fd001-regression

June 14, 2024

1 Predictive Maintenance of Turbofan Jet Engine: Remaining Useful Life Regression

Here we will be evaluating a few models for the regression of remaining useful life. The results will be compared to the baseline model below: - RMSE against Test Set: 22.3685 - MAE against Test Set: 17.8900

Once we have choose the best model, we will further evaluate it on the test set and compare with the given true RUL.

1.1 1. Load FD001 Data

```
[1]: import warnings
warnings.filterwarnings("ignore")

import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

from utils import read_dataset, calculate_RUL
```

```
[2]: train, test, test_rul = read_dataset("FD001")
train.shape, test.shape, test_rul.shape
```

```
[2]: ((20631, 26), (13096, 26), (100,))
```

1.2 2. Build Pipeline

```
[3]: from sklearn.pipeline import Pipeline
from utils import (SENSOR_COLUMNS, LowVarianceFeaturesRemover, ScalePerEngine, 
RollTimeSeries, TSFreshFeaturesExtractor, CustomPCA, 
TSFreshFeaturesSelector, tsfresh_calc)

preprocessing = Pipeline([
    ('drop-low-variance', LowVarianceFeaturesRemover(threshold=0)),
    ('scale-per-engine', ScalePerEngine(n_first_cycles=10, 
Sensors_columns=SENSOR_COLUMNS)),
```

```
→rolling_direction=1)),
         ('extract-tsfresh-features', TSFreshFeaturesExtractor(calc=tsfresh_calc)),
         ('PCA', CustomPCA(n components=20)),
         ('features-selection', TSFreshFeaturesSelector(fdr_level=0.001))
    ])
[4]: train = preprocessing.fit_transform(train)
    Dropped features: ['op_setting_3', 'sensor_1', 'sensor_5', 'sensor_10',
    'sensor_16', 'sensor_18', 'sensor_19']
    Start Rolling TS
                       | 20/20 [00:09<00:00, 2.11it/s]
    Rolling: 100%|
    Done Rolling TS in 0:00:09.924466
    Start Extracting Features
    Feature Extraction: 100%
                                  | 20/20 [06:59<00:00, 20.96s/it]
    Done Extracting Features in 0:07:27.730287
    Dropped 19 duplicate features
    Dropped 14 features with NA values
    Selected 10 out of 20 features: [0, 2, 3, 4, 1, 5, 6, 8, 7, 15]
[5]: train.index = train.index.set_names(['unit', 'time_cycles'])
    print('train shape after pipeline:', train.shape)
    train.head()
    train shape after pipeline: (17731, 10)
[5]:
                              0
                                                  3
                                                            4
                                                                                5
    unit time_cycles
    1.0 30.0
                      -9.621386 -1.371975 5.191464 0.054828 -1.199549 0.844392
         31.0
                      -9.606291 -1.232110 5.135508 0.179561 -1.077269
                                                                         2.018672
         32.0
                     -10.308093 -1.298788 5.198759 -1.302478 -0.891965 1.396961
         33.0
                     -10.131534 -0.869859 5.472415 -0.976122 -0.968814 0.938607
         34.0
                      -9.200284 -1.104652 4.923388 -0.435127 -0.761176 0.046133
                                                7
                             6
                                                           15
    unit time_cycles
                     -0.590629 -2.036566 3.959777 -1.407563
    1.0 30.0
         31.0
                     -0.816393 -2.107204 2.911140 -1.635141
         32.0
                      0.043931 -2.375148
                                          2.345193 -2.681971
         33.0
                      0.085886 -3.012547
                                          3.961745 -2.582504
         34.0
                     -0.009720 -4.006164 4.296591 -2.074314
```

('roll-time-series', RollTimeSeries(min_timeshift=19, max_timeshift=19, __

1.3 3. Split features and target

```
[6]: X_train = train.reset_index().drop(columns=['unit'])

train_units_df = train.index.to_frame(index=False)
y_train = calculate_RUL(train_units_df, upper_threshold=135)
```

1.4 4. Linear Regression

First, let's train a Linear Regression model to evaluate whether all those preprocessing steps actually helps to achieve better performance than our baseline model which is a Linear Regression model without any preprocessing.

```
[7]: from sklearn.linear_model import LinearRegression from sklearn.preprocessing import StandardScaler from sklearn.compose import make_column_selector from utils import CustomGroupKFold, evaluate
```

```
[test] :: root mean squared error : 15.62 +- 0.96
[train] :: root mean squared error : 15.47 +- 0.25
[test] :: mean absolute error : 12.61 +- 0.69
[train] :: mean absolute error : 12.43 +- 0.21
```

We can see that just by implementing our preprocessing pipeline, we were able to improve the performance of Linear Regression model as compared to the baseline model.

