Random Forest

In [1]:
```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
```

In [2]:
```
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.preprocessing import MinMaxScaler
from sklearn.pipeline import Pipeline
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import classification_report
from sklearn.metrics import confusion_matrix
from sklearn.metrics import plot_confusion_matrix
```

In [3]:
```
df = pd.read_csv('data/data_no_fliers.csv')
df.drop('Unnamed: 0', axis=1, inplace=True)
df.head()
```

Out[3]:

	neo	pha	H	epoch	epoch_mjd	epoch_cal	e	a	q	i
0	0	0	3.40	2458600.5	58600	20190427.0	0.076009	2.769165	2.558684	10.594067
1	0	0	4.20	2459000.5	59000	20200531.0	0.229972	2.773841	2.135935	34.832932
2	0	0	5.33	2459000.5	59000	20200531.0	0.256936	2.668285	1.982706	12.991043
3	0	0	3.00	2458600.5	58600	20190427.0	0.088721	2.361418	2.151909	7.141771
4	0	0	6.90	2459000.5	59000	20200531.0	0.190913	2.574037	2.082619	5.367427

5 rows × 45 columns

In [4]:
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 921430 entries, 0 to 921429
Data columns (total 45 columns):
 #   Column     Non-Null Count   Dtype  
---  ------     --------------   -----  
 0   neo        921430 non-null  int64  
 1   pha        921430 non-null  int64  
 2   H          921430 non-null  float64
 3   epoch      921430 non-null  float64
 4   epoch_mjd  921430 non-null  int64  
 5   epoch_cal  921430 non-null  float64
 6   e          921430 non-null  float64
 7   a          921430 non-null  float64
 8   q          921430 non-null  float64
 9   i          921430 non-null  float64
 10  om         921430 non-null  float64
 11  w          921430 non-null  float64
 12  ma         921430 non-null  float64
 13  ad         921430 non-null  float64
 14  n          921430 non-null  float64
 15  tp         921430 non-null  float64
 16  tp_cal     921430 non-null  float64
```

```
 17  per         921430 non-null  float64
 18  per_y       921430 non-null  float64
 19  moid        921430 non-null  float64
 20  moid_ld     921430 non-null  float64
 21  sigma_e     921430 non-null  float64
 22  sigma_a     921430 non-null  float64
 23  sigma_q     921430 non-null  float64
 24  sigma_i     921430 non-null  float64
 25  sigma_om    921430 non-null  float64
 26  sigma_w     921430 non-null  float64
 27  sigma_ma    921430 non-null  float64
 28  sigma_ad    921430 non-null  float64
 29  sigma_n     921430 non-null  float64
 30  sigma_tp    921430 non-null  float64
 31  sigma_per   921430 non-null  float64
 32  rms         921430 non-null  float64
 33  class_AMO   921430 non-null  int64
 34  class_APO   921430 non-null  int64
 35  class_AST   921430 non-null  int64
 36  class_ATE   921430 non-null  int64
 37  class_CEN   921430 non-null  int64
 38  class_IEO   921430 non-null  int64
 39  class_IMB   921430 non-null  int64
 40  class_MBA   921430 non-null  int64
 41  class_MCA   921430 non-null  int64
 42  class_OMB   921430 non-null  int64
 43  class_TJN   921430 non-null  int64
 44  class_TNO   921430 non-null  int64
dtypes: float64(30), int64(15)
memory usage: 316.3 MB
```

In [5]:
```
X = df.drop('pha', axis=1)
y = df['pha']

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.25, random
```

In [6]:
```
ss = StandardScaler()

