6dp7yxy4f

June 6, 2024

[ ]:
```
import numpy as np
import pandas as pd

!pip install rdkit-pypi
import rdkit
from rdkit import Chem
from rdkit.Chem import AllChem
```

```
Requirement already satisfied: rdkit-pypi in /usr/local/lib/python3.10/dist-
packages (2022.9.5)
Requirement already satisfied: numpy in /usr/local/lib/python3.10/dist-packages
(from rdkit-pypi) (1.25.2)
Requirement already satisfied: Pillow in /usr/local/lib/python3.10/dist-packages
(from rdkit-pypi) (9.4.0)
```

[ ]:
```
train = pd.read_csv('/content/X_train_AX2CWD7.csv')
Y_train = pd.read_csv('/content/y_train_hCIvDMj.csv')['y']
test = pd.read_csv('/content/X_test_0mB4D2v.csv')
```

[ ]:
```
# Convert SMILES to mols
train_mols = [AllChem.MolFromSmiles(smile) for smile in
train['smiles']]
test_mols = [AllChem.MolFromSmiles(smile) for smile in test['smiles']]
```

[ ]:
```
# Convert Mol to fingerprints
train_fps = np.array([AllChem.GetMorganFingerprintAsBitVect(mol,
radius=2, nBits=2048) for mol in train_mols])
test_fps = np.array([AllChem.GetMorganFingerprintAsBitVect(mol,
radius=2, nBits=2048) for mol in test_mols])
```

[ ]:
```
X_train = train_fps
X_test = test_fps
```

[ ]:
```
from sklearn.ensemble import RandomForestRegressor
from sklearn.model_selection import cross_validate
```

[ ]:
```
model = RandomForestRegressor()

cv = cross_validate(estimator=model,
 X=X_train,
 y=Y_train,
 cv=3,
 scoring=["neg_median_absolute_error"],
 n_jobs=-1,
 verbose=0)
print(f"Mean MAE over 10 folds = {-cv['test_neg_median_absolute_error'].mean():.
 ↪4f}")
```

```
Mean MAE over 10 folds = 0.4431
```