1.5 5. SVM (Support Vector Machines)

Since we know that our preprocessing pipeline worked, let's train a SVM model and see if it's better than Linear Regression

```
('model', SVR())
])

svm_cv = evaluate(
    svm,
    X=X_train.values,
    y=y_train,
    groups=train_units_df['unit'],
    cv=CustomGroupKFold(n_splits=5),
)
```

```
[test] :: root mean squared error : 15.82 +- 1.08
[train] :: root mean squared error : 14.54 +- 0.14
[test] :: mean absolute error : 12.23 +- 0.80
[train] :: mean absolute error : 10.71 +- 0.13
```

Nothing significant when comparing SVM result to Linear Regression.

1.6 6. Decision Tree

```
[test] :: root mean squared error : 19.45 +- 0.68 [train] :: root mean squared error : 0.00 +- 0.00 [test] :: mean absolute error : 14.97 +- 0.61 [train] :: mean absolute error : 0.00 +- 0.00
```

Seems like our Decision Tree model is very overfitted and it performs badly during cross-validation.

1.7 7. Random Forest

```
rf_cv = evaluate(
    rf,
    X=X_train.values,
    y=y_train,
    groups=train_units_df['unit'],
    cv=CustomGroupKFold(n_splits=5),
)
```

```
[test] :: root mean squared error : 14.26 +- 0.63
[train] :: root mean squared error : 2.74 +- 0.05
[test] :: mean absolute error : 10.99 +- 0.42
[train] :: mean absolute error : 1.81 +- 0.03
```

Our random forest model is overfitted similar to decision tree. However, it is performing better in cross-validation when compared to SVM and Linear Regression.

1.8 8. XGBoost

```
[test] :: root mean squared error : 14.55 +- 0.41
[train] :: root mean squared error : 4.79 +- 0.13
[test] :: mean absolute error : 11.12 +- 0.25
[train] :: mean absolute error : 3.37 +- 0.08
```

Our XGBoost model is also overfitted. Although XGBoost and Random Forest is performing better than Linear Regression / SVM in cross-validation, we want a model that can generalizes well to new data. For predictive maintenance setting, we would have many operation modes, thus more data and new patterns to learn.

As of right now, Linear Regression or SVM is still the best model in our opinion.

1.9 9. NGBoost

NGBoost stands for Natural Gradient Boosting and it is used for probabilistic prediction. This model is very interesting for us because the biggest problem of single point predictions is that it provides **no uncertainty estimates** of a given prediction.

