters = { 'objective' : 'reg:squarederror', 'learning_rate' : 0.01, 'eval_metric' : 'rmse', 'tree method' : 'gpu hist', 'predictor' : 'gpu_predictor',
'random_state' : 9, 'verbosity' : 0, 'max_depth' : trial.suggest_int('max_depth', 1, 8),
'subsample' : trial.suggest_uniform('subsample', 0.1, 1), 'colsample_bytree' : trial.suggest_uniform('colsample bytree', 0.1, 1), 'min split loss' : trial.suggest_uniform('min_split_loss', 0, 10), 'min_child_weight' : trial.suggest_uniform('min_child_weight', 0, 32), 'reg_alpha' : trial.suggest_uniform('reg_alpha', 0.1, 10),
'reg_lambda' : trial.suggest_uniform('reg_lambda', 0.1, 10) } Y train pred = np.zeros(len(X train)) xgb folds = StratifiedKFold(n splits = 4, shuffle = True, random state = 9) for fold, (train idx, val idx) in enumerate(xgb folds.split(X train, Outlier.values)): train_data = xgb.DMatrix(X_train.iloc[train_idx], label = Y_train.iloc[train_idx]) val_data = xgb.DMatrix(X_train.iloc[val_idx], label = Y_train.iloc[val_idx]) reggressor_XGB = xgb.train(params = parameters, dtrain = train_data, evals = [(train data, 'train'), (val data, 'eval')], num boost round = 10000 early_stopping_rounds = 500, verbose eval = False) Y_train_pred[val_idx] = reggressor_XGB.predict(xgb.DMatrix(X_train.iloc[val_idx]), iteration range = (0, reggressor XGB.best iteration)) return np.sqrt(mean squared error(Y train, Y train pred)) In [8]: study = optuna.create study() study.optimize(objective, n trials = 20) [I 2022-04-06 15:19:23,374] A new study created in memory with name: no-name-53d31acd-a906-4c5b-9c4a-2c7f6dad11 [I 2022-04-06 15:27:57,693] Trial 0 finished with value: 3.6619383657128575 and parameters: {'max depth': 4, 's ubsample: 0.9284543408473314, 'colsample_bytree': 0.6142413275865513, 'min_split_loss': 8.771818142117235, 'm in_child_weight': 28.626850478354413, 'reg_alpha': 5.950270078225057, 'reg_lambda': 5.668986265787472}. Best is trial 0 with value: 3.6619383657128575. [I 2022-04-06 15:35:32,200] Trial 1 finished with value: 3.6567083715942403 and parameters: {'max depth': 6, 's ubsample': 0.8479080538654751, 'colsample_bytree ': 0.7036818428596705, 'min_split_loss': 0.878213388299679, 'm in_child_weight': 24.51261521795519, 'reg_alpha': 9.93772670077798, 'reg_lambda': 2.611761219922766}. Best is t rial 1 with value: 3.6567083715942403. [I 2022-04-06 15:43:34,915] Trial 2 finished with value: 3.661179407715765 and parameters: {'max depth': 4, 'su bsample': 0.9230392651263223, 'colsample_bytree ': 0.5954651886785793, 'min_split_loss': 0.0991246125709011, 'm in_child_weight': 30.790700410321158, 'reg_alpha': 8.912795282576779, 'reg_lambda': 9.581735891069085}. Best is trial 1 with value: 3.6567083715942403. [I 2022-04-06 15:55:16,528] Trial 3 finished with value: 3.69023803173204 and parameters: {'max depth': 2, 'sub sample': 0.33985985329657153, 'colsample_bytree ': 0.5530136153582356, 'min_split_loss': 8.336412225346555, 'mi n_child_weight': 3.42250016008364, 'reg_alpha': 1.8834159367371457, 'reg_lambda': 1.50146369534415}. Best is tr ial 1 with value: 3.6567083715942403. [I 2022-04-06 16:07:52,306] Trial 4 finished with value: 3.6880772942702054 and parameters: {'max depth': 2, 's ubsample: 0.2911126243869341, 'colsample_bytree': 0.8189063730329996, 'min_split_loss': 2.316506362362878, 'm in_child_weight': 0.14967794537415813, 'reg_alpha': 7.959181116569342, 'reg_lambda': 7.8076422416540625}. Best is trial 1 with value: 3.6567083715942403. [I 2022-04-06 16:19:38,272] Trial 5 finished with value: 3.6569816964289097 and parameters: {'max depth': 8, 's ubsample': 0.6244273905441523, 'colsample_bytree ': 0.7191547938903964, 'min_split_loss': 3.883828047862573, in_child_weight': 13.423328704687783, 'reg_alpha': 8.830768409869819, 'reg_lambda': 4.78882921075339}. Best is trial 1 with value: 3.6567083715942403. [I 2022-04-06 16:25:33,059] Trial 6 finished with value: 3.6590863243347687 and parameters: {'max depth': 5, 's ubsample': 0.6152060398357531, 'colsample_bytree ': 0.43586852513673147, 'min_split_loss': 9.286939143166911, 'min_child_weight': 22.620957895542297, 'reg_alpha': 7.003260396141438, 'reg_lambda': 0.9892320211569767}. Bes t is trial 1 with value: 3.6567083715942403. [I 2022-04-06 16:33:08,052] Trial 7 finished with value: 3.661364761454252 and parameters: {'max depth': 5, 'su bsample': 0.9662526242796118, 'colsample bytree ': 0.9463173637783876, 'min split loss': 9.338805381090044, 'mi n_child_weight': 