[ ]:
```
#opti rf

parameters ={'max_depth':[3,5,10,None],
              'n_estimators':[10,100,200],
              'max_features':[1,3,5,7],
              'min_samples_leaf':[1,2,3],
              'min_samples_split':[1,2,3]
           }

from sklearn.model_selection import GridSearchCV

scoring = "neg_median_absolute_error"

rfGS = GridSearchCV(model,parameters,cv=3,scoring=scoring)
rfGS.fit(X_train,Y_train)
```

```
/usr/local/lib/python3.10/dist-
packages/sklearn/model_selection/_validation.py:378: FitFailedWarning:
432 fits failed out of a total of 1296.
The score on these train-test partitions for these parameters will be set to
nan.
If these failures are not expected, you can try to debug them by setting
error_score='raise'.

Below are more details about the failures:
--------------------------------------------------------------------------------
432 fits failed with the following error:
Traceback (most recent call last):
  File "/usr/local/lib/python3.10/dist-
packages/sklearn/model_selection/_validation.py", line 686, in _fit_and_score
    estimator.fit(X_train, y_train, **fit_params)
  File "/usr/local/lib/python3.10/dist-packages/sklearn/ensemble/_forest.py",
line 340, in fit
    self._validate_params()
```

```
  File "/usr/local/lib/python3.10/dist-packages/sklearn/base.py", line 600, in
_validate_params
    validate_parameter_constraints(
  File "/usr/local/lib/python3.10/dist-
packages/sklearn/utils/_param_validation.py", line 97, in
validate_parameter_constraints
    raise InvalidParameterError(
sklearn.utils._param_validation.InvalidParameterError: The 'min_samples_split'
parameter of RandomForestRegressor must be an int in the range [2, inf) or a
float in the range (0.0, 1.0]. Got 1 instead.

  warnings.warn(some_fits_failed_message, FitFailedWarning)
/usr/local/lib/python3.10/dist-packages/sklearn/model_selection/_search.py:952:
UserWarning: One or more of the test scores are non-finite: [        nan
nan         nan -1.00964122 -1.01173039 -1.01315898
 -1.01638276 -1.01017684 -1.0111199          nan         nan         nan
 -1.00722442 -1.0093324  -1.0126763  -1.01493452 -1.01048898 -1.01178652
         nan         nan         nan -1.01105657 -1.01489673 -1.01471783
 -1.01486522 -1.01117206 -1.01480303         nan         nan         nan
 -0.99665491 -1.00107675 -1.00856028 -1.00455239 -1.00225164 -1.00444011
         nan         nan         nan -1.00899647 -1.00517213 -1.00486342
 -1.00072866 -1.00402508 -1.00131622         nan         nan         nan
 -0.99223362 -1.00618676 -1.00321872 -1.00499367 -1.00507436 -1.00456394
         nan         nan         nan -0.99936056 -0.99114586 -0.9946129
 -0.98698777 -0.99600227 -0.99741215         nan         nan         nan
 -1.00069509 -0.99359601 -0.99419528 -0.98314616 -0.99397611 -0.99226767
         nan         nan         nan -0.99400115 -0.9967248  -0.99571412
 -0.98648272 -0.99501075 -0.9950583          nan         nan         nan
 -0.99537057 -0.98881321 -0.98758654 -0.98188308 -0.98424843 -0.98469798
         nan         nan         nan -0.98597738 -0.99023375 -0.98660466
 -0.99781923 -0.98497484 -0.99008784         nan         nan         nan
 -0.97774038 -0.98554891 -0.99060387 -0.98659612 -0.99088888 -0.9884243
         nan         nan         nan -0.99826392 -1.00096341 -1.00598466
 -1.00852455 -1.00617339 -1.00290436         nan         nan         nan
 -0.99741646 -1.00287652 -1.00690661 -1.01083615 -1.01022214 -1.00609651
         nan         nan         nan -1.01076914 -1.01215305 -1.00917272
 -1.01274437 -1.01140202 -1.01272844         nan         nan         nan
 -0.99177416 -0.98687184 -0.98920987 -0.99699992 -0.98555028 -0.98647671
         nan         nan         nan -0.99070153 -0.98522247 -0.99057508
 -0.99840808 -0.98612232 -0.9901768          nan         nan         nan
 -0.99250648 -0.98785992 -0.98870023 -0.99490161 -0.99410626 -0.98777354
         nan         nan         nan -0.97373623 -0.9768996  -0.96945902
 -0.97475577 -0.97068112 -0.97599031         nan         nan         nan
 -0.97684577 -0.98022315 -0.97327327 -0.98587098 -0.9804268  -0.9736871
         nan         nan         nan -0.97860345 -0.97537614 -0.97612237
 -0.97893128 -0.98207809 -0.98002379         nan         nan         nan
 -0.97442443 -0.96370993 -0.96152808 -0.97041491 -0.95665881 -0.9627602
         nan         nan         nan -0.95651837 -0.97162401 -0.96195726
```

```
-0.97419118 -0.96343492 -0.96058            nan         nan         nan
-0.97012908 -0.96345323 -0.96253443 -0.96627177 -0.96909131 -0.96749902
        nan         nan         nan -0.97065031 -0.9794422  -0.97466559
-0.98074452 -0.97916785 -0.97742774         nan         nan         nan
-0.98945704 -0.99084754 -0.99506058 -0.99250443 -0.9990644  -0.99514071
        nan         nan         nan -1.0049589  -1.00147757 -1.00235474
-1.00782257 -1.0009751  -1.00117789         nan         nan         nan
-0.9351918  -0.93815285 -0.94254149 -0.94252843 -0.9433914  -0.93958461
        nan         nan         nan -0.95017639 -0.95673617 -0.95235906
-0.95064829 -0.96270051 -0.9601322          nan         nan         nan
-0.95028545 -0.96165974 -0.9579557  -0.96143062 -0.95987349 -0.96402122
        nan         nan         nan -0.92293275 -0.9110397  -0.91215598
-0.92980228 -0.91036465 -0.90943679         nan         nan         nan
-0.9336994  -0.93349685 -0.928822   -0.92515951 -0.92549546 -0.92321741
        nan         nan         nan -0.92829495 -0.93282517 -0.9408489
-0.93652479 -0.93827831 -0.93072434         nan         nan         nan
-0.91473202 -0.89507912 -0.88561606 -0.91877099 -0.88501402 -0.889217
        nan         nan         nan -0.90980277 -0.89888302 -0.90531233
-0.92260099 -0.89448536 -0.8991795          nan         nan         nan
-0.91335217 -0.90685475 -0.90042839 -0.91550596 -0.9100975  -0.90674792
        nan         nan         nan -0.56956892 -0.53902522 -0.53901771
-0.58283131 -0.56269175 -0.57692495         nan         nan         nan
-0.96112435 -0.97414996 -0.98034772 -0.98182746 -0.97157749 -0.98017605
        nan         nan         nan -0.99421945 -0.99790681 -0.99812681
-1.00600127 -0.99286924 -0.99961286         nan         nan         nan
-0.55039478 -0.52587619 -0.52404813 -0.57244385 -0.55133926 -0.54984079
        nan         nan         nan -0.87595007 -0.86338215 -0.86722478
-0.87631411 -0.8708154  -0.86020432         nan         nan         nan
-0.89121296 -0.89019832 -0.8919875  -0.90911339 -0.89164889 -0.88809536
        nan         nan         nan -0.53324125 -0.51764146 -0.51654393
-0.53934416 -0.54215466 -0.53674965         nan         nan         nan
-0.80015329 -0.81601176 -0.80905986 -0.79458024 -0.80383012 -0.8075757
        nan         nan         nan -0.84981835 -0.84896925 -0.84671533
-0.87228239 -0.84561224 -0.84755564         nan         nan         nan
-0.52467533 -0.50351085 -0.51001228 -0.55808162 -0.52565886 -0.53149721
        nan         nan         nan -0.75544529 -0.76924283 -0.77389269
-0.77579908 -0.76363736 -0.76545975         nan         nan         nan
-0.80969299 -0.81163375 -0.81392648 -0.80945711 -0.80846864 -0.80839187]
 warnings.warn(
```

