train_recall 0.225 (+/- 0.012) 0.649 (+/- 0.005) test_precision 0.223 (+/- 0.009) 0.378 (+/- 0.007) **train_precision** 0.226 (+/- 0.009) 0.381 (+/- 0.003) 0.477 (+/- 0.009) **test_f1** 0.225 (+/- 0.009) **train_f1** 0.225 (+/- 0.010) 0.480 (+/- 0.003) test_average_precision 0.224 (+/- 0.001) 0.507 (+/- 0.016) 0.509 (+/- 0.004) train_average_precision 0.223 (+/- 0.001) # 2. Carry out hyperparameter optimization from sklearn.model selection import RandomizedSearchCV from scipy.stats import loguniform param dist lr = { "logisticregression C": loguniform(1e-3, 1e3), search lr = RandomizedSearchCV(pipe lr, param dist lr, n iter=50, verbose=1, n jobs=-1, return train score=True, scoring="f1", random state=123, search lr.fit(X train, y train); Fitting 5 folds for each of 50 candidates, totalling 250 fits In [24]: search lr.best params Out[24]: {'logisticregression__C': 0.011290431413903904} search_lr.best_score_ Out[25]: 0.47983419889173823 # 3. Report scores results["Tuned Logistic Regression"] = mean_std_cross_val_scores(search_lr.best_estimator_, X_train, y_train, return_train_score=True, scoring=scor pd.DataFrame(results) **Dummy Logistic Regression Tuned Logistic Regression fit_time** 0.001 (+/- 0.000) 0.324 (+/- 0.061) 0.068 (+/- 0.005) score_time 0.004 (+/- 0.000) 0.013 (+/- 0.002) 0.012 (+/- 0.002) test_accuracy 0.650 (+/- 0.005) 0.683 (+/- 0.007) 0.689 (+/- 0.007) **train_accuracy** 0.655 (+/- 0.004) 0.686 (+/- 0.003) 0.690 (+/- 0.003) **test_recall** 0.227 (+/- 0.010) 0.646 (+/- 0.021) 0.642 (+/- 0.021) **train_recall** 0.225 (+/- 0.012) 0.649 (+/- 0.005) 0.643 (+/- 0.004) test_precision 0.223 (+/- 0.009) 0.378 (+/- 0.007) 0.383 (+/- 0.008) **train_precision** 0.226 (+/- 0.009) 0.381 (+/- 0.003) 0.384 (+/- 0.004) test_f1 0.225 (+/- 0.009) 0.477 (+/- 0.009) 0.480 (+/- 0.009) **train_f1** 0.225 (+/- 0.010) 0.480 (+/- 0.003) 0.481 (+/- 0.004) test_average_precision 0.224 (+/- 0.001) 0.507 (+/- 0.016) 0.507 (+/- 0.015) 0.509 (+/- 0.004) 0.508 (+/- 0.004) train_average_precision 0.223 (+/- 0.001) Summarize the results: • The best hyperparameter found by our random search is C = 0.01 with a validation f1-score of • The tuned logistic regression model seems to not improve much compared to the model without hyperparameter optimization. In fact, recall decreases a bit while accuracy, precision, and f1 slightly increase. 8. Different models rubric={accuracy:10,reasoning:6} Your tasks: 1. Try at least 3 other models aside from a linear model. 2. Summarize your results in terms of overfitting/underfitting and fit and score times. Can you beat a linear model? **Answer:** from sklearn.ensemble import RandomForestClassifier from sklearn.neighbors import KNeighborsClassifier from lightgbm.sklearn import LGBMClassifier pipe_rf = make_pipeline(preprocessor, RandomForestClassifier(class_weight="balanced", pipe_knn = make_pipeline(preprocessor, KNeighborsClassifier()) pipe_lgbm = make_pipeline(preprocessor, LGBMClassifier(class_weight="balanced", randor models = { "Random Forest": pipe rf, "KNN": pipe_knn, "LightGBM": pipe_lgbm for (name, model) in models.items(): results[name] = mean_std_cross_val_scores(model, X_train, y_train, return_train_score=True, scoring=scoring pd.DataFrame(results) **Tuned Logistic** Logistic Random KNN **Dummy** LightGBM **Forest** Regression Regression 0.001 (+/-0.324 (+/-2.706 (+/-0.017 (+/-0.187 (+/-0.068 (+/- 0.005) fit_time 0.000)0.061) 0.004) 0.013) 0.034) 0.132 (+/-0.004 (+/-0.013 (+/-2.457 (+/-0.027 (+/score_time 0.012 (+/- 0.002) 0.000)0.002) 0.003)0.198) 0.001) 0.793 (+/-0.650 (+/-0.683 (+/-0.814 (+/-0.765 (+/-0.689 (+/- 0.007) test_accuracy 0.005) 0.007) 0.005)0.005)0.0070.655 (+/-0.686 (+/-0.999 (+/-0.844 (+/-0.824 (+/train_accuracy 0.690 (+/- 0.003) 0.003)0.004)0.000)0.001) 0.003) 0.615 (+/-0.227 (+/-0.646 (+/-0.348 (+/-0.355 (+/test_recall 0.642 (+/- 0.021) 0.021) 0.010)0.013)0.012)0.014) 0.649 (+/-0.775 (+/-0.225 (+/-1.000 (+/-0.471 (+/train_recall 0.643 (+/- 0.004) 0.012)0.005) 0.000)0.004)0.009)0.223 (+/-0.378 (+/-0.659 (+/-0.559 (+/-0.480 (+/-0.383 (+/- 0.008) test_precision 0.009)0.007) 0.017) 0.024) 0.012) 0.226 (+/-0.381 (+/-0.997 (+/-0.733 (+/-0.580 (+/train_precision 0.384 (+/- 0.004) 0.003) 0.000) 0.009)0.004)0.005) 0.477 (+/-0.225 (+/-0.455 (+/-0.434 (+/-0.539 (+/test_f1 0.480 (+/- 0.009) 0.009)0.009)0.013) 0.015) 0.013) 0.225 (+/-0.480 (+/-0.998 (+/-0.573 (+/-0.664 (+/train_f1 0.481 (+/- 0.004) 0.010) 0.003) 0.000)0.003) 0.004)0.224 (+/-0.507 (+/-0.541 (+/-0.418 (+/-0.562 (+/test_average_precision 0.507 (+/- 0.015) 0.001) 0.016) 0.017) 0.0090.019) 0.223 (+/-0.509 (+/-1.000 (+/-0.739 (+/-0.643 (+/-0.508 (+/- 0.004) train_average_precision 0.004)0.000) 0.003) 0.001) 0.004)Summarize the results: Regardin score, LightGBM has the highest validation f1 score while KNN has the lowest. Hence, we can see that not all non-linear model can beat the linear model. Regarding overfitting/ underfitting, Random Forest is overfitting badly. • Regarding fit and score time, most models are quite quick, except Random Forest takes a while to fit and KNN takes a while to score. Overall, LightGBM is the best performing model as it achieves the best score, is fast, and does not overfit/underfit. (Optional) 9. Feature selection rubric={reasoning:1} Your tasks: Make some attempts to select relevant features. You may try RFECV, forward selection or L1 regularization for this. Do the results improve with feature selection? Summarize your results. If you see improvements in the results, keep feature selection in your pipeline. If not, you may abandon it in the next exercises. Hyperparameter optimization rubric={accuracy:6,reasoning:4} Your tasks: Make some attempts to optimize hyperparameters for the models you've tried and summarize your results. In at least one case you should be optimizing multiple hyperparameters for a single model. You may use sklearn 's methods for hyperparameter optimization or fancier Bayesian optimization methods. GridSearchCV RandomizedSearchCV scikit-optimize Answer: We will perform hyperparameter optimization on the best-performing model LightGBM. import numpy as np param_dist_lgbm = { "lgbmclassifier__max_depth": np.arange(1, 20, 2), "lgbmclassifier__num_leaves": np.arange(20, 80, 5), "lgbmclassifier max bin": np.arange(200, 300, 20), search lgbm = RandomizedSearchCV(pipe lgbm, param_dist_lgbm, n iter=50, verbose=1, n jobs=-1, return_train_score=True, scoring="f1", random state=123, search_lgbm.fit(X_train, y_train); Fitting 5 folds for each of 50 candidates, totalling 250 fits results["Tuned LGBMClassification"] = mean std cross val scores(search_lgbm.best_estimator_, X_train, y_train, return_train_score=True, scoring=sc pd.DataFrame(results) Tuned Random Logistic Tune LightGBM Dummy Logistic KNN **LGBMClassificatio** Regression **Forest** Regression 0.001 2.706 0.017 0.187 (+/-0.324 (+/-0.068 (+/fit_time (+/-(+/-(+/-0.133 (+/- 0.003 0.061) 0.005)0.013)0.000)0.034) 0.004)0.004 0.132 2.457 0.013 (+/-0.027 (+/-0.012 (+/-(+/score_time 0.022 (+/- 0.001 (+/-(+/-0.002)0.002)0.001) 0.000)0.003) 0.198)0.650 0.814 0.793 0.683 (+/-0.689 (+/-0.765 (+/test_accuracy (+/-(+/-(+/-0.768 (+/- 0.008 0.007)0.007)0.0070.005) 0.005) 0.005) 0.655 0.999 0.844 0.686 (+/-0.690 (+/-0.824 (+/-0.801 (+/- 0.004 train_accuracy (+/-(+/-(+/-0.003) 0.003) 0.003) 0.004)0.000) 0.001)0.355 0.227 0.348 0.646 (+/-0.642 (+/-0.615 (+/test_recall 0.625 (+/- 0.016 (+/-(+/-(+/-0.021)0.021) 0.014)0.010) 0.013) 0.012)0.225 1.000 0.471 0.649 (+/-0.643 (+/-0.775 (+/train_recall (+/-(+/-0.698 (+/- 0.006 (+/-0.004)0.005)0.009)0.012)0.000) 0.004) 0.559 0.223 0.659 0.378 (+/-0.383 (+/-0.480 (+/-(+/test_precision 0.485 (+/- 0.014 (+/-(+/-0.007)0.008)0.012) 0.009) 0.024) 0.017) 0.226 0.997 0.733 0.381 (+/-0.384 (+/-0.580 (+/-0.543 (+/- 0.008 train_precision (+/-(+/-(+/-0.003) 0.004)0.005) 0.000) 0.009)0.004)0.225 0.455 0.434 0.477 (+/-0.480 (+/-0.539 (+/-0.546 (+/- 0.014 test_f1 (+/-(+/-(+/-0.009)0.009)0.013) 0.009)0.015) 0.013) 0.573 0.225 0.998 0.480 (+/-0.664 (+/-0.481 (+/-0.611 (+/- 0.005 train_f1 (+/-(+/-(+/-0.003)0.004)0.004)0.010) 0.000) 0.003)0.541 0.224 0.418 0.507 (+/-0.507 (+/-0.562 (+/test_average_precision (+/-(+/-0.567 (+/- 0.019 (+/-0.016) 0.015) 0.019) 0.017) 0.009) 0.001) 1.000 0.223 0.643 0.509 (+/-0.508 (+/-0.739 (+/-0.677 (+/- 0.005 train_average_precision (+/-(+/-(+/-0.004)0.004)0.003)0.001) 0.000) 0.004) search lgbm.best params {'lgbmclassifier__num_leaves': 60,
'lgbmclassifier__max_depth': 5, 'lgbmclassifier max bin': 240} search lgbm.best score Out[32]: 0.5459147030871935 The best hyperparameters found by our random search are: num_leaves = 0.01129, max_depth=5, max_bin=240 with a validation f1-score of 0.546. 11. Interpretation and feature importances rubric={accuracy:6,reasoning:4} Your tasks: 1. Use the methods we saw in class (e.g., eli5, shap), or any other methods of your choice, to examine the most important features of one of the non-linear models. 2. Summarize your observations. Answer: import shap In [34]: preprocessor.fit(X_train, y_train) ohe feature names = (preprocessor .named transformers ["pipeline-3"] .named steps["onehotencoder"] .get feature names out(categorical features) .tolist() feature names = numeric features + binary features + ohe feature names X_train_enc = pd.DataFrame(data=preprocessor.transform(X train), columns=feature names, index=X train.index, X_train_enc.head() BILL_AMT1 PAY_AMT4 BILL_AMT5 BILL_AMT2 PAY_AMT3 LIMIT_BAL PAY_6 PAY_AMT2 16395 -0.300665 -0.114944 -0.494781 -0.293394 -0.234603 1.168355 0.257059 -0.040229 6.785208 0.257059 21448 -0.685307 -0.113778 1.805461 -0.679495 2.090017 3.739796 20034 -0.696132 -0.309323 -0.661045 -0.688319 -0.289017 -0.060527 -1.485154 -0.270403 25755 -0.113843 0.752583 0.687456 0.501203 -0.060260 -0.367748 0.257059 -0.018028 -0.040230 1438 -0.212134 -0.204599 -0.031399 -0.223720 -0.905384 0.257059 -0.206185 5 rows × 32 columns X test enc = pd.DataFrame(data=preprocessor.transform(X test), columns=feature names, index=X test.index, X test enc.head() BILL_AMT2 PAY_AMT3 PAY_AMT2 BILL_AMT1 PAY_AMT4 BILL_AMT5 LIMIT_BAL PAY_6 25665 -0.301142 1.140290 0.058763 -0.346448 -0.289017 -0.982189 0.257059 -0.224533 16464 0.334336 -0.205460 0.162513 0.293371 -0.180189 -0.674969 0.257059 -0.173801 22386 1.427002 0.532986 2.086523 1.536341 -0.289017 0.016278 1.999273 0.027750 10149 -0.374955 -0.309323 -0.660751 -0.677772 -0.289017 0.246693 -1.485154 -0.270403 -0.506842 -0.584044 -0.287229 -0.575543 -0.271006 -0.905384 -0.217653 8729 0.257059 5 rows × 32 columns pipe lgbm.fit(X_train, y_train); lgbm_explainer = shap.TreeExplainer(pipe_lgbm.named_steps["lgbmclassifier"]) train lgbm shap values = lgbm explainer.shap values(X train enc) LightGBM binary classifier with TreeExplainer shap values output has changed to a list # We are only extracting shapely values for the first 100 test examples for speed. test_lgbm_shap_values = lgbm_explainer.shap_values(X_test_enc[:100]) In [40]: shap.initjs() (js) In [41]: shap.summary plot(train lgbm shap values, X train