0.7464848479982074, 'reg_alpha': 1.6701445686696066, 'reg_lambda': 2.790671934700568}. Best is trial 1 with value: 3.6567083715942403. [I 2022-04-06 16:43:21,758] Trial 8 finished with value: 3.6604296002061023 and parameters: {'max depth': 8, 's ubsample': 0.358509655175724, 'colsample bytree ': 0.9958780665916114, 'min_split_loss': 6.939544709338007, 'mi n_child_weight': 30.279103429646913, 'reg_alpha': 2.84232042355615, 'reg_lambda': 0.3670849389279919}. Best is trial 1 with value: 3.6567083715942403. [I 2022-04-06 16:52:16,042] Trial 9 finished with value: 3.6573103372949856 and parameters: {'max_depth': 7, 's ubsample': 0.8443194357002407, 'colsample_bytree ': 0.9277765493557409, 'min_split_loss': 4.860710523470409, 'm in_child_weight': 29.478152824142235, 'reg_alpha': 2.5614727782492954, 'reg_lambda': 5.0395706385219174}. Best is trial 1 with value: 3.6567083715942403. [I 2022-04-06 16:58:33,723] Trial 10 finished with value: 3.6744161622040465 and parameters: {'max depth': 6, 'subsample': 0.10990672992390699, 'colsample_bytree ': 0.12555869239676365, 'min_split_loss': 0.02419095641027 0914, 'min_child_weight': 16.791758181406195, 'reg_alpha': 4.630714944024064, 'reg_lambda': 3.076697500642170 6}. Best is trial 1 with value: 3.6567083715942403. [I 2022-04-06 17:10:33,363] Trial 11 finished with value: 3.6580256181442854 and parameters: {'max_depth': 8, 'subsample': 0.7117073467758669, 'colsample_bytree ': 0.7549007838853784, 'min_split_loss': 3.181905667852382 7, 'min_child_weight': 10.320708628611172, 'reg_alpha': 9.956747439302987, 'reg_lambda': 4.922268935028661}. Be st is trial 1 with value: 3.6567083715942403. [I 2022-04-06 17:17:38,292] Trial 12 finished with value: 3.6543842961463846 and parameters: {'max depth': 7, 'subsample': 0.7145610313690366, 'colsample_bytree': 0.364896100159906, 'min_split_loss': 2.2685374838074592, 'min_child_weight': 16.579787389902428, 'reg_alpha': 9.874511648120071, 'reg_lambda': 3.474818860996104}. Best is trial 12 with value: 3.6543842961463846. [I 2022-04-06 17:23:50,396] Trial 13 finished with value: 3.655308624034834 and parameters: {'max depth': 6, 's ubsample': 0.7546894736891103, 'colsample_bytree ': 0.35953055604455697, 'min_split_loss': 1.7430072736882494, 'min child weight': 20.871581025950157, 'reg alpha': 9.754453743092853, 'reg lambda': 2.9917869001417916}. Bes t is trial 12 with value: 3.6543842961463846. [I 2022-04-06 17:30:20,329] Trial 14 finished with value: 3.655754255676229 and parameters: {'max_depth': 6, 's ubsample': 0.7378770130703372, 'colsample_bytree ': 0.338046217432016, 'min_split_loss': 1.9645302780920293, 'm in child weight': 19.93997754531223, 'reg alpha': 4.656227042466928, 'reg lambda': 3.7495764104611213}. Best is trial 12 with value: 3.6543842961463846. [I 2022-04-06 17:37:43,899] Trial 15 finished with value: 3.6559629537567555 and parameters: {'max depth': 7, 'subsample': 0.5420137286855751, 'colsample_bytree ': 0.27513457857490214, 'min_split_loss': 6.131848208646049 5, 'min_child_weight': 7.669472157495031, 'reg_alpha': 6.971738449754822, 'reg_lambda': 7.296388374083267}. Bes t is trial 12 with value: 3.6543842961463846. [I 2022-04-06 17:52:00,139] Trial 16 finished with value: 3.6700415332758265 and parameters: {'max depth': 3, 'subsample': 0.49550856948340094, 'colsample_bytree ': 0.40492581092133645, 'min_split_loss': 1.76557917635189 62, 'min_child_weight': 16.698224788006556, 'reg_alpha': 0.4164559475927003, 'reg_lambda': 6.368655741414436}. Best is trial 12 with value: 3.6543842961463846. [I 2022-04-06 18:06:45,351] Trial 17 finished with value: 3.6554290803978655 and parameters: {'max depth': 7, 'subsample': 0.7352937090284963, 'colsample bytree ': 0.18838194998649513, 'min split loss': 3.881307218225757 5, 'min child weight': 20.728257731411414, 'reg alpha': 8.663844153637069, 'reg lambda': 1.894964817150832}. Be st is trial 12 with value: 3.6543842961463846. [I 2022-04-06 18:31:34,418] Trial 18 finished with value: 3.734257977121652 and parameters: {'max depth': 1, 's ubsample': 0.4306898046818125, 'colsample_bytree ': 0.46324135253079496, 'min_split_loss': 3.0587942845005154, 'min_child_weight': 25.125964232381428, 'reg_alpha': 7.383607233605659, 'reg_lambda': 3.7416948958534593}. Bes t is trial 12 with value: 3.6543842961463846. [I 2022-04-06 18:37:46,675] Trial 19 finished with value: 3.6552227392232033 and parameters: {'max depth': 6, 'subsample': 0.8036160540143876, 