[ ]:
```
GridSearchCV(cv=3, estimator=RandomForestRegressor(),
             param_grid={'max_depth': [3, 5, 10, None],
                         'max_features': [1, 3, 5, 7],
                         'min_samples_leaf': [1, 2, 3],
                         'min_samples_split': [1, 2, 3],
                         'n_estimators': [10, 100, 200]},
             scoring='neg_median_absolute_error')
```

[ ]:
```
best_rf = rfGS.best_estimator_
```

[ ]:
```
model = best_rf

cv = cross_validate(estimator=model,
 X=X_train,
 y=Y_train,
 cv=3,
 scoring=["neg_median_absolute_error"],
 n_jobs=-1,
 verbose=0)
print(f"Mean MAE over 10 folds = {-cv['test_neg_median_absolute_error'].mean():.
 ↪4f}")
```

```
Mean MAE over 10 folds = 0.5155
```

[ ]:
```
from sklearn.tree import DecisionTreeRegressor

model = DecisionTreeRegressor()

cv = cross_validate(estimator=model,
 X=X_train,
 y=Y_train,
 cv=3,
 scoring=["neg_median_absolute_error"],
 n_jobs=-1,
 verbose=0)
print(f"Mean MAE over 10 folds = {-cv['test_neg_median_absolute_error'].mean():.
 ↪4f}")
```

```
Mean MAE over 10 folds = 0.4785
```