Thus, we would like to focus on methods that are above to provide **prediction intervals**. One of it is NGBoost that outputs a full probability distribution over the entire outcome space.

```
[iter 0] loss=17.6044 val_loss=0.0000 scale=2.0000 norm=0.9514
[iter 100] loss=5.0638 val_loss=0.0000 scale=2.0000 norm=0.4187
[iter 200] loss=4.3844 val_loss=0.0000 scale=1.0000 norm=0.1767
[iter 300] loss=4.2607 val_loss=0.0000 scale=1.0000 norm=0.1706
[iter 400] loss=4.2061 val loss=0.0000 scale=1.0000 norm=0.1678
[iter 0] loss=17.6165 val_loss=0.0000 scale=2.0000 norm=0.9521
[iter 100] loss=5.1596 val_loss=0.0000 scale=2.0000 norm=0.4242
[iter 200] loss=4.4490 val_loss=0.0000 scale=1.0000 norm=0.1801
[iter 300] loss=4.2569 val loss=0.0000 scale=2.0000 norm=0.3431
[iter 400] loss=4.1923 val_loss=0.0000 scale=1.0000 norm=0.1684
[iter 0] loss=17.6104 val_loss=0.0000 scale=2.0000 norm=0.9517
[iter 100] loss=5.0563 val_loss=0.0000 scale=2.0000 norm=0.4160
[iter 200] loss=4.3719 val loss=0.0000 scale=1.0000 norm=0.1792
[iter 300] loss=4.2300 val_loss=0.0000 scale=1.0000 norm=0.1725
[iter 400] loss=4.1718 val loss=0.0000 scale=2.0000 norm=0.3385
[iter 0] loss=17.6107 val_loss=0.0000 scale=2.0000 norm=0.9517
[iter 100] loss=5.0794 val_loss=0.0000 scale=2.0000 norm=0.4203
[iter 200] loss=4.3860 val loss=0.0000 scale=1.0000 norm=0.1779
[iter 300] loss=4.2266 val_loss=0.0000 scale=1.0000 norm=0.1700
[iter 400] loss=4.1566 val_loss=0.0000 scale=1.0000 norm=0.1659
[iter 0] loss=17.6121 val_loss=0.0000 scale=2.0000 norm=0.9518
[iter 100] loss=5.1213 val loss=0.0000 scale=2.0000 norm=0.4227
[iter 200] loss=4.4319 val_loss=0.0000 scale=1.0000 norm=0.1801
[iter 300] loss=4.3022 val loss=0.0000 scale=1.0000 norm=0.1739
```

```
[iter 400] loss=4.2307 val_loss=0.0000 scale=1.0000 norm=0.1706
[test] :: root mean squared error : 14.09 +- 0.82
[train] :: root mean squared error : 13.11 +- 0.17
[test] :: mean absolute error : 10.82 +- 0.62
[train] :: mean absolute error : 10.21 +- 0.13
```

Wow! The results for NGBoost are amazing. It is not overfitting and yet it still performs better than XGBoost and Random Forest. Thus, we will select NGBoost as our best model and proceed to hyperparameter tuning.

1.10 10. Hyperparameter Tuning

For hyperparameter tuning of the NGBoost model, first let's just try to tune the n_estimators, learning_rate, and minibatch fraction of the NGBoost Regressor.

```
[15]: from sklearn.model selection import GridSearchCV
[16]: param_grid = {
          'minibatch_frac': [1, 0.8, 0.5],
          'n estimators': [100, 200, 300, 400],
          'learning_rate': [0.01, 0.05, 0.1],
      }
      ngb = NGBRegressor(Dist=Poisson)
      grid_search = GridSearchCV(
          estimator=ngb,
          param_grid=param_grid,
          scoring='neg_mean_squared_error',
          n_jobs=-1,
          cv=CustomGroupKFold(n_splits=5),
          verbose=1
      grid_search.fit(X_train.values, y_train, groups=train_units_df['unit'])
     Fitting 5 folds for each of 36 candidates, totalling 180 fits
     [iter 0] loss=17.6108 val_loss=0.0000 scale=2.0000 norm=0.9517
     [iter 100] loss=4.1534 val loss=0.0000 scale=1.0000 norm=0.1667
     [iter 200] loss=4.0524 val_loss=0.0000 scale=1.0000 norm=0.1599
[16]: GridSearchCV(cv=CustomGroupKFold(n_splits=5),
                   estimator=NGBRegressor(Dist=<class
      'ngboost.distns.poisson.Poisson'>,
                                          random_state=RandomState(MT19937) at
      0x1847F83B740),
                   n_jobs=-1,
                   param_grid={'learning_rate': [0.01, 0.05, 0.1],
                               'minibatch_frac': [1, 0.8, 0.5],
```

```
'n_estimators': [100, 200, 300, 400]},
                   scoring='neg_mean_squared_error', verbose=1)
[17]: grid_search.best_params_
[17]: {'learning_rate': 0.05, 'minibatch_frac': 1, 'n_estimators': 300}
     Using the best parameters above, let's now try to find out the best base learner for the NGBoost
     Regressor.
[18]: param_grid = {
          'Base': [
              DecisionTreeRegressor(criterion='friedman_mse', max_depth=4),
              DecisionTreeRegressor(criterion='friedman_mse', max_depth=5,__
       →max_features=0.8, min_samples_leaf=50),
      }
      ngb = NGBRegressor(Dist=Poisson, n_estimators=grid_search.
       ⇔best_params_['n_estimators'], learning_rate=grid_search.
       ⇔best_params_['learning_rate'], minibatch_frac=grid_search.
       ⇔best_params_['minibatch_frac'])
      grid_search = GridSearchCV(
          estimator=ngb,
          param_grid=param_grid,
          scoring='neg_mean_squared_error',
          n_{jobs=-1},
          cv=CustomGroupKFold(n_splits=5),
          verbose=1
      )
      grid_search.fit(X_train.values, y_train, groups=train_units_df['unit'])
     Fitting 5 folds for each of 2 candidates, totalling 10 fits
     [iter 0] loss=17.6108 val loss=0.0000 scale=2.0000 norm=0.9517
     [iter 100] loss=3.8365 val_loss=0.0000 scale=1.0000 norm=0.1399
     [iter 200] loss=3.8045 val_loss=0.0000 scale=0.0312 norm=0.0043
[18]: GridSearchCV(cv=CustomGroupKFold(n_splits=5),
                   estimator=NGBRegressor(Dist=<class
      'ngboost.distns.poisson.Poisson'>,
                                           learning_rate=0.05, minibatch_frac=1,
                                           n estimators=300,
                                           random_state=RandomState(MT19937) at
```