X_train_scaled = ss.fit_transform(X_train)
X_test_scaled = ss.transform(X_test)
```

In [7]:
```
RF = RandomForestClassifier(class_weight={0:1, 1:200})
RF.fit(X_train_scaled, y_train)
```

Out[7]:
```
RandomForestClassifier(class_weight={0: 1, 1: 200})
```

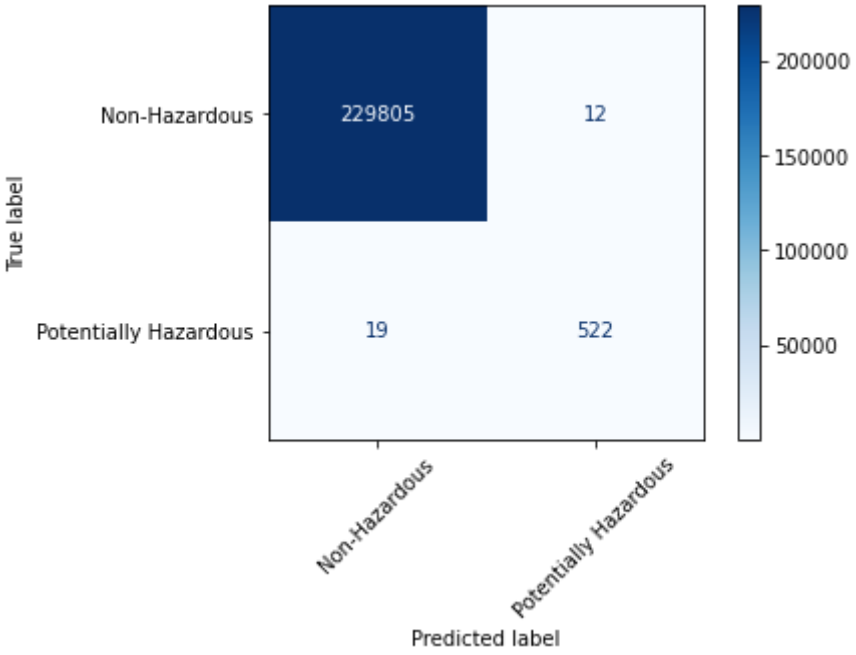
In [8]:
```
y_pred = RF.predict(X_test_scaled)

print('Train Report')
print(classification_report(y_train, RF.predict(X_train_scaled)))
print('\n')
print('Test Report')
print(classification_report(y_test, y_pred))
```

```
Train Report
              precision    recall  f1-score   support

           0       1.00      1.00      1.00    689548
           1       1.00      1.00      1.00      1524

    accuracy                           1.00    691072
   macro avg       1.00      1.00      1.00    691072
```

```
weighted avg       1.00      1.00      1.00    691072


Test Report
              precision    recall  f1-score   support

           0       1.00      1.00      1.00    229817
           1       0.98      0.96      0.97       541

    accuracy                           1.00    230358
   macro avg       0.99      0.98      0.99    230358
weighted avg       1.00      1.00      1.00    230358
```

The baseline model is overfit to the training data, as we let the tree depths grow out.

In [9]:
```
plot_confusion_matrix(RF, X_test_scaled, y_test, cmap=plt.cm.Blues,
                      display_labels=['Non-Hazardous', 'Potentially Hazardous'],
```



In [10]:
```
depths = [estimator.tree_.max_depth for estimator in RF.estimators_]
print('Mean depth:', np.mean(depths))
depths
```

```
Mean depth: 26.93
```

Out[10]:
```
[23,
 23,
 27,
 25,
 25,
 31,
 27,
 36,
 24,
 24,
 21,
 23,
 23,
 37,
 25,
 26,
```

```
24,
18,
26,
35,
24,
20,
26,
17,
30,
32,
29,
29,
25,
23,
28,
34,
21,
20,
35,
24,
43,
23,
29,
29,
32,
25,
25,
33,
35,
27,
30,
26,
22,
23,
24,
22,
22,
31,
22,
29,
28,
24,
22,
28,
27,
41,
24,
23,
23,
29,
23,
19,
32,
29,
38,
22,
25,
32,
27,
26,
24,
23,
21,
28,
26,
```

