parameter_tuning_grid_search

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1 Hyperparameter tuning by grid-search

In the previous notebook, we saw that hyperparameters can affect the statistical performance of a model. In this notebook, we will show how to optimize hyperparameters using a grid-search approach.

1.1 Our predictive model

Let us reload the dataset as we did previously:

[1]:
```
from sklearn import set_config

set_config(display="diagram")
```

[2]:
```
import pandas as pd

adult_census = pd.read_csv("../datasets/adult-census.csv")
```

We extract the column containing the target.

[3]:
```
target_name = "class"
target = adult_census[target_name]
target
```

[3]:
```
0         <=50K
1         <=50K
2          >50K
3          >50K
4         <=50K
          …
48837     <=50K
48838      >50K
48839     <=50K
48840     <=50K
48841      >50K
Name: class, Length: 48842, dtype: object
```

We drop from our data the target and the "education-num" column which duplicates the information from the "education" column.

```
[4]: data = adult_census.drop(columns=[target_name, "education-num"])
     data.head()
```

```
[4]:    age  workclass      education       marital-status          occupation  \
     0   25    Private           11th        Never-married   Machine-op-inspct
     1   38    Private        HS-grad   Married-civ-spouse     Farming-fishing
     2   28  Local-gov     Assoc-acdm   Married-civ-spouse     Protective-serv
     3   44    Private   Some-college   Married-civ-spouse   Machine-op-inspct
     4   18          ?   Some-college        Never-married                   ?

       relationship   race     sex  capital-gain  capital-loss  hours-per-week  \
     0    Own-child  Black    Male             0             0              40
     1      Husband  White    Male             0             0              50
     2      Husband  White    Male             0             0              40
     3      Husband  Black    Male          7688             0              40
     4    Own-child  White  Female             0             0              30

       native-country
     0  United-States
     1  United-States
     2  United-States
     3  United-States
     4  United-States
```

Once the dataset is loaded, we split it into a training and testing sets.

```
[5]: from sklearn.model_selection import train_test_split

     data_train, data_test, target_train, target_test = train_test_split(
         data, target, random_state=42)
```

We will define a pipeline as seen in the first module. It will handle both numerical and categorical features.

As we will use a tree-based model as a predictor, here we apply an ordinal encoder on the categorical features: it encodes every category with an arbitrary integer. For simple models such as linear models, a one-hot encoder should be preferred. But for complex models, in particular tree-based models, the ordinal encoder is useful as it avoids having high-dimensional representations.

First we select all the categorical columns.

```
[6]: from sklearn.compose import make_column_selector as selector

     categorical_columns_selector = selector(dtype_include=object)
     categorical_columns = categorical_columns_selector(data)
```

Then we build our ordinal encoder, giving it the known categories.

[7]:
```
from sklearn.preprocessing import OrdinalEncoder

categorical_preprocessor = OrdinalEncoder(handle_unknown="use_encoded_value",
                                          unknown_value=-1)
```

We now use a column transformer with code to select the categorical columns and apply to them the ordinal encoder.

[8]:
```
from sklearn.compose import ColumnTransformer

preprocessor = ColumnTransformer([
    ('cat-preprocessor', categorical_preprocessor, categorical_columns)],
    remainder='passthrough', sparse_threshold=0)
```

Finally, we use a tree-based classifier (i.e. histogram gradient-boosting) to predict whether or not a person earns more than 50 k$ a year.