enc) PAY_1 LIMIT_BAL BILL_AMT1 PAY AMT2 PAY_AMT1 PAY AMT3 PAY_2 PAY AMT4 PAY_3 PAY_6 PAY_5 PAY AMT5 MARRIAGE 2 BILL AMT2 BILL AMT3 PAY_4 SEX PAY AMT6 AGE Class 0 BILL AMT6 Class 1 1.0 0.2 0.4 0.6 0.8 mean(|SHAP value|) (average impact on model output magnitude) **Summary of Observations:** The plot shows global feature importances, where the features are ranked in descending order of feature importances. Colour shows the class of feature (red for default payment and blue for non-default payment) PAY_1 is likely the most important feature while BILL_AMT6 is likely the least important one. 12. Results on the test set rubric={accuracy:6,reasoning:4} Your tasks: 1. Try your best performing model on the test data and report test scores. 2. Do the test scores agree with the validation scores from before? To what extent do you trust your results? Do you think you've had issues with optimization bias? 3. Take one or two test predictions and explain them with SHAP force plots. **Answer:** 1. Try on test data and report test scores. In [42]: best lgbm = search lgbm.best estimator In [43]: best lgbm.predict(X test) Out[43]: array([0, 0, 1, ..., 1, 1, 1]) In [44]: f1 score(y test,best lgbm.predict(X test)) Out[44]: 0.5299528831052278 1. The test score agrees with the validation score from Section 10. I would trust the result because the test score of 0.53 is just slightly lower than validation score of 0.546. Therefore, I think there's no issue with optimization bias in this case. 1. Test predictions and explain with SHAP force plots. In [45]: X train enc = X train enc.round(3) X_test_enc = X_test_enc.round(3) In [46]: shap.force plot(lgbm explainer.expected value[1], test_lgbm_shap_values[1][31,:], X test enc.iloc[31, :], matplotlib=True, base value 0.15 PAY 5 = 3.75 PAY AMT2 = -0.27 PAY 3 = 5.16 PAY 6 = 2.87 $PAY_1 = 7.154$ BILL_AMT1 = 1.03 PAY_2 = 5.975 $PAY_4 = 4.472$ The raw model score is higher than the base value so the prediction is default (1) because this example was pushed higher by all the factors shown in red such as PAY_1, PAY_6. Meanwhile, PAY_4, BILL_AMT1 are pushing the prediction towards lower score. In [47]: shap.force plot(lgbm explainer.expected value[1], test lgbm shap values[1][6,:], X test enc.iloc[6, :], matplotlib=True, higher f(x) base value -0.55 -0.4 -0.2 PAY_AMT2 = -0.211 PAY_AMT1 = -0.252 LIMIT_BAL = -0.905 BILL AMT1 = -0.352 PAY 1 = 0.014• The raw model score is lower than the base value so the prediction is non-default (0) because this example was pushed lower by all the factors shown in blue such as PAY_1, BILL_AMT1. • Meanwhile, LIMIT_BAL, PAY_AMT2 are pushing the prediction towards higher score. 13. Summary of results rubric={reasoning:12} Imagine that you want to present the summary of these results to your boss and co-workers. Your tasks: 1. Create a table summarizing important results. 2. Write concluding remarks. 3. Discuss other ideas that you did not try but could potentially improve the performance/interpretability. 4. Report your final test score along with the metric you used at the top of this notebook in the Submission instructions section. Answer: 1. Summary Table In [48]: models = { "Dummy": dummy_model, "Logistic Regression": pipe lr, "Tuned Logistic Regression": search lr.best estimator , "Random Forest": pipe rf, "KNN": pipe knn, "LGBM": pipe lgbm, "Best LightGBM": best lgbm important scores = ["f1"] final result={} for (name, model) in models.items(): final_result[name] = mean_std_cross_val_scores(model, X_train, y_train, return train score=True, scoring=important scores pd.DataFrame(final result) **Tuned Logistic** Logistic Random **Best KNN LGBM Dummy** LightGBM