```
36,
34,
34,
24,
34,
24,
26,
34,
27,
21,
28,
19,
24,
23,
28,
41,
31,
25,
24]
```

In [11]:
```
RF.get_params()
```

Out[11]:
```
{'bootstrap': True,
 'ccp_alpha': 0.0,
 'class_weight': {0: 1, 1: 200},
 'criterion': 'gini',
 'max_depth': None,
 'max_features': 'auto',
 'max_leaf_nodes': None,
 'max_samples': None,
 'min_impurity_decrease': 0.0,
 'min_impurity_split': None,
 'min_samples_leaf': 1,
 'min_samples_split': 2,
 'min_weight_fraction_leaf': 0.0,
 'n_estimators': 100,
 'n_jobs': None,
 'oob_score': False,
 'random_state': None,
 'verbose': 0,
 'warm_start': False}
```

Iteration 2

This iteration will search `max_depth` values less than 27 and a small range of values for `min_samples_leaf`. `min_samples_leaf` is kept at 2, the smallest possible value. This is also the value that worked best for the decision tree model, and one would expect the trees in a forest to be more grown out.

In [8]:
```
RF2 = RandomForestClassifier(random_state=123)

param_grid = {
    'class_weight': ['balanced', {0:1, 1:200}],
    'n_estimators': [50, 100],
    'max_depth': [7, 14, 21],
    'min_samples_leaf': [1, 3, 6]
}

RF2_grid = GridSearchCV(RF2, param_grid=param_grid, cv=3, scoring='recall')
```

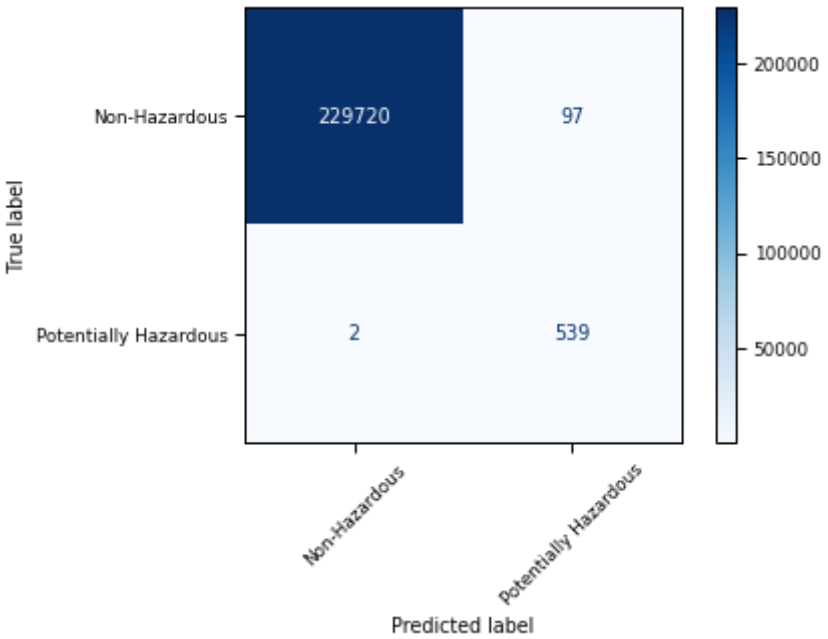
In [ ]:
```
RF2_grid.fit(X_train_scaled, y_train)
```

In [15]:
```
y_pred = RF2_grid.predict(X_test_scaled)

print('Train Report')
print(classification_report(y_train, RF2_grid.predict(X_train_scaled)))
print('\n')
print('Test Report')
print(classification_report(y_test, y_pred))
```

```
Train Report
              precision    recall  f1-score   support

           0       1.00      1.00      1.00    689548
           1       0.85      1.00      0.92      1524

    accuracy                           1.00    691072
   macro avg       0.93      1.00      0.96    691072
weighted avg       1.00      1.00      1.00    691072



Test Report
              precision    recall  f1-score   support

           0       1.00      1.00      1.00    229817
           1       0.85      1.00      0.92       541

    accuracy                           1.00    230358
   macro avg       0.92      1.00      0.96    230358
weighted avg       1.00      1.00      1.00    230358
```

The model is no longer overfit to the training data.

In [39]:
```
plot_confusion_matrix(RF2_grid, X_test_scaled, y_test, cmap=plt.cm.Blues,
                      display_labels=['Non-Hazardous', 'Potentially Hazardous'],
```



In [17]:
```
RF2_grid.best_params_
```

Out[17]:
```
{'class_weight': {0: 1, 1: 200},
 'max_depth': 7,
```