0x1847F83B740),

 $n_{jobs=-1}$,

```
param_grid={'Base':
      [DecisionTreeRegressor(criterion='friedman_mse',
                                                               max_depth=4),
      DecisionTreeRegressor(criterion='friedman_mse',
                                                               max_depth=5,
                                                               max_features=0.8,
                                                               min_samples_leaf=50)]},
                   scoring='neg_mean_squared_error', verbose=1)
[19]: # find out the best base learner
      grid search best params
[19]: {'Base': DecisionTreeRegressor(criterion='friedman_mse', max_depth=5,
      max_features=0.8,
                             min samples leaf=50)}
     Let's use all the best parameters for base learner, learning rate, minibatch frac, and n estimators
     and evaluate the cross-validation.
[27]: ngb_base = DecisionTreeRegressor(criterion='friedman_mse', max_depth=5,__
       →max_features=0.8, min_samples_leaf=50)
      ngb_tuned = NGBRegressor(Dist=Poisson, Base=ngb_base, n_estimators=300,__
       →learning_rate=0.05, minibatch_frac=1)
      ngb_tuned_cv = evaluate(
          ngb_tuned,
          X=X_train.values,
          y=y_train,
          groups=train_units_df['unit'],
          cv=CustomGroupKFold(n splits=5),
      )
     [iter 0] loss=17.6044 val_loss=0.0000 scale=2.0000 norm=0.9514
     [iter 100] loss=3.8102 val loss=0.0000 scale=1.0000 norm=0.1375
     [iter 200] loss=3.7851 val_loss=0.0000 scale=1.0000 norm=0.1354
     [iter 0] loss=17.6165 val loss=0.0000 scale=2.0000 norm=0.9521
     [iter 100] loss=3.8136 val_loss=0.0000 scale=1.0000 norm=0.1376
     [iter 200] loss=3.7792 val_loss=0.0000 scale=1.0000 norm=0.1345
     [iter 0] loss=17.6104 val_loss=0.0000 scale=1.0000 norm=0.4759
     [iter 100] loss=3.8020 val_loss=0.0000 scale=1.0000 norm=0.1385
     [iter 200] loss=3.7614 val_loss=0.0000 scale=1.0000 norm=0.1345
```

[iter 0] loss=17.6107 val_loss=0.0000 scale=2.0000 norm=0.9517 [iter 100] loss=3.8021 val_loss=0.0000 scale=1.0000 norm=0.1379 [iter 200] loss=3.7584 val_loss=0.0000 scale=1.0000 norm=0.1340 [iter 0] loss=17.6121 val_loss=0.0000 scale=2.0000 norm=0.9518 [iter 100] loss=3.8187 val_loss=0.0000 scale=1.0000 norm=0.1387 [iter 200] loss=3.7646 val_loss=0.0000 scale=0.5000 norm=0.0669