[ ]:
```
parameters={"splitter":["best","random"],
            "max_depth" : [1,3,5,7,9,11,12],
           "min_samples_leaf":[1,2,3,4,5,6,7,8,9,10],
           "min_weight_fraction_leaf":[0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9],
           "max_features":["auto","log2","sqrt",None],
           "max_leaf_nodes":[None,10,20,30,40,50,60,70,80,90] }

scoring = "neg_median_absolute_error"

dtGS = GridSearchCV(model,parameters,cv=3,scoring=scoring)
#dtGS.fit(X_train,Y_train) trop long
```

```
Le flux de sortie a été tronqué et ne contient que les 5000 dernièreslignes.
/usr/local/lib/python3.10/dist-packages/sklearn/tree/_classes.py:277:
FutureWarning: `max_features='auto'` has been deprecated in 1.1 and will be
removed in 1.3. To keep the past behaviour, explicitly set `max_features=1.0'`.
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```
---------------------------------------------------------------------------
KeyboardInterrupt                         Traceback (most recent call last)
<ipython-input-34-bbf97a8f1f31> in <cell line: 11>()
      9
     10 dtGS = GridSearchCV(model,parameters,cv=3,scoring=scoring)
---> 11 dtGS.fit(X_train,Y_train)

/usr/local/lib/python3.10/dist-packages/sklearn/model_selection/_search.py in␣
 ↪fit(self, X, y, groups, **fit_params)
    872             return results
    873
--> 874         self._run_search(evaluate_candidates)
    875
    876         # multimetric is determined here because in the case of a␣
 ↪callable

/usr/local/lib/python3.10/dist-packages/sklearn/model_selection/_search.py in␣
 ↪_run_search(self, evaluate_candidates)
   1386     def _run_search(self, evaluate_candidates):
   1387         """Search all candidates in param_grid"""
-> 1388         evaluate_candidates(ParameterGrid(self.param_grid))
   1389
   1390

/usr/local/lib/python3.10/dist-packages/sklearn/model_selection/_search.py in␣
 ↪evaluate_candidates(candidate_params, cv, more_results)
    819                 )
    820
--> 821             out = parallel(
    822                 delayed(_fit_and_score)(
    823                     clone(base_estimator),
```

```
/usr/local/lib/python3.10/dist-packages/sklearn/utils/parallel.py in␣
 ↪__call__(self, iterable)
     61             for delayed_func, args, kwargs in iterable
     62         )
---> 63         return super().__call__(iterable_with_config)
     64
     65

/usr/local/lib/python3.10/dist-packages/joblib/parallel.py in __call__(self,␣
 ↪iterable)
   1916             output = self._get_sequential_output(iterable)
   1917             next(output)
-> 1918             return output if self.return_generator else list(output)
   1919
   1920         # Let's create an ID that uniquely identifies the current call.␣
 ↪If the

/usr/local/lib/python3.10/dist-packages/joblib/parallel.py in␣
 ↪_get_sequential_output(self, iterable)
   1845                 self.n_dispatched_batches += 1
   1846                 self.n_dispatched_tasks += 1
-> 1847                 res = func(*args, **kwargs)
   1848                 self.n_completed_tasks += 1
   1849                 self.print_progress()

/usr/local/lib/python3.10/dist-packages/sklearn/utils/parallel.py in␣
 ↪__call__(self, *args, **kwargs)
    121             config = {}
    122         with config_context(**config):
--> 123             return self.function(*args, **kwargs)

/usr/local/lib/python3.10/dist-packages/sklearn/model_selection/_validation.py␣
 ↪in _fit_and_score(estimator, X, y, scorer, train, test, verbose, parameters,␣
 ↪fit_params, return_train_score, return_parameters, return_n_test_samples,␣
 ↪return_times, return_estimator, split_progress, candidate_progress,␣
 ↪error_score)
    684             estimator.fit(X_train, **fit_params)
    685         else:
--> 686             estimator.fit(X_train, y_train, **fit_params)
    687
    688     except Exception:

/usr/local/lib/python3.10/dist-packages/sklearn/tree/_classes.py in fit(self, X␣
 ↪y, sample_weight, check_input)
   1245         """
   1246
-> 1247         super().fit(

   1248             X,
```

```
   1249             y,

/usr/local/lib/python3.10/dist-packages/sklearn/tree/_classes.py in fit(self, X␣
↪y, sample_weight, check_input)
    184             check_X_params = dict(dtype=DTYPE, accept_sparse="csc")
    185             check_y_params = dict(ensure_2d=False, dtype=None)
--> 186             X, y = self._validate_data(
    187                 X, y, validate_separately=(check_X_params,␣
↪check_y_params)
    188             )

/usr/local/lib/python3.10/dist-packages/sklearn/base.py in _validate_data(self,␣
↪X, y, reset, validate_separately, **check_params)
    577                 if "estimator" not in check_X_params:
    578                     check_X_params = {**default_check_params,␣
↪**check_X_params}
--> 579                 X = check_array(X, input_name="X", **check_X_params)
    580                 if "estimator" not in check_y_params:
    581                     check_y_params = {**default_check_params,␣
↪**check_y_params}

/usr/local/lib/python3.10/dist-packages/sklearn/utils/validation.py in␣
↪check_array(array, accept_sparse, accept_large_sparse, dtype, order, copy,␣
↪force_all_finite, ensure_2d, allow_nd, ensure_min_samples,␣
↪ensure_min_features, estimator, input_name)
    877                     array = xp.astype(array, dtype, copy=False)
    878                 else:
--> 879                     array = _asarray_with_order(array, order=order,␣
↪dtype=dtype, xp=xp)
    880             except ComplexWarning as complex_warning:
    881                 raise ValueError(

/usr/local/lib/python3.10/dist-packages/sklearn/utils/_array_api.py in␣
↪_asarray_with_order(array, dtype, order, copy, xp)
    183     if xp.__name__ in {"numpy", "numpy.array_api"}:
    184         # Use NumPy API to support order
--> 185         array = numpy.asarray(array, order=order, dtype=dtype)
    186         return xp.asarray(array, copy=copy)
    187     else:

KeyboardInterrupt:
```