'colsample_bytree ': 0.3078380360844784, 'min_split_loss': 1.286284593877773 8, 'min child weight': 13.362410445443684, 'reg alpha': 5.934780234540893, 'reg lambda': 3.967702509333143}. Be st is trial 12 with value: 3.6543842961463846. In [9]: b_trial = study.best_trial print('RSME : ', b_trial.value) best_params = b_trial.params print("Best Hyperparameters") print('-' * 20) for hyperparameter, value in best_params.items(): print(hyperparameter, ' : ', value) RSME : 3.6543842961463846 Best Hyperparameters max depth : 7 subsample : 0.7145610313690366 colsample bytree : 0.364896100159906 min split loss : 2.2685374838074592 min child weight: 16.579787389902428 reg_alpha : 9.874511648120071 reg_lambda : 3.474818860996104 In [10]: with open('data/XGB_parameters', 'ab') as df file: pickle.dump(best_params, df_file) We will use the best hyperparameters obtained from optuna trial for building the final XGBoost model. with open('data/XGB_parameters', 'rb') as df_file: best_params_xgb = pickle.load(df_file) In [10]: parameters = { 'objective' : 'reg:squarederror', 'learning_rate' : 0.01, 'eval_metric' : 'rmse',
'tree_method' : 'gpu_hist',
'predictor' : 'gpu_predictor', 'random_state' : 9,
'verbosity' : 0,
'max_depth' : best_params_xgb.get('max_depth'),
'subsample' : best_params_xgb.get('subsample'), 'colsample_bytree' : best_params_xgb.get('colsample_bytree'), 'min_split_loss' : best_params_xgb.get('min_split_loss'), 'min_child_weight' : best_params_xgb.get('min_child_weight'), 'reg_alpha' : best_params_xgb.get('reg_alpha'),
'reg_lambda' : best_params_xgb.get('reg_lambda') In [11]: Y_train_pred_xgb = np.zeros(len(X_train)) xgb folds = StratifiedKFold(n splits = 4, shuffle = True, random state = 9) for fold, (train idx, val idx) in enumerate(xgb folds.split(X train, Outlier.values)): print("Training for fold {}.........".format(fold + 1)) train_data = xgb.DMatrix(X_train.iloc[train_idx], label = Y_train.iloc[train_idx]) val_data = xgb.DMatrix(X_train.iloc[val_idx], label = Y_train.iloc[val_idx]) reggressor_XGB = xgb.train(params = parameters, dtrain = train_data, evals = [(train_data, 'train'), (val_d num_boost_round = 10000, early_stopping_rounds = 500, verbose_eval = 1000) Y_train_pred_xgb[val_idx] = reggressor_XGB.predict(xgb.DMatrix(X_train.iloc[val_idx]), iteration_range = (0, reggressor_XGB.best_iteration)) Training for fold 1..... [0] train-rmse:3.98423 eval-rmse:3.83439 [1000] train-rmse:3.26844 eval-rmse:3.53679 [1369] train-rmse:3.16492 eval-rmse:3.53823 Training for fold 2..... [0] train-rmse:3.93100 eval-rmse:3.99622 [1000] train-rmse:3.21182 eval-rmse:3.72947 [1268] train-rmse:3.13924 eval-rmse:3.73045 Training for fold 3..... [0] train-rmse:3.93589 eval-rmse:3.98138 [1000] train-rmse:3.21848 eval-rmse:3.69194 [1355] train-rmse:3.12377 eval-rmse:3.69378 Training for fold 4..... [0] train-rmse:3.93726 eval-rmse:3.97762 [1000] train-rmse:3.22834 eval-rmse:3.67231 [1589] train-rmse:3.07012 eval-rmse:3.67334 In [12]: rsme_xgb = np.sqrt(mean_squared_error(Y_train, Y_train_pred_xgb)) print("RSME score for XGBoost model: ", rsme xgb) RSME score for XGBoost model: 3.6579771246304467 The XGBoost model with RSME score of 3.6579 has much better performance than the KNNRegressor and shows big improvement in RSME score from the Baseline model. **LightGBM Model** We will also build a LightGBM model for the problem to analyze if it performs better than the XGBoost model. Similar to XGBoost, we will use Optuna to find the best hyperparameters before building the final LightGBM model. In [13]: def objective(trial): parameters = { 'objective' : 'regression', 'metric' : 'rmse', 'boosting_type' : 'gbdt', 'learning_rate' : 0.01, 'device' : 'cpu', 'n_jobs' : -1, 'verbosity' : -1, 'random_state' : 9, 'bagging_freq' : 1, 'bagging_seed' : 9, 'max depth' : trial.suggest_int('max_depth', 1, 16), 'num leaves' : trial.suggest_int('num_leaves', 16, 128), 'min_data_in_leaf' : trial.suggest_int('min_data_in_leaf', 8, 64), 'min_child_weight' : trial.suggest_uniform('min_child_weight', 0, 32), 'feature_fraction' : trial.suggest_uniform('feature_fraction', 0.1, 1.0), 'bagging_fraction' : trial.suggest_uniform('bagging_fraction', 0.1, 1.0), 'min_split_gain' : trial.suggest_uniform('min_split_gain', 0, 10), : trial.suggest_uniform('reg_alpha', 0, 10), 'reg alpha' 'reg_lambda' : trial.suggest_uniform('reg_lambda', 0, 10) } Y_train_pred = np.zeros(len(X_train)) lgb folds = StratifiedKFold(n splits = 4, shuffle = True, random state = 9) for fold, (train_idx, val_idx) in enumerate(lgb_folds.split(X_train, Outlier.values)): train_data = lgb.Dataset(X_train.iloc[train_idx], label = Y_train.iloc[train_idx]) val_data = lgb.Dataset(X_train.iloc[val_idx], label = Y_train.iloc[val_idx]) reggressor_LGB = lgb.train(params = parameters, train_set = train_data, valid_sets = [train_data, val_d num_boost_round = 10000, early_stopping_rounds = 500, verbose_eval = False) Y_train_pred[val_idx] = reggressor_LGB.predict(X_train.iloc[val_idx], num_iteration = reggressor_LGB.be return np.sqrt(mean_squared_error(Y_train, Y_train_pred)) In [14]: study = optuna.create study() study.optimize(objective, n trials = 20) [I 2022-04-07 00:47:47,852] A new study created in memory with name: no-name-9168335d-dbc9-496e-8895-179b481815 [I 2022-04-07 00:54:35,935] Trial 0 finished with value: 3.6630423850962637 and parameters: {'max depth': 12, 'num_leaves': 71, 'min_data_in_leaf': 22, 'min_child_weight': 21.669760862270813, 'feature_fraction': 0.599153 2629972278, 'bagging_fraction': 0.40395548684511795, 'min_split_gain': 4.348054423432296, 'reg_alpha': 2.217543 805827545, 'reg_lambda': 3.039140014881019}. Best is trial 0 with value: 3.6630423850962637. [I 2022-04-07 01:04:50,792] Trial 1 finished with value: 3.6574406809362014 and parameters: {'max_depth': 9, 'n um_leaves': 42, 'min_data_in_leaf': 53, 'min_child_weight': 26.058615434144063, 'feature_fraction': 0.822052706 10647, 'bagging_fraction': 0.8922895465650358, 'min_split_gain': 3.768155610827323, 'reg_alpha': 9.119062148441 706, 'reg_lambda': 6.553709195366454}. Best is trial 1 with value: 3.6574406809362014. [I 2022-04-07 01:26:40,094] Trial 2 finished with value: 3.687509677709659 and parameters: {'max_depth': 2, 'nu m_leaves': 53, 'min_data_in_leaf': 20, 'min_child_weight': 31.34975651966691, 'feature_fraction': 0.94127633834 04444, 'bagging_fraction': 0.7882988513258217, 'min_split_gain': 2.9882013397167073, 'reg_alpha': 2.66817406294 19326, 'reg_lambda': 0.12642142265436251}. Best is trial 1 with value: 3.6574406809362014. [I 2022-04-07 01:31:50,941] Trial 3 finished with value: 3.6617145946640917 and parameters: {'max_depth': 8, 'n um_leaves': 23, 'min_data_in_leaf': 34, 'min_child_weight': 6.0921731789187135, 'feature_fraction': 0.480737363 0519206, 'bagging_fraction': 0.4318080651273023, 'min_split_gain': 6.19801713860399, 'reg_alpha': 1.29390847221 17233, 'reg_lambda': 2.336503781610312}. Best is trial 1 with value: 3.6574406809362014. [I 2022-04-07 01:42:10,222] Trial 4 finished with value: 3.6625471833940697 and parameters: {'max_depth': 4, 'n um_leaves': 77, 'min_data_in_leaf': 9, 'min_child_weight': 21.76258486439517, 'feature_fraction': 0.56011618184 56099, 'bagging_fraction': 0.9464732131946071, 'min_split_gain': 3.9458547409624725, 'reg_alpha': 5.81827231638 3561, 'reg_lambda': 8.874537586433622}. Best is trial 1 with value: 3.6574406809362014. [I 2022-04-07 01:49:15,208] Trial 5 finished with value: 3.6663725637949165 and parameters: {'max_depth': 16, 'num_leaves': 120, 'min_data_in_leaf': 58, 'min_child_weight': 2.144902755552689, 'feature_fraction': 0.155574 04142879028, 'bagging_fraction': 0.29981072618721505, 'min_split_gain': 3.3275569173944763, 'reg_alpha': 5.2869 98887674157, 'reg_lambda': 4.709183214556333}. Best is trial 1 with value: 3.6574406809362014. [I 2022-04-07 01:58:06,639] Trial 6 finished with value: 3.6704289050163696 and parameters: {'max_depth': 5, 'n um_leaves': 120, 'min_data_in_leaf': 36, 'min_child_weight': 11.679726089495535, 'feature_fraction': 0.15914698 918145215, 'bagging_fraction': 0.14385242383875402, 'min_split_gain': 5.953101021397269, 'reg_alpha': 6.9342713 64173691, 'reg_lambda': 5.840012476765176}. Best is trial 1 with value: 3.6574406809362014. [I 2022-04-07 02:05:54,039] Trial 7 finished with value: 3.671626781391197 and parameters: {'max_depth': 14, 'n um_leaves': 94, 'min_data_in_leaf': 52, 'min_child_weight': 23.791540519168898, 'feature_fraction': 0.857090907 0148612, 'bagging_fraction': 0.12859621679162855, 'min_split_gain': 1.1542536990525287, 'reg_alpha': 4.09914205 683505, 'reg_lambda': 5.411445316124768}. Best is trial 1 with value: 3.6574406809362014. [I 2022-04-07 02:18:34,728] Trial 8 finished with value: 3.737315632837233 and parameters: {'max_depth': 1, 'nu m_leaves': 80, 'min_data_in_leaf': 19, 'min_child_weight': 18.12503015676918, 'feature_fraction': 