Introducing Grid Search

HYPERPARAMETER TUNING IN PYTHON

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Automating 2 Hyperparameters

Your previous work:

```
neighbors_list = [3,5,10,20,50,75]
accuracy_list = []
for test_number in neighbors_list:
    model = KNeighborsClassifier(n_neighbors=test_number)
    predictions = model.fit(X_train, y_train).predict(X_test)
    accuracy = accuracy_score(y_test, predictions)
    accuracy_list.append(accuracy)
```

Which we then collated in a dataframe to analyse.

Automating 2 Hyperparameters

What about testing values of 2 hyperparameters?

Using a GBM algorithm:

- `learn_rate` `[0.001, 0.01, 0.05]`
- `max_depth` `[4,6,8,10]`

We could use a (*nested*) for loop!

Automating 2 Hyperparameters

Firstly a model creation function:

```
def gbm_grid_search(learn_rate, max_depth):
    model = GradientBoostingClassifier(
            learning_rate=learn_rate,
            max_depth=max_depth)
    predictions = model.fit(X_train, y_train).predict(X_test)
    return([learn_rate, max_depth, accuracy_score(y_test, predictions)])
```

Automating 2 Hyperparameters

Now we can loop through our lists of hyperparameters and call our function:

```
results_list = []

for learn_rate in learn_rate_list:
    for max_depth in max_depth_list:
        results_list.append(gbm_grid_search(learn_rate,max_depth))
```

Automating 2 Hyperparameters

We can put these results into a DataFrame as well and print out:

```
results_df = pd.DataFrame(results_list, columns=['learning_rate', 'max_depth', 'accuracy'])
print(results_df)
```

learning_rate	max_depth	accuracy
0.001	4	0.75
0.001	6	0.75
0.01	4	0.77
0.01	6	0.76

How many models?

There were many more models built by adding more hyperparameters and values.

- The relationship is not linear, it is exponential
- One more value of a hyperparameter is not *just* one model
- 5 for Hyperparameter 1 and 10 for Hyperparameter 2 is 50 models!

What about cross-validation?

- 10-fold cross-validation would make 50x10 = 500 models!

From 2 to N hyperparameters

What about adding more hyperparameters?

We could nest our loop!

```
# Adjust the list of values to test
learn_rate_list = [0.001, 0.01, 0.1, 0.2, 0.3, 0.4, 0.5]
max_depth_list = [4,6,8, 10, 12, 15, 20, 25, 30]
subsample_list = [0.4,0.6, 0.7, 0.8, 0.9]
max_features_list = ['auto', 'sqrt']
```

From 2 to N hyperparameters

Adjust our function:

```
def gbm_grid_search(learn_rate, max_depth,subsample,max_features):
    model = GradientBoostingClassifier(
        learning_rate=learn_rate,
        max_depth=max_depth,
        subsample=subsample,
        max_features=max_features)
    predictions = model.fit(X_train, y_train).predict(X_test)
    return([learn_rate, max_depth, accuracy_score(y_test, predictions)])
```

From 2 to N hyperparameters

Adjusting our for loop (nesting):

```
for learn_rate in learn_rate_list:
    for max_depth in max_depth_list:
        for subsample in subsample_list:
            for max_features in max_features_list:
                results_list.append(gbm_grid_search(learn_rate,max_depth,
                                         subsample,max_features))
results_df = pd.DataFrame(results_list, columns=['learning_rate',
                         'max_depth', 'subsample', 'max_features','accuracy'])
print(results_df)
```

From 2 to N hyperparameters

How many models now?

- $7 \times 9 \times 5 \times 2 = 630$ (6,300 if cross-validated!)

We can't keep nesting forever!

Plus, what if we wanted:

- Details on training times & scores
- Details on cross-validation scores

Introducing Grid Search

Let's create a grid:

- Down the left all values of max_depth
- Across the top all values of learning_rate

	learn_rate			
max_depth		0.001	0.01	0.05
	4	(4 , 0.001)	(4 , 0.01)	(4 , 0.05)
	6	(6 , 0.001)	(6 , 0.01)	(6 , 0.05)
	8	(8 , 0.001)	(8 , 0.01)	(8 , 0.05)