Regression Regression Forest 0.003 (+/-0.016 (+/-0.167 (+/-0.269 (+/-2.665 (+/-0.230 (+/fit_time 0.065 (+/- 0.004) 0.003) 0.001) 0.021) 0.054)0.076)0.024) 1.248 (+/-0.002 (+/-0.005 (+/-0.064 (+/-0.012 (+/-0.010 (+/score_time 0.005 (+/- 0.000) 0.001) 0.000)0.001) 0.121) 0.001) 0.001) 0.221 (+/-0.477 (+/-0.539 (+/-0.546 (+/-0.455 (+/-0.434 (+/test_f1 0.480 (+/- 0.009) 0.016) 0.013) 0.009)0.015) 0.013) 0.014) 0.225 (+/-0.480 (+/-0.998 (+/-0.573 (+/-0.664 (+/-0.611 (+/train_f1 0.481 (+/- 0.004) 0.003)0.004)0.005) 0.005) 0.000)0.003)1. Concluding remarks: Best and worst performing models: With default hyperparameters for all models, the LGBM model seems to be performing best, whereas KNN seems to be performing worst. With hyper parameters optimization, the best hyperparameters found by our random search for LGBM model are: num_leaves = 0.01129, max_depth=5, max_bin=240 with a validation f1-score of 0.546. Overfitting/underfitting: Random Forest model seems to overfit; the training score is high and the gap between train and validation score f1 is big compared to other models. (Of course, our baseline model, dummy regressor, is also underfitting.) All other models seem to underfit; the training score is low and the gap between train and validation score is not that big. Fit time Random Forest model is much slower compared to other models. KNN performs worst but it fits much faster than other models. Score time Scoring is fast for almost all models except KNN. · Stability of scores The scores look more or less stable with std in the range 0.009 to 0.016 for f1 score. 1. Due to time limit, there are shortcomings in our mini project; hence the f1 score of the best model is not quite satisfactory. If we are able to try different models (such as SVC, SVM, tree models) and implement feature engineering such as polinomial, it is possible that we can improve the performance/interpretability of this project. 1. TEST SCORE: 0.53, METRIC: F1 (Optional) 14. Creating a data analysis pipeline rubric={reasoning:2} Your tasks: • In 522 you learned how build a reproducible data analysis pipeline. Convert this notebook into scripts and create a reproducible data analysis pipeline with appropriate documentation. (Optional) 15. Your takeaway from the course rubric={reasoning:1} Your tasks: What is your biggest takeaway from this course? Answer: The biggest takeaway of our group from this course is: To define and use evaluation metrics for classification and regression, • To learn the importance of feature engineering in building machine learning models. • To learn the importance of interpretability in Machine Learning. PLEASE READ BEFORE YOU SUBMIT: When you are ready to submit your assignment do the following: 1. Run all cells in your notebook to make sure there are no errors by doing Kernel -> Restart Kernel and Clear All Outputs and then Run -> Run All Cells. 2. Notebooks with cell execution numbers out of order or not starting from "1" will have marks deducted. Notebooks without the output displayed may not be graded at all (because we need to see the output in order to grade your work). 3. Push all your work to your GitHub lab repository. 4. Upload the assignment using Gradescope's drag and drop tool. Check out this Gradescope Student Guide if you need help with Gradescope submission. 5. Make sure that the plots and output are rendered properly in your submitted file. If the .ipynb file is too big and doesn't render on Gradescope, also upload a pdf or html in addition to the .ipynb so that the TAs can view your submission on Gradescope. Well done!! Have a great weekend! from IPython.display import Image Image("eva-well-done.png")