0.43868107902 01414, 'bagging_fraction': 0.3559475215161121, 'min_split_gain': 5.1298000392298775, 'reg_alpha': 9.70843415796 1342, 'reg_lambda': 8.159726750172482}. Best is trial 1 with value: 3.6574406809362014. [I 2022-04-07 02:28:15,670] Trial 9 finished with value: 3.6557832249966506 and parameters: {'max_depth': 8, 'n um_leaves': 128, 'min_data_in_leaf': 28, 'min_child_weight': 18.712065960638746, 'feature_fraction': 0.56886132 00905298, 'bagging_fraction': 0.7775705635193393, 'min_split_gain': 1.348505568825985, 'reg_alpha': 7.474796380 8521245, 'reg_lambda': 3.597114670480944}. Best is trial 9 with value: 3.6557832249966506. [I 2022-04-07 02:36:10,408] Trial 10 finished with value: 3.658582587846033 and parameters: {'max_depth': 9, 'n um_leaves': 106, 'min_data_in_leaf': 43, 'min_child_weight': 12.7634358361123, 'feature_fraction': 0.6793235328 878287, 'bagging_fraction': 0.6715660608010557, 'min_split_gain': 9.465408406844215, 'reg_alpha': 7.70764142279 8685, 'reg_lambda': 0.06895362504385805}. Best is trial 9 with value: 3.6557832249966506. [I 2022-04-07 02:45:49,664] Trial 11 finished with value: 3.657962875779366 and parameters: {'max_depth': 9, 'n um_leaves': 37, 'min_data_in_leaf': 47, 'min_child_weight': 29.73267330437201, 'feature_fraction': 0.7700104545 097888, 'bagging_fraction': 0.9990589411241023, 'min_split_gain': 0.39769147902561297, 'reg_alpha': 9.984417672 011926, 'reg_lambda': 7.129707869325249}. Best is trial 9 with value: 3.6557832249966506. [I 2022-04-07 02:56:14,514] Trial 12 finished with value: 3.6560084785763785 and parameters: {'max_depth': 6, 'num_leaves': 52, 'min_data_in_leaf': 64, 'min_child_weight': 26.167439606538956, 'feature fraction': 0.368875 73276598606, 'bagging_fraction': 0.7975711598497612, 'min_split_gain': 1.8368667966461514, 'reg_alpha': 8.18813 552385062, 'reg_lambda': 3.4181327302114215}. Best is trial 9 with value: 3.6557832249966506. [I 2022-04-07 03:02:02,355] Trial 13 finished with value: 3.6558622632283373 and parameters: {'max_depth': 6, 'num_leaves': 60, 'min_data_in_leaf': 64, 'min_child_weight': 16.499103534101472, 'feature_fraction': 0.393610 719209942, 'bagging_fraction': 0.6475390952499872, 'min_split_gain': 1.6693583942874644, 'reg_alpha': 7.9229501 90857678, 'reg_lambda': 3.360524687295772}. Best is trial 9 with value: 3.6557832249966506. [I 2022-04-07 03:11:58,696] Trial 14 finished with value: 3.659372400334074 and parameters: {'max_depth': 12, 'num_leaves': 62, 'min_data_in_leaf': 29, 'min_child_weight': 17.087599310358023, 'feature_fraction': 0.308332 0076825721, 'bagging_fraction': 0.6368495205157543, 'min_split_gain': 0.04083347943075921, 'reg_alpha': 7.01336 8742462264, 'reg_lambda': 1.6512446030953574}. Best is trial 9 with value: 3.6557832249966506. [I 2022-04-07 03:21:26,572] Trial 15 finished with value: 3.658863713345061 and parameters: {'max_depth': 7, 'n um_leaves': 95, 'min_data_in_leaf': 42, 'min_child_weight': 11.529503798106507, 'feature_fraction': 0.278697952 0577261, 'bagging_fraction': 0.5576345885858514, 'min_split_gain': 2.0598778444750665, 'reg_alpha': 6.126715632 617882, 'reg_lambda': 4.3855034044905485}. Best is trial 9 with value: 3.6557832249966506. [I 2022-04-07 03:31:40,817] Trial 16 finished with value: 3.670509939142782 and parameters: {'max_depth': 3, 'n um_leaves': 22, 'min_data_in_leaf': 28, 'min_child_weight': 14.75491911647246, 'feature_fraction': 0.6814024308 355047, 'bagging_fraction': 0.7533163414910654, 'min_split_gain': 8.576141864288697, 'reg_alpha': 8.44372803353 525, 'reg_lambda': 3.8264756089796728}. Best is trial 9 with value: 3.6557832249966506. [I 2022-04-07 03:39:06,274] Trial 17 finished with value: 3.6631446808868633 and parameters: {'max_depth': 11, 'num_leaves': 90, 'min_data_in_leaf': 14, 'min_child_weight': 7.8857898799835, 'feature_fraction': 0.457415185 2978893, 'bagging_fraction': 0.5172766626730054, 'min_split_gain': 2.0791580181573965, 'reg_alpha': 6.848048132 38946, 'reg_lambda': 1.8005027088613534}. Best is trial 9 with value: 3.6557832249966506. [I 2022-04-07 03:46:34,076] Trial 18 finished with value: 3.6550641942500763 and parameters: {'max_depth': 6, 'num_leaves': 108, 'min_data_in_leaf': 64, 'min_child_weight': 19.542744175146908, 'feature_fraction': 0.64636 94894206278, 'bagging_fraction': 0.6959253014980463, 'min_split_gain': 7.309719954929109, 'reg_alpha': 4.610038 3504763505, 'reg_lambda': 9.827071071570177}. Best is trial 