Introducing Grid Search

Working through each cell on the grid:

		learn_rate		
max_depth		0.001	0.01	0.05
	4	(4 , 0.001)	(4 , 0.01)	(4 , 0.05)
	6	(6 , 0.001)	(6 , 0.01)	(6 , 0.05)
	8	(8 , 0.001)	(8 , 0.01)	(8 , 0.05)

(4,0.001) is equivalent to making an estimator like so:

```
GradientBoostingClassifier(max_depth=4, learning_rate=0.001)
```

Grid Search Pros & Cons

Some advantages of this approach:

Advantages:

- You don't have to write thousands of lines of code
- Finds the best model within the grid (*special note here!)
- Easy to explain

Grid Search Pros & Cons

Some disadvantages of this approach:

- Computationally expensive! Remember how quickly we made 6,000+ models?
- It is 'uninformed'. Results of one model don't help creating the next model.

We will cover 'informed' methods later!

Let's practice!

HYPERPARAMETER TUNING IN PYTHON

Grid Search with Scikit Learn

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GridSearchCV Object

Introducing a `GridSearchCV` object:

```
sklearn.model_selection.GridSearchCV(
    estimator,
    param_grid, scoring=None, fit_params=None,
    n_jobs=None, refit=True, cv='warn',
    verbose=0, pre_dispatch='2*n_jobs',
    error_score='raise-deprecating',
    return_train_score='warn')
```

Steps in a Grid Search

Steps in a Grid Search:

1. An algorithm to tune the hyperparameters. (Sometimes called an 'estimator')
2. Defining which hyperparameters we will tune
3. Defining a range of values for each hyperparameter
4. Setting a cross-validation scheme; and
5. Define a score function so we can decide which square on our grid was 'the best'.
6. Include extra useful information or functions

GridSearchCV Object Inputs

The important inputs are:

- `estimator`
- `param_grid`
- `cv`
- `scoring`
- `refit`
- `n_jobs`
- `return_train_score`

GridSearchCV 'estimator'

The `estimator` input:

- Essentially our algorithm
- You have already worked with KNN, Random Forest, GBM, Logistic Regression

Remember:

- Only one estimator per GridSearchCV object

GridSearchCV 'param_grid'

The `param_grid` input:

- Setting which hyperparameters and values to test

Rather than a list:

```
max_depth_list = [2, 4, 6, 8]
min_samples_leaf_list = [1, 2, 4, 6]
```

This would be:

```
param_grid = {'max_depth': [2, 4, 6, 8],
              'min_samples_leaf': [1, 2, 4, 6]}
```

GridSearchCV 'param_grid'

The `param_grid` input:

Remember: The keys in your `param_grid` dictionary must be valid hyperparameters.

For example, for a Logistic regression estimator:

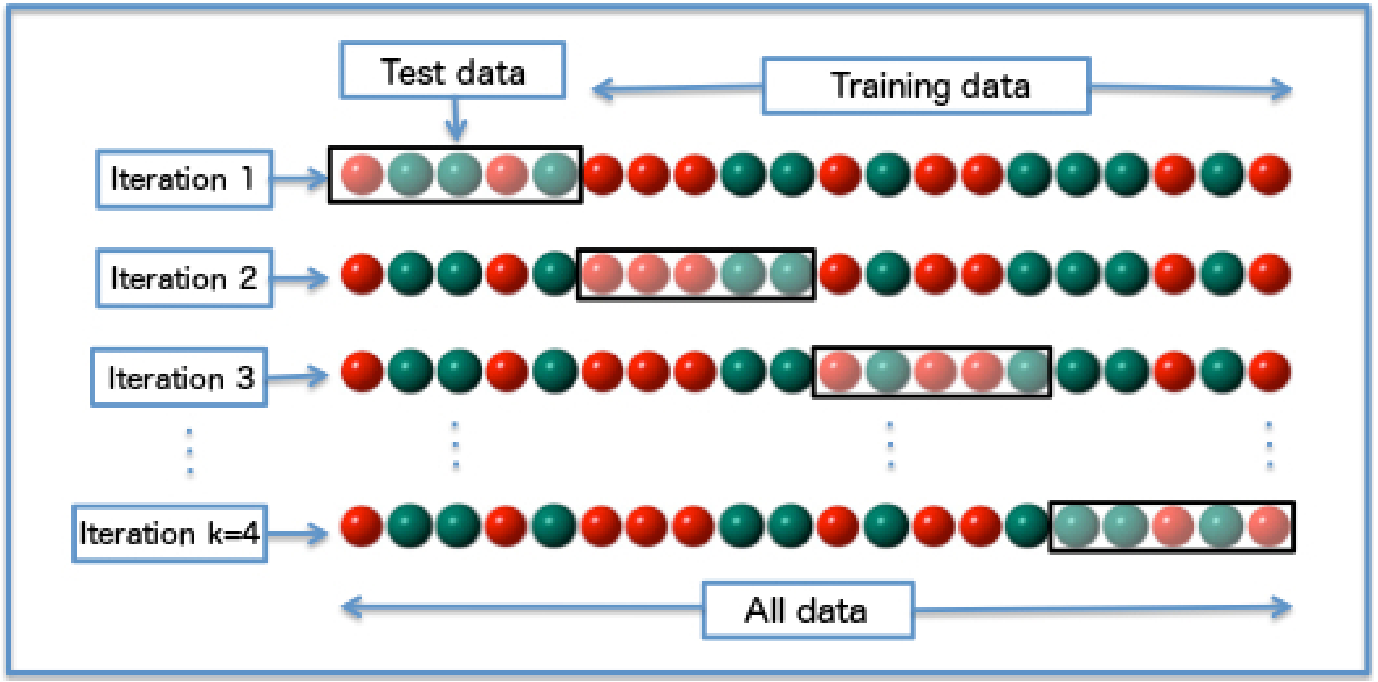
```
# Incorrect
param_grid = {'C': [0.1,0.2,0.5],
              'best_choice': [10,20,50]}
```

```
ValueError: Invalid parameter best_choice for estimator LogisticRegression
```