[9]:
```
# for the moment this line is required to import HistGradientBoostingClassifier
from sklearn.experimental import enable_hist_gradient_boosting
from sklearn.ensemble import HistGradientBoostingClassifier
from sklearn.pipeline import Pipeline

model = Pipeline([
    ("preprocessor", preprocessor),
    ("classifier",
     HistGradientBoostingClassifier(random_state=42, max_leaf_nodes=4))])
model
```

[9]:
```
Pipeline(steps=[('preprocessor',
                 ColumnTransformer(remainder='passthrough', sparse_threshold=0,
                                   transformers=[('cat-preprocessor',
OrdinalEncoder(handle_unknown='use_encoded_value',
unknown_value=-1),
                                                  ['workclass', 'education',
                                                   'marital-status',
                                                   'occupation', 'relationship',
                                                   'race', 'sex',
                                                   'native-country'])])),
                ('classifier',
                 HistGradientBoostingClassifier(max_leaf_nodes=4,
                                                random_state=42))])
```

1.2 Tuning using a grid-search

Instead of manually writing the two `for` loops, scikit-learn provides a class called `GridSearchCV` which implement the exhaustive search implemented during the exercise.

Let see how to use the `GridSearchCV` estimator for doing such search. Since the grid-search will be costly, we will only explore the combination learning-rate and the maximum number of nodes.

```
[10]: %%time
from sklearn.model_selection import GridSearchCV

param_grid = {
    'classifier__learning_rate': (0.05, 0.1, 0.5, 1, 5),
    'classifier__max_leaf_nodes': (3, 10, 30, 100)}
model_grid_search = GridSearchCV(model, param_grid=param_grid,
                                 n_jobs=4, cv=2)
model_grid_search.fit(data_train, target_train)
```

```
CPU times: user 2.74 s, sys: 141 ms, total: 2.88 s
Wall time: 5.08 s
```

```
[10]: GridSearchCV(cv=2,
             estimator=Pipeline(steps=[('preprocessor',
ColumnTransformer(remainder='passthrough',
                                                          sparse_threshold=0,
                                                          transformers=[('cat-
preprocessor',
OrdinalEncoder(handle_unknown='use_encoded_value',
        unknown_value=-1),
['workclass',
'education',
'marital-status',
'occupation',
'relationship',
'race',
                                                                         'sex',
'native-country'])])),
                                       ('classifier',
HistGradientBoostingClassifier(max_leaf_nodes=4,
random_state=42))]),
             n_jobs=4,
             param_grid={'classifier__learning_rate': (0.05, 0.1, 0.5, 1, 5),
                         'classifier__max_leaf_nodes': (3, 10, 30, 100)})
```

Finally, we will check the accuracy of our model using the test set.

```
[11]: accuracy = model_grid_search.score(data_test, target_test)
print(
    f"The test accuracy score of the grid-searched pipeline is: "
    f"{accuracy:.2f}"
)
```

```
The test accuracy score of the grid-searched pipeline is: 0.88
```

Warning

Be aware that the evaluation should normally be performed in a cross-validation framework by providing model_grid_search as a model to the cross_validate function.

Here, we are using a single train-test split to highlight the specificities of the model_grid_search instance. We will show such examples in the last section of this notebook.

The `GridSearchCV` estimator takes a `param_grid` parameter which defines all hyperparameters and their associated values. The grid-search will be in charge of creating all possible combinations and test them.

The number of combinations will be equal to the product of the number of values to explore for each parameter (e.g. in our example 4 x 4 combinations). Thus, adding new parameters with their associated values to be explored become rapidly computationally expensive.

Once the grid-search is fitted, it can be used as any other predictor by calling `predict` and `predict_proba`. Internally, it will use the model with the best parameters found during `fit`.

Get predictions for the 5 first samples using the estimator with the best parameters.

[12]:
```
model_grid_search.predict(data_test.iloc[0:5])
```

[12]:
```
array([' <=50K', ' <=50K', ' >50K', ' <=50K', ' >50K'], dtype=object)
```

You can know about these parameters by looking at the `best_params_` attribute.

[13]:
```
print(f"The best set of parameters is: "
      f"{model_grid_search.best_params_}")
```

```
The best set of parameters is: {'classifier__learning_rate': 0.1,
'classifier__max_leaf_nodes': 30}
```

The accuracy and the best parameters of the grid-searched pipeline are similar to the ones we found in the previous exercise, where we searched the best parameters "by hand" through a double for loop.

In addition, we can inspect all results which are stored in the attribute `cv_results_` of the grid-search. We will filter some specific columns from these results.