18 with value: 3.6550641942500763. [I 2022-04-07 03:57:33,329] Trial 19 finished with value: 3.6570494402472997 and parameters: {'max_depth': 11, 'num_leaves': 125, 'min_data_in_leaf': 28, 'min_child_weight': 19.72828031110244, 'feature_fraction': 0.656213 0735667374, 'bagging_fraction': 0.8581991424448983, 'min_split_gain': 7.128826954687689, 'reg_alpha': 4.1714822 30038237, 'reg_lambda': 9.206931485860473}. Best is trial 18 with value: 3.6550641942500763. In [19]: b_trial = study.best trial print('RSME : ', b_trial.value) best_params = b_trial.params print("Best Hyperparameters") print('-' * 20) for hyperparameter, value in best params.items(): print(hyperparameter, ' : ', value) RSME : 3.6550641942500763 Best Hyperparameters max depth : 6 num leaves : 108 min data in leaf : 64 min child weight : 19.542744175146908 feature fraction : 0.6463694894206278 bagging fraction : 0.6959253014980463 min_split_gain : 7.309719954929109 reg_alpha : 4.6100383504763505 reg lambda : 9.827071071570177 with open('data/LGB parameters', 'ab') as df file: In [15]: pickle.dump(best_params, df_file) Now the best hyperparameters obtained from Optuna will be used to build the final LightGBM model. with open('data/LGB_parameters', 'rb') as df_file: best params lgb = pickle.load(df file) In [14]: parameters = { 'objective' : 'regression', 'metric' 'metric' : 'rmse',
'boosting_type' : 'gbdt',
'learning_rate' : 0.01,
'device' 'device' : 'cpu', 'n_jobs' : -1, 'verbosity' 'verbosity' : -1,
'random_state' : 9,
'bagging_freq' : 1,
'bagging_seed' : 9, 'max_depth' : best_params_lgb.get('max_depth'),
'num_leaves' : best_params_lgb.get('num_leaves'), 'min_data_in_leaf' : best_params_lgb.get('min_data_in_leaf'), 'min_child_weight' : best_params_lgb.get('min_child_weight'), 'feature_fraction' : best_params_lgb.get('feature_fraction'), 'bagging_fraction' : best_params_lgb.get('bagging_fraction'), 'min_split_gain' : best_params_lgb.get('min_split_gain'), 'reg_alpha' : best_params_lgb.get('reg_alpha'),
'reg_lambda' : best_params_lgb.get('reg_lambda') } In [15]: Y_train_pred_lgb = np.zeros(len(X_train)) lgb_folds = StratifiedKFold(n_splits = 4, shuffle = True, random_state = 9) for fold, (train_idx, val_idx) in enumerate(lgb_folds.split(X_train, Outlier.values)): print("Training for fold {}.........".format(fold + 1)) train_data = lgb.Dataset(X_train.iloc[train_idx], label = Y_train.iloc[train_idx]) val_data = lgb.Dataset(X_train.iloc[val_idx], label = Y_train.iloc[val_idx]) reggressor_LGB = lgb.train(params = parameters, train_set = train_data, valid_sets = [train_data, val_data] num_boost_round = 10000, verbose_eval = 1000, early_stopping_rounds = 500) Y_train_pred_lgb[val_idx] = reggressor_LGB.predict(X_train.iloc[val_idx], num_iteration = reggressor_LGB.be Training for fold 1..... Training until validation scores don't improve for 500 rounds [1000] training's rmse: 3.51008 valid_1's rmse: 3.53725 valid_1's rmse: 3.53775 [2000] training's rmse: 3.39051 Early stopping, best iteration is: [1608] training's rmse: 3.435 valid_1's rmse: 3.53617 Training for fold 2..... Training until validation scores don't improve for 500 rounds [1000] training's rmse: 3.44442 valid_1's rmse: 3.72588 Early stopping, best iteration is: [1038] training's rmse: 3.43916 valid_1's rmse: 3.72561 Training for fold 3..... Training until validation scores don't improve for 500 rounds [1000] training's rmse: 3.45567 valid_1's rmse: 3.68775 Early stopping, best iteration is: [1229] training's rmse: 3.42736 valid_1's rmse: 3.68719 Training for fold 4..... Training until validation scores don't improve for 500 rounds [1000] training's rmse: 3.46697 valid_1's rmse: 3.67038 [2000] training's rmse: 3.35138 valid_1's rmse: 3.66958 Early stopping, best iteration is: valid_1's rmse: 3.66851 [1514] training's rmse: 3.40552 In [16]: rsme_lgb = np.sqrt(mean_squared_error(Y_train, Y_train_pred_lgb)) print("RSME score for LGBM model: ", rsme_lgb) RSME score for LGBM model: 3.6550641942500763 The LightGBM model with RSME score of 3.6551 is the best of all the models with XGBoost not far behind. To improve the RSME score even more, we will use stacked models of LightGBM and XGBoost with different weightage. Stacked Model We will use different weightage for the XGBoost and LightGBM models to decide the weightage for our final Stacked model. In [17]: for i in range(10,100,10): Y train pred stack = ((i / 100) * Y train pred xgb) + (((100 - i) / 