[test] :: root mean squared error : 13.62 +- 0.62

```
[train] :: root mean squared error : 10.80 +- 0.14
[test] :: mean absolute error : 10.40 +- 0.45
[train] :: mean absolute error : 7.92 +- 0.11
```

Well, after hyperparameter tuning, we can see that the performance improved a little bit as below: - Train RMSE: 13.11 -> 10.80 - Train MAE: 10.21 -> 7.92 - CV RMSE: 14.09 -> 13.62 - CV MAE: 10.82 -> 10.40

1.11 11. Evaluate on Test Set

Lastly, let's evaluate the performance of the model on an unseen test set. We will be predicting the RUL from the last available cycle of each engine unit and comparing it with the true RUL values given by the NASA CMAPSS's Turbofan Jet Engine dataset.

Before testing the model, we need to train the model on a whole train set using fit().

```
Then, we need to transform the test dataset with our preprocessing pipeline.
[22]: test = preprocessing.transform(test)
     Dropped features: ['op_setting_3', 'sensor_1', 'sensor_5', 'sensor_10',
     'sensor_16', 'sensor_18', 'sensor_19']
     Start Rolling TS
                         | 20/20 [00:05<00:00, 3.93it/s]
     Rolling: 100%
     Done Rolling TS in 0:00:05.297616
     Start Extracting Features
     Feature Extraction: 100%
                                    | 20/20 [04:06<00:00, 12.34s/it]
     Done Extracting Features in 0:04:22.001927
     Dropped 19 duplicate features
     Dropped 14 features with NA values
[23]: test.index = test.index.set_names(['unit', 'time_cycles'])
      print('test shape after pipeline:', test.shape)
      test.head()
```

test shape after pipeline: (10196, 10)

```
[23]:
                             0
                                       2
                                                 3
                                                                     1
     unit time_cycles
     1.0 30.0
                      -9.256385 -0.490375 6.074795 -0.449975 -0.576160 -6.715231
          31.0
                      -9.381528 -0.558332 6.106739 -1.206451 -0.220868 -5.100832
     2.0 30.0
                      -7.653845 -0.880013 4.063427 -1.274309 1.547471 -4.917313
          31.0
                      -7.815636 -1.282548
                                           3.427045 -0.840907 0.538139 -3.874088
          32.0
                      -7.405561 -1.151824 3.588774 -0.815627
                                                               1.004709 -3.433972
                                       8
                                                 7
                             6
                                                           15
     unit time_cycles
     1.0 30.0
                       7.550608 0.834388 -4.062945 1.993335
          31.0
                       5.631008 1.099968 -4.798740 1.567725
     2.0 30.0
                       2.644615 -3.372040 -3.008906
                                                     0.318385
          31.0
                       2.340176 -3.338283 -2.777530 -0.810257
          32.0
                       2.057121 -3.976815 -2.692903 -0.650431
[24]: X_test = test.reset_index().drop(columns=['unit'])
     test_units = test.index.to_frame(index=False)
     print(X_test)
     print(test_units)
            time_cycles
                                                     3
                                                                           \
                                 0
                                           2
                                                                         1
     0
                   30.0 -9.256385 -0.490375 6.074795 -0.449975
                                                                 -0.576160
     1
                   31.0 -9.381528 -0.558332 6.106739 -1.206451
                                                                 -0.220868
     2
                   30.0 -7.653845 -0.880013 4.063427 -1.274309
                                                                  1.547471
     3
                   31.0 -7.815636 -1.282548 3.427045 -0.840907
                                                                  0.538139
                   32.0 -7.405561 -1.151824 3.588774 -0.815627
     4
                                                                  1.004709
                                  ...
                                                  •••
     10191
                  194.0 13.096492 -1.176219 -1.317391 1.801781 21.304902
     10192
                  195.0 13.586926 -0.942031 -1.207001 0.273047
                                                                 20.533458
     10193
                  196.0 14.515057 -0.627367 -0.823441 0.930284
                                                                 21.043452
     10194
                  197.0 15.554129 -0.203595 -0.484195 1.336224
                                                                 22.420758
     10195
                  198.0 17.002795 0.267946 0.424074 2.156849
                                                                 22.857258
                                      8
                                                7
                                                         15
     0
           -6.715231 7.550608 0.834388 -4.062945 1.993335
                                                   1.567725
     1
           -5.100832 5.631008 1.099968 -4.798740
     2
           -4.917313 2.644615 -3.372040 -3.008906 0.318385
     3
           -3.874088 2.340176 -3.338283 -2.777530 -0.810257
     4
           -3.433972 2.057121 -3.976815 -2.692903 -0.650431
     10191 -0.910152 -0.382022 -2.723103 1.212824 -2.101157
     10192 -1.680287 -0.436096 -4.283490 0.396544 -2.296455
     10193 -2.166492 1.273038 -3.255015 -0.723864 -2.218065
     10194 -1.959344 2.098871 -3.352730 -1.734722 -3.435271
     10195 -2.160963 1.900672 -3.287815 -1.863974 -2.713282
```

```
[10196 rows x 11 columns]
        unit
              time_cycles
0
         1.0
                      30.0
1
         1.0
                      31.0
2
                      30.0
         2.0
3
         2.0
                      31.0
4
         2.0
                      32.0
10191
                     194.0
      100.0
                     195.0
10192
       100.0
10193
       100.0
                     196.0
10194
       100.0
                     197.0
10195
       100.0
                     198.0
```

[10196 rows x 2 columns]

Let's define the model testing methodology. We need to select the instances with the high time_cycles, so that the model can predict the remaining RUL and compare it with the true RUL given by the dataset itself. Of course, logically this should be the last row of each engine unit.

```
[25]: from utils import rul_evaluation_score

def test_model(model, X_test, engines, test_rul):
    '''Evaluate on test set'''
    X_test_last = X_test_groupby(engines, as_index=False).last()
    return rul_evaluation_score(model, X_test_last.values, test_rul, usinetrics='all')
```

Finally we can test our tuned NGBoost model on the test FD001 data.

```
[30]: test_model(ngb_tuned, X_test, test_units['unit'], test_rul)
```

```
[30]: {'RMSE': 13.189623973028215, 'MAE': 10.139092587105042}
```

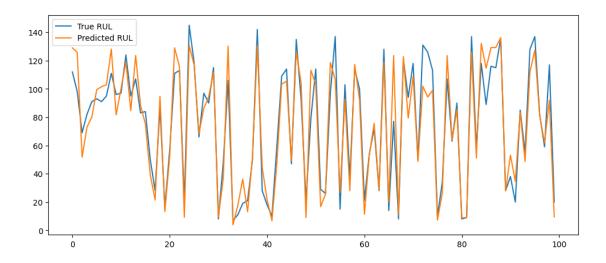
This is a huge improvement when we compared to the baseline model. - RMSE: 22.3685 -> 13.1896 (-41.03% reduction in RMSE) - MAE: 17.8900 -> 10.1391 (-43.33% reduction in MAE)

In conclusion, due to the robust Exploratory Data Analysis performed, we were able to identify appropriate data preprocessing methods. Plus, by using tsfresh for features engineering with PCA, we were able to achieve better performance while reducing the dimensionality of the model.

1.12 Additional Visualization

```
[33]: from utils import plot_rul

X_test_last = X_test.groupby(test_units['unit'], as_index=False).last()
y_pred = ngb_tuned.predict(X_test_last.values)
plot_rul(test_rul, y_pred)
```



We can see that the Predicted RUL follow closely the True RUL compared to the result of Baseline Model.

```
[32]: # Print the predicted value vs true value pd.DataFrame({'True RUL': test_rul, 'Predicted RUL': y_pred})
```

[32]:		True RUL	Predicted RUL
	0	112.0	129.028261
	1	98.0	125.847364
	2	69.0	51.760241
	3	82.0	72.974155
	4	91.0	80.064634
		•••	•••
	95	137.0	127.228299
	96	82.0	81.335217
	97	59.0	61.887104
	98	117.0	91.919749
	99	20.0	9.434601

[100 rows x 2 columns]