[ ]:
```
#best_dt = dtGS.best_estimator_
```

[ ]:
```
#model = best_dt
model_dt = DecisionTreeRegressor().fit(X_train, Y_train)
best_dt = model_dt
```

[ ]:
```
#cv = cross_validate(estimator=model, X=X_train, y=Y_train, cv=3,␣
 ↪scoring=["neg_median_absolute_error"], n_jobs=-1, verbose=0)
#print(f"Mean MAE over 10 folds = {-cv['test_neg_median_absolute_error'].mean():
 ↪.4f}")
```

[ ]:
```
from sklearn.neighbors import KNeighborsRegressor

model = KNeighborsRegressor()

cv = cross_validate(estimator=model,
 X=X_train,
 y=Y_train,
 cv=3,
 scoring=["neg_median_absolute_error"],
 n_jobs=-1,
 verbose=0)
print(f"Mean MAE over 10 folds = {-cv['test_neg_median_absolute_error'].mean():.
 ↪4f}")
```

```
Mean MAE over 10 folds = 0.4669
```

[ ]:
```
parameters = {'n_neighbors': list(range(1,31))}

scoring = "neg_median_absolute_error"

knnGS = GridSearchCV(model,parameters,cv=3,scoring=scoring)
knnGS.fit(X_train,Y_train)
```

[ ]:
```
GridSearchCV(cv=3, estimator=KNeighborsRegressor(),
             param_grid={'n_neighbors': [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12,
                                         13, 14, 15, 16, 17, 18, 19, 20, 21, 22,
                                         23, 24, 25, 26, 27, 28, 29, 30]},
             scoring='neg_median_absolute_error')
```

[ ]:
```
best_knn = knnGS.best_estimator_
```

[ ]:
```
model = best_knn

cv = cross_validate(estimator=model,
 X=X_train,
 y=Y_train,
 cv=3,
 scoring=["neg_median_absolute_error"],
 n_jobs=-1,
 verbose=0)
print(f"Mean MAE over 10 folds = {-cv['test_neg_median_absolute_error'].mean():.
 ↪4f}")
```

```
Mean MAE over 10 folds = 0.4014
```

[ ]:
```
import sklearn.metrics as metrics

rf_acc = metrics.median_absolute_error(Y_train, best_rf.predict(X_train))
knn_acc = metrics.median_absolute_error(Y_train, best_knn.predict(X_train))
dt_acc = metrics.median_absolute_error(Y_train, best_dt.predict(X_train))
```

[ ]:
```
model_acc = pd.DataFrame({
    'Model': ['KNN', 'Decision Tree',
              'Random Forest'],

    'median_absolute_error': [knn_acc, dt_acc,
              rf_acc]})

model_acc.sort_values(by='median_absolute_error', ascending=False)
```

[ ]:
```
            Model  median_absolute_error
2  Random Forest               0.175092
0            KNN               0.000000
1  Decision Tree               0.000000
```

[ ]:
```
mean_acc = np.mean([rf_acc, knn_acc, dt_acc])
weight_rf = rf_acc / mean_acc
weight_knn = knn_acc / mean_acc
weight_dt = dt_acc / mean_acc
```

[ ]:
```
from sklearn.ensemble import VotingRegressor

ensemble = VotingRegressor(estimators=[("rf", best_rf), ("knn", best_knn),␣
 ↪("dt", best_dt)], weights=[weight_rf, weight_knn, weight_dt])
```

[ ]:
```
ensemble.fit(X_train, Y_train)

ens_prediction = ensemble.predict(X_train)
metrics.median_absolute_error(Y_train, ens_prediction)
```

[ ]:
```
0.17546683859685075
```

[ ]:
```
ensemble.fit(X_train, Y_train)

y_pred = ensemble.predict(X_test)

submission_df = pd.DataFrame()
submission_df['id'] = test['id']
submission_df['y'] = y_pred
submission_df.to_csv("y_benchmark.csv", index=False)
```

[ ]:
```
from google.colab import files
files.download('y_benchmark.csv')
```

```
<IPython.core.display.Javascript object>
```

```
<IPython.core.display.Javascript object>
```