100) * Y train pred lgb)print("RSME score for Stacked Model with {}% weightage to XGBoost and {}% weightage to LightGBM : {}".forma RSME score for Stacked Model with 10% weightage to XGBoost and 90% weightage to LightGBM: 3.654806730014835 RSME score for Stacked Model with 20% weightage to XGBoost and 80% weightage to LightGBM : 3.6546712326313924 RSME score for Stacked Model with 30% weightage to XGBoost and 70% weightage to LightGBM: 3.6546577156656053 RSME score for Stacked Model with 40% weightage to XGBoost and 60% weightage to LightGBM: 3.6547661804708893 RSME score for Stacked Model with 50% weightage to XGBoost and 50% weightage to LightGBM: 3.6549966161875393 RSME score for Stacked Model with 60% weightage to XGBoost and 40% weightage to LightGBM: 3.6553489997481643 RSME score for Stacked Model with 70% weightage to XGBoost and 30% weightage to LightGBM: 3.655823295889232 RSME score for Stacked Model with 80% weightage to XGBoost and 20% weightage to LightGBM: 3.656419457168701 RSME score for Stacked Model with 90% weightage to XGBoost and 10% weightage to LightGBM: 3.657137423989734 In [26]: rsme_stack = np.sqrt(mean_squared_error(Y_train, ((0.3 * Y_train_pred_xgb) + (0.7 * Y_train_pred_lgb)))) print("RSME score for Stacked model: ", rsme_stack) RSME score for Stacked model: 3.6546577156656053 The Stacked Model with 30% weightage to XGBoost and 70% weightage to LightGBM provides a small improvement in RSME score from our previous best of LightGBM. Stacked Model using Meta Learner Now we will build another Stacked model but with a meta learner and see if it is better than the rest of our models. We will be using Ridge Regressor with predictions of XGBoost and LightGBM as input and the Y train as target values. In [19]: meta_train = np.vstack([Y_train_pred_xgb, Y_train_pred_lgb]).transpose() In [20]: meta_model = Ridge() parameters = {"alpha" : [0.0001, 0.001, 0.01,0.1, 1.0]} meta_folds = StratifiedKFold(n_splits = 3, random_state = 9, shuffle = True).split(meta_train, Outlier.values) regressor_meta = GridSearchCV(meta_model, parameters, cv = meta_folds, scoring = 'neg_mean_squared_error',) In [21]: regressor_meta.fit(meta_train, Y_train) GridSearchCV(cv=<generator object _BaseKFold.split at 0x000001F5627BB300>, Out[21]: estimator=Ridge(), param_grid={'alpha': [0.0001, 0.001, 0.01, 0.1, 1.0]}, scoring='neg_mean_squared_error') In [22]: best_params = regressor_meta.best_params_ print("Best Hyperparameters") print('-' * 20) for hyperparameter, value in best_params.items(): print(hyperparameter, ' : ', value) Best Hyperparameters _____ alpha : 1.0 In [24]: Y_train_pred_meta = np.zeros(len(meta_train)) meta_folds = StratifiedKFold(n_splits = 4, random_state = 9, shuffle = True) for fold, (train_idx, val_idx) in enumerate(meta_folds.split(meta_train, Outlier.values)): print("Training for fold {}........".format(fold + 1)) regressor_meta = Ridge(alpha = 1.0) regressor_meta.fit(meta_train[train_idx], Y_train.iloc[train_idx].values) Y train pred_meta[val_idx] = regressor_meta.predict(meta_train[val_idx]) Training for fold 1..... Training for fold 2..... Training for fold 3..... Training for fold 4..... In [25]: rsme_meta_stack = np.sqrt(mean_squared_error(Y_train, Y_train_pred_meta)) print("RSME score for Stacked model with Meta Learner: ", rsme_meta_stack) RSME score for Stacked model with Meta Learner: 3.654871417535515 The Meta Leaner Stacked model with RSME score of 3.6548 has performed little better than LightGBM but poorly compared to Weighted Stacked models. Final RSME Scores of all Models In [27]: myTable = PrettyTable(["Model", "RSME Score"]) mvTable.add row(["Baseline", rsme baseline]) myTable.add row(["KNNRegressor", rsme knn]) myTable.add row(["XGBoost", rsme xgb]) myTable.add row(["LightGBM", rsme lgb]) myTable.add row(["Simple Stacked", rsme stack]) myTable.add_row(["Meta-learner Stacked", rsme_meta_stack]) print(myTable) +----+ Model | RSME Score | +----+ Baseline | 3.850440680607971 | KNNRegressor | 3.824844001316022 XGBoost | 3.6579771246304467 | LightGBM | 3.6550641942500763 | LightGBM | 3.6550641942500763 | Simple Stacked | 3.6546577156656053 | | Meta-learner Stacked | 3.654871417535515 | **Submission** In [28]: with open('data/XGB_parameters', 'rb') as df file: best_params_xgb = pickle.load(df_file) In [29]: with open('data/LGB_parameters', 'rb') as df file: best_params_lgb = pickle.load(df_file) In [30]: def predict(X_train, Y_train, X_test, Outlier, param, num_splits = 4, num_round = 10000, model = 'lgb'): '''This function predicts and returns the target value of test data by training model on train data. It takes X train, X test and Y train as dataframe, parameters for model as dictionary, number of boosting rounds for model and whether to train LightGBM or XGBoost model as string."" Y_test_pred = np.zeros(len(X_test)) folds = StratifiedKFold(n splits = num splits, shuffle = True, random state = 9) if model == 'lgb': parameters = { 'objective' : 'regression', 'metric' : 'rmse',