```
 'min_samples_leaf': 3,
 'n_estimators': 100}
```

Iteration 3

Searching around `max_depth` = 7 and `min_samples_leaf` = 3

In [10]:
```
RF3 = RandomForestClassifier(random_state=123)

class_weights = ['balanced', {0:1, 1:200}]

param_grid = {
    'class_weight': class_weights,
    'max_depth': [6, 7, 8, 9],
    'min_samples_leaf': [2, 3, 4, 5]
}

RF3_grid = GridSearchCV(RF3, param_grid=param_grid, cv=3, scoring='recall')
```

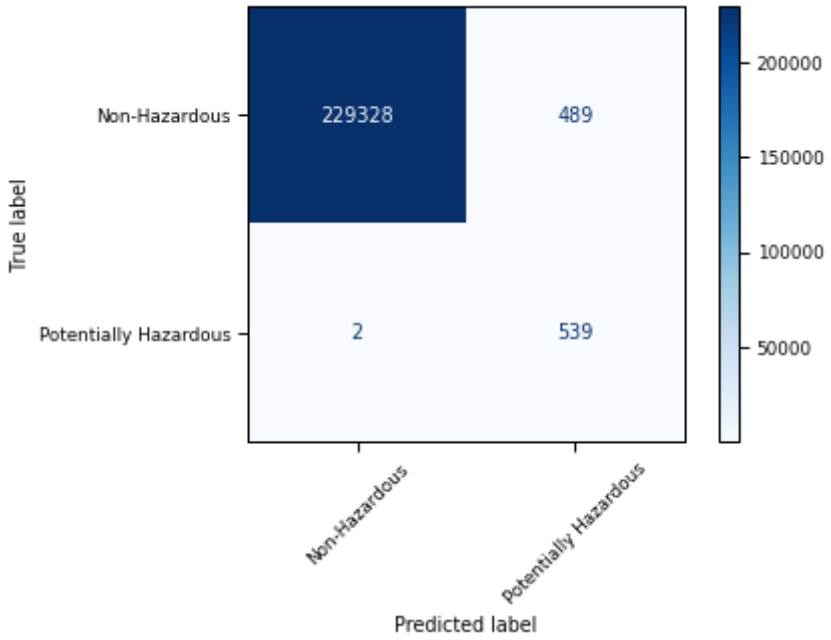
In [11]:
```
RF3_grid.fit(X_train_scaled, y_train)
```

Out[11]:
```
GridSearchCV(cv=3, estimator=RandomForestClassifier(random_state=123),
             param_grid={'class_weight': ['balanced', {0: 1, 1: 200}],
                         'max_depth': [6, 7, 8, 9],
                         'min_samples_leaf': [2, 3, 4, 5]},
             scoring='recall')
```

In [12]:
```
y_pred = RF3_grid.predict(X_test_scaled)

print('Train Report')
print(classification_report(y_train, RF3_grid.predict(X_train_scaled)))
print('\n')
print('Test Report')
print(classification_report(y_test, y_pred))
```

```
Train Report
              precision    recall  f1-score   support

           0       1.00      1.00      1.00    689548
           1       0.50      1.00      0.67      1524

    accuracy                           1.00    691072
   macro avg       0.75      1.00      0.83    691072
weighted avg       1.00      1.00      1.00    691072



Test Report
              precision    recall  f1-score   support

           0       1.00      1.00      1.00    229817
           1       0.52      1.00      0.69       541

    accuracy                           1.00    230358
   macro avg       0.76      1.00      0.84    230358
weighted avg       1.00      1.00      1.00    230358
```

In [13]:
```
sns.set_context('paper')

plot_confusion_matrix(RF3_grid, X_test_scaled, y_test, cmap=plt.cm.Blues,
                      display_labels=['Non-Hazardous', 'Potentially Hazardous'],
```



In [14]:
```
RF3_grid.best_params_
```

Out[14]:
```
{'class_weight': 'balanced', 'max_depth': 6, 'min_samples_leaf': 2}
```

Iteration 4

Last gridsearch will omit `max_depth` = 6 to see if we can address the high number of false positives.

In [17]:
```
RF4 = RandomForestClassifier(random_state=123)

param_grid = {
    'class_weight': class_weights,
    'max_depth': [7, 8, 9],
    'min_samples_leaf': [2, 3, 4, 5]
}