GridSearchCV 'cv'

The `cv` input:

- Choice of how to undertake cross-validation
- Using an integer undertakes k-fold cross validation where 5 or 10 is usually standard



GridSearchCV 'scoring'

The `scoring` input:

- Which score to use to choose the best grid square (model)
- Use your own or Scikit Learn's `metrics` module

You can check all the built in scoring functions this way:

```
from sklearn import metrics
sorted(metrics.SCORERS.keys())
```

GridSearchCV 'refit'

The `refit` input:

- Fits the best hyperparameters to the training data
- Allows the `GridSearchCV` object to be used as an estimator (for prediction)
- A very handy option!

GridSearchCV 'n_jobs'

The `n_jobs` input:

- Assists with parallel execution
- Allows multiple models to be created at the same time, rather than one after the other

Some handy code:

```
import os
print(os.cpu_count())
```

Careful using all your cores for modelling if you want to do other work!

GridSearchCV 'return_train_score'

The `return_train_score` input:

- Logs statistics about the training runs that were undertaken
- Useful for analyzing bias-variance trade-off but adds computational expense.
- Does not assist in picking the best model, only for analysis purposes

Building a GridSearchCV object

Building our own GridSearchCV Object:

```
# Create the grid
param_grid = {'max_depth': [2, 4, 6, 8], 'min_samples_leaf': [1, 2, 4, 6]}

#Get a base classifier with some set parameters.
rf_class = RandomForestClassifier(criterion='entropy', max_features='auto')
```

Building a GridSearchCv Object

Putting the pieces together:

```
grid_rf_class = GridSearchCV(
    estimator = rf_class,
    param_grid = parameter_grid,
    scoring='accuracy',
    n_jobs=4,
    cv = 10,
    refit=True,
    return_train_score=True)
```

Using a GridSearchCV Object

Because we set `refit` to `True` we can directly use the object:

```
#Fit the object to our data
grid_rf_class.fit(X_train, y_train)

# Make predictions
grid_rf_class.predict(X_test)
```

Let's practice!

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Understanding a grid search output

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Analyzing the output

Let's analyze the GridSearchCV outputs.

Three different groups for the GridSearchCV properties;

- A results log
  - `cv_results_`
- The best results
  - `best_index_` , `best_params_` & `best_score_`
- 'Extra information'
  - `scorer_` , `n_splits_` & `refit_time_`

Accessing object properties

Properties are accessed using the dot notation.

For example:

```
grid_search_object.property
```

Where `property` is the actual property you want to retrieve

The .cv_results_ property

The `cv_results_` property:

Read this into a DataFrame to print and analyze:

```
cv_results_df = pd.DataFrame(grid_rf_class.cv_results_)

print(cv_results_df.shape)
```

```
(12, 23)
```

- The 12 rows for the 12 squares in our grid or 12 models we ran

The .cv_results_ 'time' columns

The `time` columns refer to the time it took to fit (and score) the model.