'boosting_type' : 'gbdt',
'learning_rst' 'learning_rate' : 0.01, 'device' 'n_jobs' 'verbose' 'random_state' 'bagging_freq' 'bagging_seed' : 9,
'max_depth' : param.get('max_depth'),
'num_leaves' : param.get('num_leaves') : param.get('num leaves'), 'min data in leaf' : param.get('min data in leaf'), 'min child weight' : param.get('min child weight'), 'feature_fraction' : param.get('feature_fraction'), 'bagging_fraction' : param.get('bagging_fraction'), 'min_split_gain' : param.get('min_split_gain'),
'reg_alpha' : param.get('reg_alpha'),
'reg_lambda' : param.get('reg_lambda') for fold, (train idx, val idx) in enumerate(folds.split(X_train, Outlier.values)): train_data = lgb.Dataset(X_train.iloc[train_idx], label = Y_train.iloc[train_idx]) val data = lgb.Dataset(X train.iloc[val_idx], label = Y_train.iloc[val_idx]) reggressor LGB = lgb.train(params = parameters, train set = train data, valid sets = [train data, v num boost round = num round, early stopping rounds = 500, verbose eval = Fa Y_test_pred += (reggressor_LGB.predict(X_test, num_iteration = reggressor_LGB.best_iteration) / num return Y test pred elif model == 'xgb': parameters = { 'objective' : 'reg:squarederror', 'learning_rate' : 0.01, 'eval_metric' : 'rmse', tree_method' 'gpu_hist', : 'gpu_predictor', 'predictor' 'random state' 'max depth' : param.get('subsample'), 'subsample' 'colsample_bytree' : param.get('colsample_bytree'),
'min_split_loss' : param.get('min_split_loss'), 'min_child_weight' : param.get('min_child_weight'), : param.get('reg_alpha'), 'reg_alpha' : param.get('reg lambda') 'reg_lambda' for fold, (train idx, val idx) in enumerate(folds.split(X train, Outlier.values)): train_data = xgb.DMatrix(X_train.iloc[train_idx], label = Y_train.iloc[train_idx]) val data = xgb.DMatrix(X train.iloc[val idx], label = Y train.iloc[val idx]) reggressor_XGB = xgb.train(params = parameters, dtrain = train_data, evals = [(train_data, 'train'), (val_data, 'eval')], num_boost_round = n early_stopping_rounds = 500, verbose eval = False) Y test pred += (reggressor XGB.predict(xgb.DMatrix(X test), iteration_range = (0, reggressor_XGB.best_iteration)) / num_ return Y test pred In [31]: Y_test_pred_xgb = predict(X_train, Y_train, X_test, Outlier, best_params_xgb, model = 'xgb') In [32]: sub_xgb = pd.DataFrame({"card_id":test["card id"].values}) sub xgb["target"] = Y test pred xgb sub xgb.to csv("data/submit xgb.csv", index = False) XGBoost Model Kaggle Score In [33]: Y_test_pred_lgb = predict(X_train, Y_train, X_test, Outlier, best params lgb, model = 'lgb') In [34]: sub_lgb = pd.DataFrame({"card id":test["card id"].values}) sub_lgb["target"] = Y_test_pred_lgb sub lgb.to csv("data/submit lgb.csv", index = False) LightGBM Model Kaggle Score In [35]: Y_test_pred_stack = (0.1 * Y_test_pred_xgb) + (0.9 * Y_test_pred_lgb) In [36]: sub_stack = pd.DataFrame({"card_id":test["card id"].values}) sub_stack["target"] = Y_test_pred_stack sub stack.to csv("data/submit stack.csv", index = False) Stacked Model Kaggle Score In [37]: meta_train = np.vstack([Y_train_pred_xgb, Y_train_pred_lgb]).transpose() meta_test = np.vstack([Y_test_pred_xgb, Y_test_pred_lgb]).transpose() In [40]: Y_train_pred_meta = np.zeros(len(meta_train)) Y_test_pred_meta = np.zeros(len(meta_test)) meta_folds = StratifiedKFold(n_splits = 4, random_state = 9, shuffle = True) for fold, (train_idx, val_idx) in enumerate(meta_folds.split(meta_train, Outlier.values)): regressor_meta = Ridge(alpha = 1.0) regressor_meta.fit(meta_train[train_idx], Y_train.iloc[train_idx].values) Y_train_pred_meta[val_idx] = regressor_meta.predict(meta_train[val_idx]) Y_test_pred_meta += (regressor_meta.predict(meta_test) / meta_folds.n_splits) In [41]: sub_meta = pd.DataFrame({"card_id":test["card id"].values}) sub meta["target"] = Y test pred meta sub meta.to csv("data/submit meta.csv", index = False) Meta Learner Stacked Model Kaggle Score