RF4_grid = GridSearchCV(RF4, param_grid=param_grid, cv=3, scoring='recall')
```

In [18]:
```
RF4_grid.fit(X_train_scaled, y_train)
```

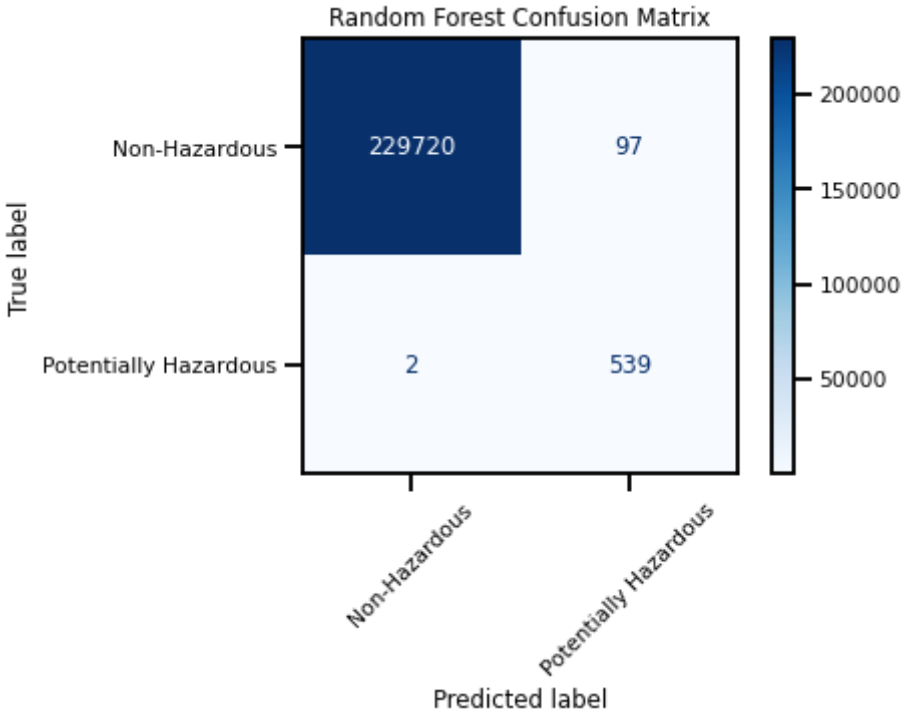
Out[18]:
```
GridSearchCV(cv=3, estimator=RandomForestClassifier(random_state=123),
             param_grid={'class_weight': ['balanced', {0: 1, 1: 200}],
                         'max_depth': [7, 8, 9],
                         'min_samples_leaf': [2, 3, 4, 5]},
             scoring='recall')
```

In [19]:
```
y_pred = RF4_grid.predict(X_test_scaled)

print('Train Report')
print(classification_report(y_train, RF4_grid.predict(X_train_scaled)))
print('\n')
print('Test Report')
print(classification_report(y_test, y_pred))
```

```
Train Report
              precision    recall  f1-score   support
```

```
              0       1.00      1.00      1.00    689548
              1       0.85      1.00      0.92      1524

    accuracy                            1.00    691072
   macro avg       0.93      1.00      0.96    691072
weighted avg       1.00      1.00      1.00    691072



Test Report
              precision    recall  f1-score   support

           0       1.00      1.00      1.00    229817
           1       0.85      1.00      0.92       541