[14]:
```
cv_results = pd.DataFrame(model_grid_search.cv_results_).sort_values(
    "mean_test_score", ascending=False)
cv_results.head()
```

[14]:
```
    mean_fit_time  std_fit_time  mean_score_time  std_score_time  \
6        0.402035      0.036689         0.096746        0.002013
2        0.529683      0.044697         0.114243        0.003284
10       0.144486      0.001599         0.065035        0.001020
5        0.314567      0.048679         0.098290        0.005070
8        0.182427      0.001276         0.080603        0.002204

   param_classifier__learning_rate param_classifier__max_leaf_nodes  \
6                              0.1                               30
2                             0.05                               30
10                             0.5                               30
```

```
5                              0.1                                10
8                              0.5                                 3

                                               params  split0_test_score  \
6   {'classifier__learning_rate': 0.1, 'classifier…           0.868912
2   {'classifier__learning_rate': 0.05, 'classifie…           0.868530
10  {'classifier__learning_rate': 0.5, 'classifier…           0.867056
5   {'classifier__learning_rate': 0.1, 'classifier…           0.866783
8   {'classifier__learning_rate': 0.5, 'classifier…           0.864872

    split1_test_score  mean_test_score  std_test_score  rank_test_score
6            0.867213         0.868063        0.000850                1
2            0.866667         0.867598        0.000932                2
10           0.865902         0.866479        0.000577                3
5            0.866066         0.866425        0.000359                4
8            0.866776         0.865824        0.000952                5
```

Let us focus on the most interesting columns and shorten the parameter names to remove the `"param_classifier__"` prefix for readability:

[15]:
```
# get the parameter names
column_results = [f"param_{name}" for name in param_grid.keys()]
column_results += [
    "mean_test_score", "std_test_score", "rank_test_score"]
cv_results = cv_results[column_results]
```

[16]:
```
def shorten_param(param_name):
    if "__" in param_name:
        return param_name.rsplit("__", 1)[1]
    return param_name


cv_results = cv_results.rename(shorten_param, axis=1)
cv_results
```

[16]:
```
   learning_rate max_leaf_nodes  mean_test_score  std_test_score  \
6            0.1             30         0.868063        0.000850
2           0.05             30         0.867598        0.000932
10           0.5             30         0.866479        0.000577
5            0.1             10         0.866425        0.000359
8            0.5              3         0.865824        0.000952
9            0.5             10         0.865824        0.000031
3           0.05            100         0.865797        0.001259
7            0.1            100         0.864732        0.000795
1           0.05             10         0.862029        0.000222
11           0.5            100         0.859491        0.001069
13             1             10         0.858863        0.004036
```

```
12            1           3      0.857389       0.003545
4           0.1           3      0.853266       0.000515
14            1          30      0.851028       0.002707
15            1         100      0.835194       0.004609
0          0.05           3      0.827196       0.000214
19            5         100      0.727579       0.055780
18            5          30      0.638062       0.144696
17            5          10      0.527527       0.175411
16            5           3      0.283476       0.003775

    rank_test_score
6                 1
2                 2
10                3
5                 4
8                 5
9                 6
3                 7
7                 8
1                 9
11               10
13               11
12               12
4                13
14               14
15               15
0                16
19               17
18               18
17               19
16               20
```

With only 2 parameters, we might want to visualize the grid-search as a heatmap. We need to transform our `cv_results` into a dataframe where:

- the rows will correspond to the learning-rate values;
- the columns will correspond to the maximum number of leaf;
- the content of the dataframe will be the mean test scores.