Remember how we did a 5-fold cross-validation? This ran 5 times and stored the average and standard deviation of the times it took in seconds.

	mean_fit_time	std_fit_time	mean_score_time	std_score_time
0	0.321069	0.007236	0.015008	0.000871
1	0.678216	0.066385	0.034155	0.003767
2	0.939865	0.009502	0.055868	0.004148
3	0.296547	0.006261	0.017990	0.002803
4	0.686065	0.016163	0.040048	0.001304
5	1.097201	0.006327	0.057136	0.004468
6	0.416973	0.085533	0.021157	0.003901
7	0.788864	0.021954	0.042638	0.004802
8	1.198466	0.054694	0.049674	0.006884
9	0.398824	0.027500	0.025307	0.009473
10	0.719588	0.019231	0.035629	0.005712
11	0.847477	0.036584	0.029104	0.005220

The .cv_results_ 'param_' columns

The `param_` columns store the parameters it tested on that row, one column per parameter

param_max_depth	param_min_samples_leaf	param_n_estimators
10	1	100
10	1	200
10	2	100
10	2	200
10	2	300

The .cv_results_ 'param' column

The `params` column contains dictionary of all the parameters:

```
pd.set_option("display.max_colwidth", -1)
print(cv_results_df.loc[:, "params"])
```

params
{'max_depth': 10, 'min_samples_leaf': 1, 'n_estimators': 100}
{'max_depth': 10, 'min_samples_leaf': 1, 'n_estimators': 200}
{'max_depth': 10, 'min_samples_leaf': 2, 'n_estimators': 100}
{'max_depth': 10, 'min_samples_leaf': 2, 'n_estimators': 200}
{'max_depth': 10, 'min_samples_leaf': 2, 'n_estimators': 300}

The .cv_results_ 'test_score' columns

The `test_score` columns contain the scores on our test set for each of our cross-folds as well as some summary statistics:

split0_test_score	split1_test_score	...	mean_test_score	std_test_score
0.72820401	0.7859811	...	0.76010401	0.02995142
0.73539669	0.7963085	...	0.76590708	0.02721413
0.72929381	0.78686003	...	0.7718143	0.02775648
0.72820401	0.78554164	...	0.77044862	0.02794597
0.72885789	0.78795869	...	0.77122424	0.03288053

The .cv_results_ 'rank_test_score' column

The rank column, ordering the `mean_test_score` from best to worst:

rank_test_score
9
4
1
3
2

Extracting the best row

We can select the best grid square easily from `cv_results_` using the `rank_test_score` column

```
best_row = cv_results_df[cv_results_df["rank_test_score"] == 1]
print(best_row)
```

mean_fit_time	...	params	...	mean_test_score	rank_test_score
0.97765441	...	{'max_depth': 10, 'min_samples_leaf': 2, 'n_estimators': 200}	...	0.7718143	1

The .cv_results_ 'train_score' columns

The `test_score` columns are then repeated for the `training_scores` .

Some important notes to keep in mind:

- `return_train_score` must be `True` to include training scores columns.
- There is no ranking column for the training scores, as we only care about test set performance

The best grid square

Information on the best grid square is neatly summarized in the following three properties:

- `best_params_` , the dictionary of parameters that gave the best score.
- `best_score_` , the actual best score.
- `best_index_` , the row in our `cv_results_.rank_test_score` that was the best.

The best_estimator_ property

The `best_estimator_` property is an estimator built using the best parameters from the grid search.

For us this is a Random Forest estimator:

```
type(grid_rf_class.best_estimator_)
```

`sklearn.ensemble.forest.RandomForestClassifier`

We could also directly use this object as an estimator if we want!

The best_estimator_ property

```
print(grid_rf_class.best_estimator_)
```

```
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='entropy',
            max_depth=10, max_features='auto', max_leaf_nodes=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=300, n_jobs=None,
            oob_score=False, random_state=None, verbose=0,
            warm_start=False)
```

Extra information

Some extra information is available in the following properties:

- `scorer_`

What scorer function was used on the held out data. (we set it to AUC)

- `n_splits_`

How many cross-validation splits. (We set to 5)

- `refit_time_`

The number of seconds used for refitting the best model on the whole dataset.

Let's practice!

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