    accuracy                           1.00    230358
   macro avg       0.92      1.00      0.96    230358
weighted avg       1.00      1.00      1.00    230358
```

In [30]:
```
sns.set_context('talk', font_scale=0.65)
plot_confusion_matrix(RF4_grid, X_test_scaled, y_test, cmap=plt.cm.Blues,
                      display_labels=['Non-Hazardous', 'Potentially Hazardous'],
plt.title('Random Forest Confusion Matrix')
plt.savefig('Images/RF-matrix.png', bbox_inches='tight')
plt.savefig('Images/RF-matrix-hr.png', dpi=200, bbox_inches='tight');
```



This model missed the same number of phas as the previous iteration, but there are much fewer false positives.

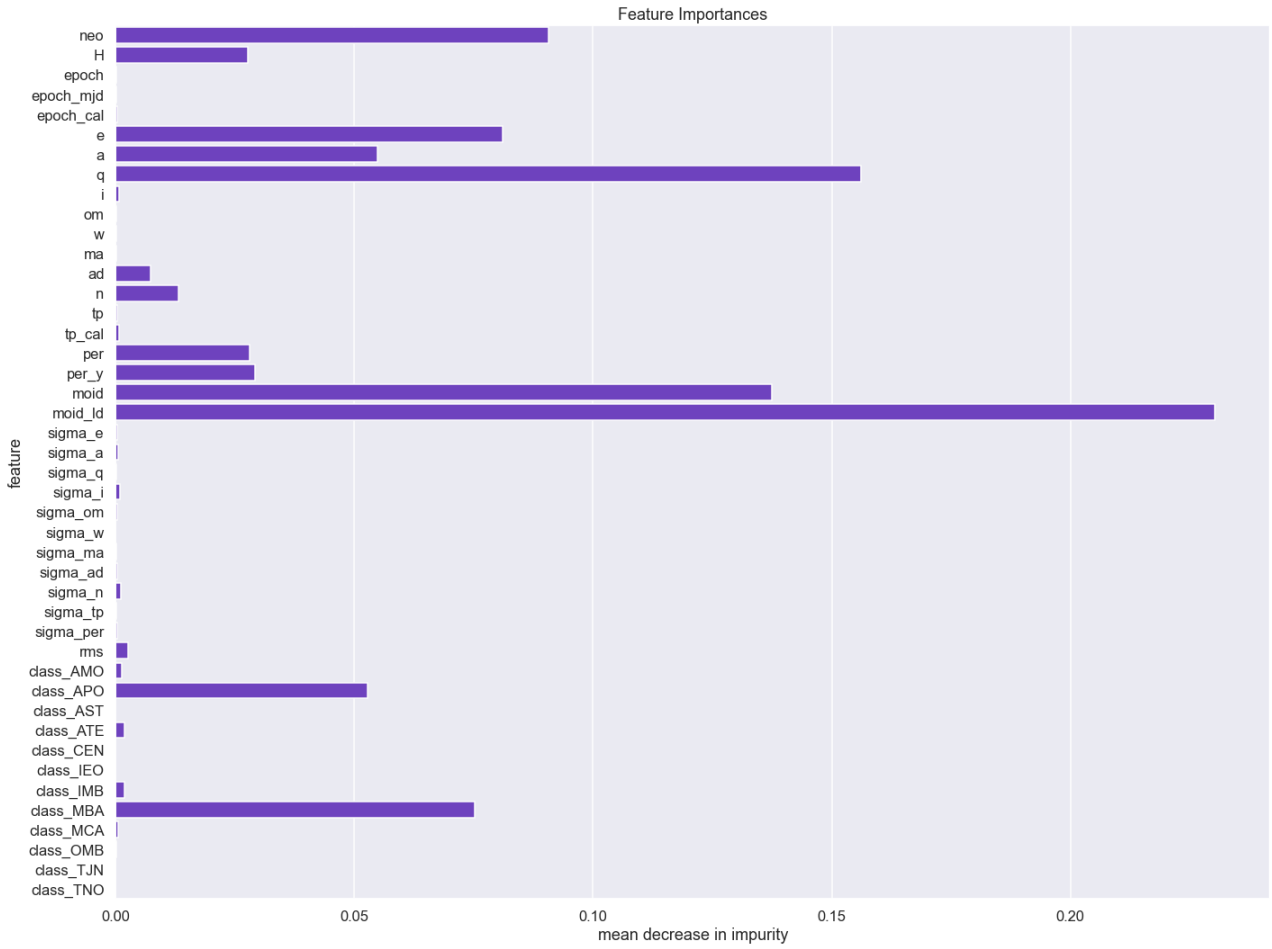
In [21]:
```
RF4_grid.best_params_
```

Out[21]:
```
{'class_weight': {0: 1, 1: 200}, 'max_depth': 7, 'min_samples_leaf': 3}
```

In [22]:
```
RF4 = RandomForestClassifier(random_state=123, class_weight={0:1, 1:200}, max_de