[17]:
```
pivoted_cv_results = cv_results.pivot_table(
    values="mean_test_score", index=["learning_rate"],
    columns=["max_leaf_nodes"])

pivoted_cv_results
```

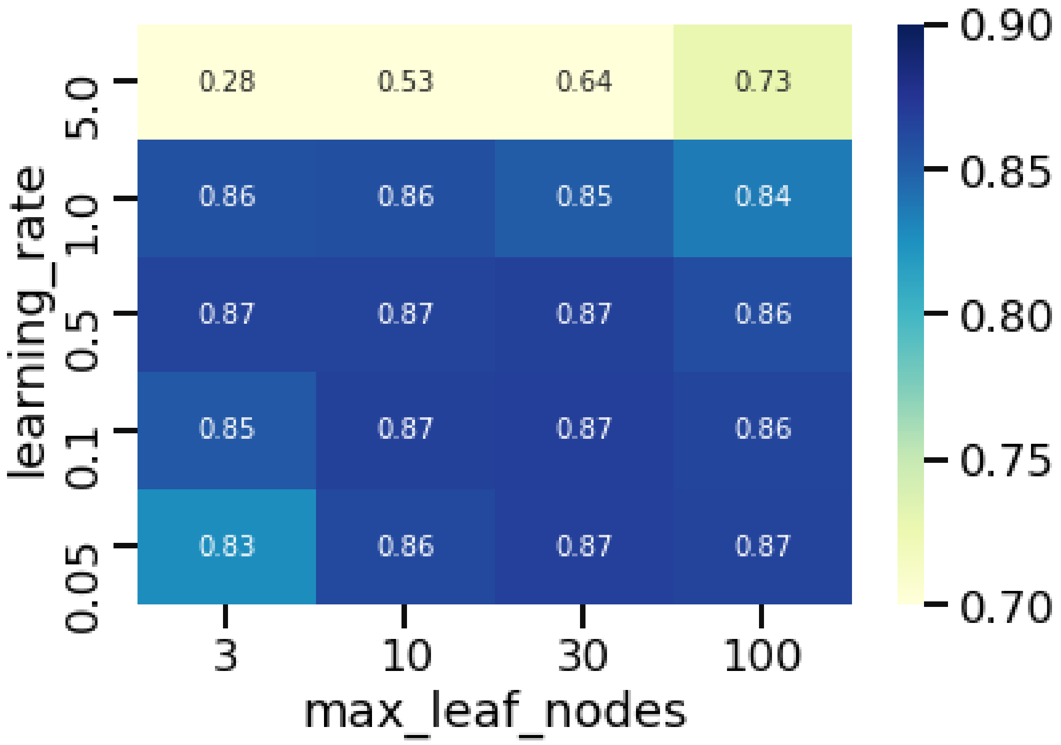
[17]:
```
max_leaf_nodes       3         10         30        100
learning_rate
0.05            0.827196  0.862029  0.867598  0.865797
```

```
0.10           0.853266  0.866425  0.868063  0.864732
0.50           0.865824  0.865824  0.866479  0.859491
1.00           0.857389  0.858863  0.851028  0.835194
5.00           0.283476  0.527527  0.638062  0.727579
```

We can use a heatmap representation to show the above dataframe visually.

[18]:
```python
import seaborn as sns

ax = sns.heatmap(pivoted_cv_results, annot=True, cmap="YlGnBu", vmin=0.7,
                 vmax=0.9)
ax.invert_yaxis()
```



The above tables highlights the following things:

- for too high values of `learning_rate`, the statistical performance of the model is degraded and adjusting the value of `max_leaf_nodes` cannot fix that problem;
- outside of this pathological region, we observe that the optimal choice of `max_leaf_nodes` depends on the value of `learning_rate`;
- in particular, we observe a "diagonal" of good models with an accuracy close to the maximal of 0.87: when the value of `max_leaf_nodes` is increased, one should increase the value of `learning_rate` accordingly to preserve a good accuracy.

The precise meaning of those two parameters will be explained in a latter notebook.

For now we will note that, in general, **there is no unique optimal parameter setting**: 6 models out of the 16 parameter configuration reach the maximal accuracy (up to small random fluctuations caused by the sampling of the training set).

In this notebook we have seen:

- how to optimize the hyperparameters of a predictive model via a grid-search;
- that searching for more than two hyperparamters is too costly;
- that a grid-search does not necessarily find an optimal solution.