RF4.fit(X_train_scaled, y_train)
```

Out[22]:
```
RandomForestClassifier(class_weight={0: 1, 1: 200}, max_depth=7,
                       min_samples_leaf=3, random_state=123)
```

In [33]:
```
sns.set_context('talk')
sns.set_style('darkgrid')

plt.figure(figsize=(20, 15))
sns.barplot(x = RF4.feature_importances_,
            y = X.columns, color='#682dd3')
plt.title('Feature Importances')
plt.xlabel('mean decrease in impurity')
plt.ylabel('feature')
plt.tight_layout()
plt.savefig('Images/RF-importances.png')
plt.savefig('Images/RF-importances.png', dpi=200);
```



In [34]:
```
from sklearn.decomposition import PCA

pca = PCA(n_components=5)
X_transformed = pca.fit_transform(X_train_scaled)
```

In [35]:
```
pca.explained_variance_ratio_
```

Out[35]:
```
array([0.19685156, 0.19090429, 0.10615482, 0.06094324, 0.04144515])
```

In [36]:
```
pca.components_
```

Out[36]:
```
array([[ 1.27542039e-02,  1.52473281e-02, -1.58175961e-02,
        -1.58175961e-02, -1.58290957e-02,  1.03213098e-02,
```

```
 -1.84319288e-02, -1.91784300e-02, -9.85767667e-04,
 -1.53721468e-04, -2.08587819e-04, -7.20260799e-04,
 -1.27459463e-02,  1.72449064e-02, -1.40138695e-02,
 -1.39574146e-02, -1.80149625e-02, -1.80149625e-02,
 -1.89824635e-02, -1.89824635e-02,  2.66314755e-01,
  3.25919764e-01,  2.61916406e-01,  2.95404804e-01,
  2.18694776e-01,  3.27418165e-01,  3.14062198e-01,
  3.25233226e-01,  3.10534332e-01,  3.15362133e-01,
  3.27373260e-01,  6.31337904e-05,  6.32400184e-03,
  9.99037782e-03, -4.70669720e-04,  4.97793807e-03,
 -1.61738770e-03,  6.51942931e-04,  4.60691810e-03,
 -7.75711353e-03,  4.49679407e-03, -4.95202787e-03,
 -3.48840881e-03, -0.00000000e+00],
[-2.08029712e-01, -2.40662799e-01,  7.68968374e-02,
  7.68968374e-02,  7.71649506e-02, -1.60202421e-01,
  3.22067675e-01,  3.23862930e-01,  8.51264474e-03,
 -3.11736182e-03, -6.85094289e-04,  1.00094776e-02,
  2.32694313e-01, -2.97992289e-01,  6.94856364e-02,
  6.92863096e-02,  3.15567275e-01,  3.15567275e-01,
  3.20495242e-01,  3.20495242e-01,  1.68380010e-02,
  2.03905489e-02,  1.65722501e-02,  1.84570066e-02,
  1.38336019e-02,  2.06088716e-02,  1.97079832e-02,
  2.03446266e-02,  1.93577886e-02,  1.98349027e-02,
  2.05025611e-02, -5.31778459e-04, -1.03243575e-01,
 -1.60801526e-01,  1.00234944e-02, -8.67192111e-02,
  3.13270355e-02, -1.12712827e-02, -8.50278890e-02,
  1.22477613e-01, -7.17198709e-02,  9.29215879e-02,
  6.48945204e-02, -0.00000000e+00],
[ 5.04435854e-02,  5.83809628e-02, -4.32708461e-01,
 -4.32708461e-01, -4.32535015e-01,  6.25047189e-02,
  1.04064623e-01,  4.68136216e-02,  3.48130986e-02,
  1.15992828e-03, -1.14031619e-05, -6.77016015e-02,
  1.26494873e-01, -6.27556860e-02, -4.15360787e-01,
 -4.13288498e-01,  1.09148295e-01,  1.09148295e-01,
  5.20714451e-02,  5.20714451e-02, -5.84144254e-03,
 -7.50950291e-03, -5.97478597e-03, -5.68749618e-03,
 -4.52441514e-03, -8.34013461e-03, -8.37113078e-03,
 -7.24631210e-03, -7.69435015e-03, -8.23011758e-03,
 -7.37636539e-03, -4.35061294e-03,  2.99983142e-02,
  4.96721615e-02,  1.25854102e-02, -1.83330542e-02,
  3.15973158e-02, -1.80021235e-03, -3.87973934e-02,
 -6.10775270e-02,  2.17590275e-02,  6.40394092e-02,
  4.46874827e-02, -0.00000000e+00],
[ 3.49079774e-01,  1.17435399e-01,  9.78174596e-02,
  9.78174596e-02,  9.74774021e-02,  3.84050341e-01,
  1.69901726e-01, -7.41751051e-02,  2.10554277e-01,
  2.57886182e-03,  1.99757534e-03,  3.50296037e-02,
  3.40140764e-01, -5.92203625e-03,  1.15746698e-01,
  1.15089382e-01,  1.98510619e-01,  1.98510619e-01,
 -4.59436561e-02, -4.59436561e-02,  6.20690275e-04,
  9.58514072e-04,  1.94201484e-04, -2.13043390e-04,
  2.90036706e-03,  1.89919267e-03,  1.57317827e-03,
  1.08053548e-03,  6.13289381e-04,  1.97692477e-03,
  1.07268351e-03,  1.95833442e-03,  2.32637610e-01,
  2.62978844e-01,  4.46999929e-02,  3.40105736e-02,
  1.22431685e-01,  4.91122677e-03, -3.78098086e-02,
 -3.84291767e-01,  1.18280885e-01,  2.50424547e-01,
  1.24844518e-01, -0.00000000e+00],
[-4.81640185e-02, -4.83080825e-02, -1.86687861e-02,
 -1.86687861e-02, -1.82572273e-02, -3.41812612e-01,
 -6.22154540e-02,  1.43063750e-01,  2.93117501e-01,
  1.13414211e-02, -2.13854392e-02,  3.83502783e-02,
 -2.27383270e-01,  1.68970365e-01, -3.23543596e-03,
 -2.24895674e-03, -4.07083816e-02, -4.07083816e-02,
  1.57011240e-01,  1.57011240e-01, -4.27329590e-03,
```

```
 1.55537734e-03, -4.25554016e-03, -2.61907550e-03,
-2.22158113e-03,  4.13474069e-04,  2.42752590e-03,
 1.36051718e-03,  2.48219699e-03,  1.63276697e-03,
 1.34093337e-03,  1.26008409e-02, -4.90320037e-02,
-7.18510381e-02, -3.56658417e-02,  1.24289327e-01,
-4.29049908e-02,  4.11308753e-02,  5.18329579e-01,
-4.67414008e-01,  1.10942505e-01,  3.19623044e-01,
 5.12157241e-02, -0.00000000e+00]])
```

In [37]:
```
pd.DataFrame(data=pca.components_, columns=X.columns).iloc[1]
```

Out[37]:
```
neo         -0.208030
H           -0.240663
epoch        0.076897
epoch_mjd    0.076897
epoch_cal    0.077165
e           -0.160202
a            0.322068
q            0.323863
i            0.008513
om          -0.003117
w           -0.000685
ma           0.010009
ad           0.232694
n           -0.297992
tp           0.069486
tp_cal       0.069286
per          0.315567
per_y        0.315567
moid         0.320495
moid_ld      0.320495
sigma_e      0.016838
sigma_a      0.020391
sigma_q      0.016572
sigma_i      0.018457
sigma_om     0.013834
sigma_w      0.020609
sigma_ma     0.019708
sigma_ad     0.020345
sigma_n      0.019358
sigma_tp     0.019835
sigma_per    0.020503
rms         -0.000532
class_AMO   -0.103244
class_APO   -0.160802
class_AST    0.010023
class_ATE   -0.086719
class_CEN    0.031327
class_IEO   -0.011271
class_IMB   -0.085028
class_MBA    0.122478
class_MCA   -0.071720
class_OMB    0.092922
class_TJN    0.064895
class_TNO   -0.000000
Name: 1, dtype: float64
```

In [ ]: