wines_knn_hyper

November 26, 2021

1 Sélection des hyper-paramètres

Le modèle des plus proches voisins KNeighborsRegressor est paramétrable. Le nombre de voisins est variables, la prédiction peut dépendre du plus proche voisins ou des k plus proches proches. Comment choisir k ?

[1]:
```
%matplotlib inline
```

[2]:
```
from papierstat.datasets import load_wines_dataset
df = load_wines_dataset()
```

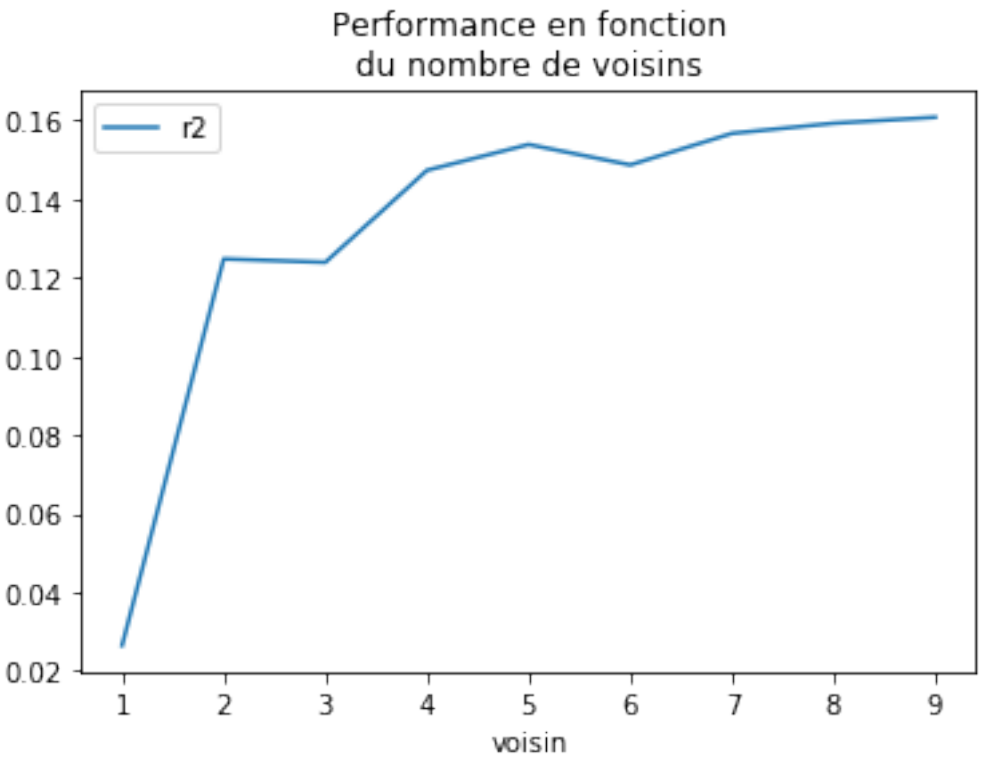
[3]:
```
import numpy.random as rnd
index = list(df.index)
rnd.shuffle(index)
df_alea = df.iloc[index, :].reset_index(drop=True)
X = df_alea.drop(['quality', 'color'], axis=1)
y = df_alea['quality']
```

[4]:
```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y)
```

On fait une boucle sur un paramètre.

[5]:
```
from sklearn.neighbors import KNeighborsRegressor
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import r2_score
voisins = []
r2s = []
for n in range(1, 10):
    knn = KNeighborsRegressor(n_neighbors=n)
    knn.fit(X_train, y_train)
    r2 = r2_score(y_test, knn.predict(X_test))
    voisins.append(n)
    r2s.append(r2)
```

[6]:
```
import pandas
df = pandas.DataFrame(dict(voisin=voisins, r2=r2s))
ax = df.plot(x='voisin', y='r2')
ax.set_title("Performance en fonction\ndu nombre de voisins");
```



La fonction GridSearchCV automatise la recherche d'un optimum parmi les hyperparamètre, elle utilise notamment la validation croisée. On teste toutes les valeurs de k de 1 à 20.

[7]:
```
parameters = {'n_neighbors': list(range(1,31))}
```

[8]:
```
from sklearn.neighbors import KNeighborsRegressor
from sklearn.model_selection import GridSearchCV
knn = KNeighborsRegressor()
grid = GridSearchCV(knn, parameters, verbose=2, return_train_score=True)
```

[9]:
```
grid.fit(X, y)
```

```
Fitting 3 folds for each of 30 candidates, totalling 90 fits
[CV] n_neighbors=1 …
[CV] … n_neighbors=1, total=   0.0s
[CV] n_neighbors=1 …
[CV] … n_neighbors=1, total=   0.0s
[CV] n_neighbors=1 …
[CV] … n_neighbors=1, total=   0.0s
[CV] n_neighbors=2 …

[Parallel(n_jobs=1)]: Done   1 out of   1 | elapsed:    0.0s remaining:    0.0s

[CV] … n_neighbors=2, total=   0.0s
[CV] n_neighbors=2 …
[CV] … n_neighbors=2, total=   0.0s
[CV] n_neighbors=2 …
```

```
[CV] … n_neighbors=2, total=   0.0s
[CV] n_neighbors=3 …
[CV] … n_neighbors=3, total=   0.0s
[CV] n_neighbors=3 …
[CV] … n_neighbors=3, total=   0.0s
[CV] n_neighbors=3 …
[CV] … n_neighbors=3, total=   0.0s
[CV] n_neighbors=4 …
[CV] … n_neighbors=4, total=   0.0s
[CV] n_neighbors=4 …
[CV] … n_neighbors=4, total=   0.0s
[CV] n_neighbors=4 …
[CV] … n_neighbors=4, total=   0.0s
[CV] n_neighbors=5 …
[CV] … n_neighbors=5, total=   0.0s
[CV] n_neighbors=5 …
[CV] … n_neighbors=5, total=   0.0s
[CV] n_neighbors=5 …
[CV] … n_neighbors=5, total=   0.0s
[CV] n_neighbors=6 …
[CV] … n_neighbors=6, total=   0.0s
[CV] n_neighbors=6 …
[CV] … n_neighbors=6, total=   0.0s
[CV] n_neighbors=6 …
[CV] … n_neighbors=6, total=   0.0s
[CV] n_neighbors=7 …
[CV] … n_neighbors=7, total=   0.0s
[CV] n_neighbors=7 …
[CV] … n_neighbors=7, total=   0.0s
[CV] n_neighbors=7 …
[CV] … n_neighbors=7, total=   0.0s
[CV] n_neighbors=8 …
[CV] … n_neighbors=8, total=   0.0s
[CV] n_neighbors=8 …
[CV] … n_neighbors=8, total=   0.0s
[CV] n_neighbors=8 …
[CV] … n_neighbors=8, total=   0.0s
[CV] n_neighbors=9 …
[CV] … n_neighbors=9, total=   0.0s
[CV] n_neighbors=9 …
[CV] … n_neighbors=9, total=   0.0s
[CV] n_neighbors=9 …
[CV] … n_neighbors=9, total=   0.0s
[CV] n_neighbors=10 …
[CV] … n_neighbors=10, total=   0.0s
[CV] n_neighbors=10 …
[CV] … n_neighbors=10, total=   0.0s
[CV] n_neighbors=10 …
[CV] … n_neighbors=10, total=   0.0s
[CV] n_neighbors=11 …
[CV] … n_neighbors=11, total=   0.0s
[CV] n_neighbors=11 …
[CV] … n_neighbors=11, total=   0.0s
[CV] n_neighbors=11 …
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[CV] … n_neighbors=11, total=   0.0s
[CV] n_neighbors=12 …
[CV] … n_neighbors=12, total=   0.0s
[CV] n_neighbors=12 …
[CV] … n_neighbors=12, total=   0.0s
[CV] n_neighbors=12 …
[CV] … n_neighbors=12, total=   0.0s
[CV] n_neighbors=13 …
[CV] … n_neighbors=13, total=   0.0s
[CV] n_neighbors=13 …
[CV] … n_neighbors=13, total=   0.0s
[CV] n_neighbors=13 …
[CV] … n_neighbors=13, total=   0.0s
[CV] n_neighbors=14 …
[CV] … n_neighbors=14, total=   0.0s
[CV] n_neighbors=14 …
[CV] … n_neighbors=14, total=   0.0s
[CV] n_neighbors=14 …
[CV] … n_neighbors=14, total=   0.0s
[CV] n_neighbors=15 …
[CV] … n_neighbors=15, total=   0.0s
[CV] n_neighbors=15 …
[CV] … n_neighbors=15, total=   0.0s
[CV] n_neighbors=15 …
[CV] … n_neighbors=15, total=   0.0s
[CV] n_neighbors=16 …
[CV] … n_neighbors=16, total=   0.0s
[CV] n_neighbors=16 …
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[CV] n_neighbors=16 …
[CV] … n_neighbors=16, total=   0.0s
[CV] n_neighbors=17 …
[CV] … n_neighbors=17, total=   0.0s
[CV] n_neighbors=17 …
[CV] … n_neighbors=17, total=   0.0s
[CV] n_neighbors=17 …
[CV] … n_neighbors=17, total=   0.0s
[CV] n_neighbors=18 …
[CV] … n_neighbors=18, total=   0.0s
[CV] n_neighbors=18 …
[CV] … n_neighbors=18, total=   0.0s
[CV] n_neighbors=18 …
[CV] … n_neighbors=18, total=   0.0s
[CV] n_neighbors=19 …
[CV] … n_neighbors=19, total=   0.0s
[CV] n_neighbors=19 …
[CV] … n_neighbors=19, total=   0.0s
[CV] n_neighbors=19 …
[CV] … n_neighbors=19, total=   0.0s
[CV] n_neighbors=20 …
[CV] … n_neighbors=20, total=   0.0s
[CV] n_neighbors=20 …
[CV] … n_neighbors=20, total=   0.0s
[CV] n_neighbors=20 …
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[CV] … n_neighbors=20, total=   0.0s
[CV] n_neighbors=21 …
[CV] … n_neighbors=21, total=   0.0s
[CV] n_neighbors=21 …
[CV] … n_neighbors=21, total=   0.0s
[CV] n_neighbors=21 …
[CV] … n_neighbors=21, total=   0.0s
[CV] n_neighbors=22 …
[CV] … n_neighbors=22, total=   0.0s
[CV] n_neighbors=22 …
[CV] … n_neighbors=22, total=   0.0s
[CV] n_neighbors=22 …
[CV] … n_neighbors=22, total=   0.0s
[CV] n_neighbors=23 …
[CV] … n_neighbors=23, total=   0.0s
[CV] n_neighbors=23 …
[CV] … n_neighbors=23, total=   0.0s
[CV] n_neighbors=23 …
[CV] … n_neighbors=23, total=   0.0s
[CV] n_neighbors=24 …
[CV] … n_neighbors=24, total=   0.0s
[CV] n_neighbors=24 …
[CV] … n_neighbors=24, total=   0.0s
[CV] n_neighbors=24 …
[CV] … n_neighbors=24, total=   0.0s
[CV] n_neighbors=25 …
[CV] … n_neighbors=25, total=   0.0s
[CV] n_neighbors=25 …
[CV] … n_neighbors=25, total=   0.0s
[CV] n_neighbors=25 …
[CV] … n_neighbors=25, total=   0.0s
[CV] n_neighbors=26 …
[CV] … n_neighbors=26, total=   0.0s
[CV] n_neighbors=26 …
[CV] … n_neighbors=26, total=   0.0s
[CV] n_neighbors=26 …
[CV] … n_neighbors=26, total=   0.0s
[CV] n_neighbors=27 …
[CV] … n_neighbors=27, total=   0.0s
[CV] n_neighbors=27 …
[CV] … n_neighbors=27, total=   0.0s
[CV] n_neighbors=27 …
[CV] … n_neighbors=27, total=   0.0s
[CV] n_neighbors=28 …
[CV] … n_neighbors=28, total=   0.0s
[CV] n_neighbors=28 …
[CV] … n_neighbors=28, total=   0.0s
[CV] n_neighbors=28 …
[CV] … n_neighbors=28, total=   0.0s
[CV] n_neighbors=29 …
[CV] … n_neighbors=29, total=   0.0s
[CV] n_neighbors=29 …
[CV] … n_neighbors=29, total=   0.0s
[CV] n_neighbors=29 …
```
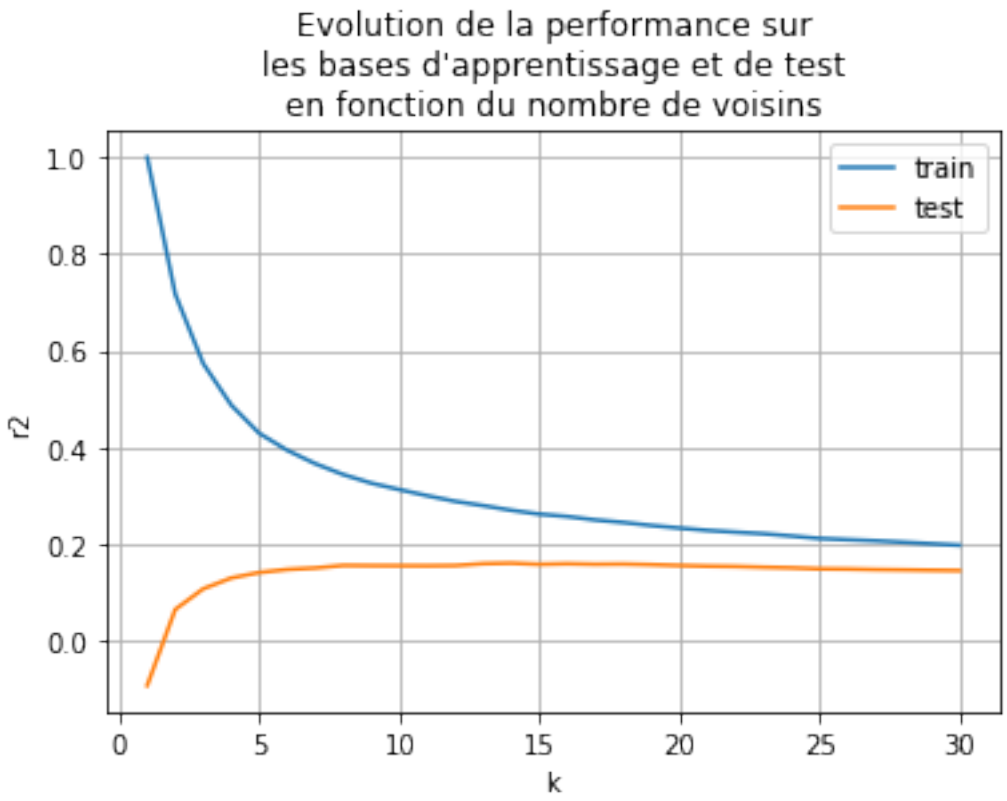

```
[CV] … n_neighbors=29, total=   0.0s
[CV] n_neighbors=30 …
[CV] … n_neighbors=30, total=   0.0s
[CV] n_neighbors=30 …
[CV] … n_neighbors=30, total=   0.0s
[CV] n_neighbors=30 …
[CV] … n_neighbors=30, total=   0.0s

[Parallel(n_jobs=1)]: Done  90 out of  90 | elapsed:   13.1s finished
```

[9]:
```
GridSearchCV(cv=None, error_score='raise',
       estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30,
metric='minkowski',
          metric_params=None, n_jobs=1, n_neighbors=5, p=2,
          weights='uniform'),
       fit_params=None, iid=True, n_jobs=1,
       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]},
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring=None, verbose=2)
```

[10]:
```
res = grid.cv_results_
k = res['param_n_neighbors']
train_score = res['mean_train_score']
test_score = res['mean_test_score']

import pandas
df_score = pandas.DataFrame(dict(k=k, test=test_score, train=train_score))
ax = df_score.plot(x='k', y='train', figsize=(6, 4))
df_score.plot(x='k', y='test', ax=ax, grid=True)
ax.set_title("Evolution de la performance sur\nles bases d'apprentissage et de test" +
             "\nen fonction du nombre de voisins")
ax.set_ylabel("r2");
```



On voit que le modèle gagne en pertinence sur la base de test et que le nombre de voisins optimal parmi ceux essayés se situe autour de 15.

[11]:
```
df_score[12:17]
```

[11]:

	k	test	train
12	13	0.159266	0.279302
13	14	0.160284	0.269703
14	15	0.157910	0.261720
15	16	0.159066	0.256823
16	17	0.158029	0.249684

L'erreur sur la base d'apprentissage augmente de manière sensible (R^2 baisse). Voyons ce qu'il en est un peu plus loin.

[12]:
```
parameters = {'n_neighbors': list(range(5, 51, 5)) + list(range(50, 201, 20))}
grid = GridSearchCV(knn, parameters, verbose=2, return_train_score=True)
grid.fit(X, y)
```

```
Fitting 3 folds for each of 18 candidates, totalling 54 fits
[CV] n_neighbors=5 …
[CV] … n_neighbors=5, total=   0.0s
[CV] n_neighbors=5 …
[CV] … n_neighbors=5, total=   0.0s
[CV] n_neighbors=5 …

[Parallel(n_jobs=1)]: Done   1 out of   1 | elapsed:    0.0s remaining:    0.0s
```

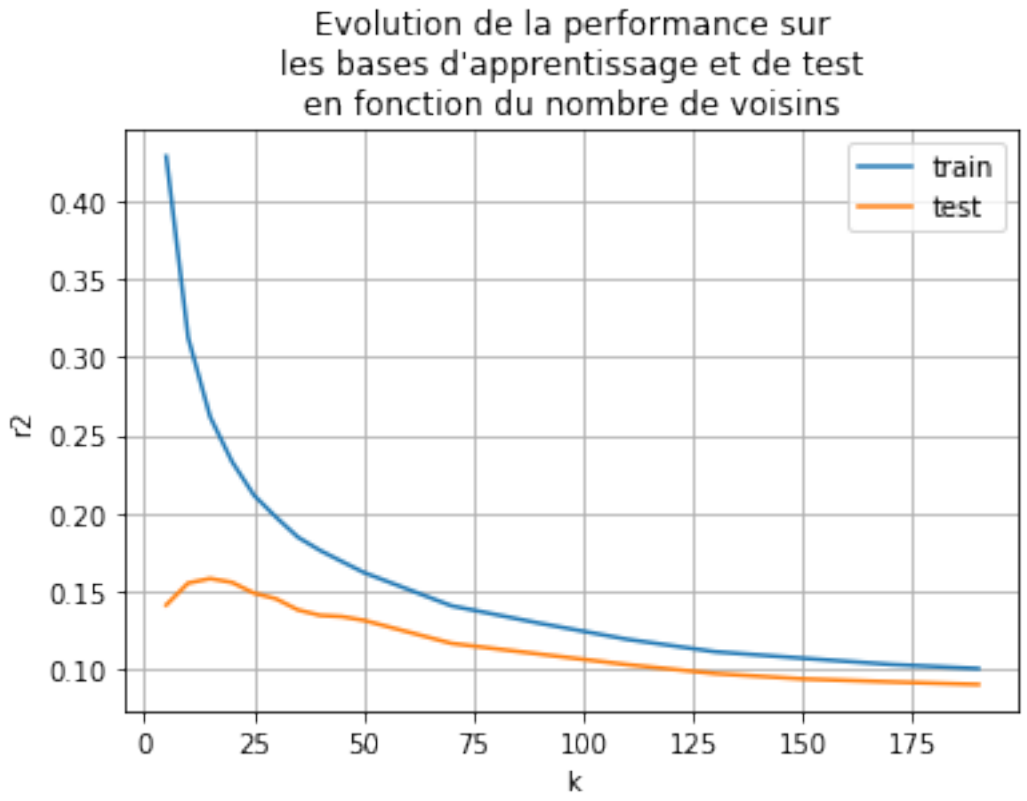
```
[CV] … n_neighbors=5, total=   0.0s
[CV] n_neighbors=10 …
[CV] … n_neighbors=10, total=   0.0s
[CV] n_neighbors=10 …
[CV] … n_neighbors=10, total=   0.0s
[CV] n_neighbors=10 …
[CV] … n_neighbors=10, total=   0.0s
[CV] n_neighbors=15 …
[CV] … n_neighbors=15, total=   0.0s
[CV] n_neighbors=15 …
[CV] … n_neighbors=15, total=   0.0s
[CV] n_neighbors=15 …
[CV] … n_neighbors=15, total=   0.0s
[CV] n_neighbors=20 …
[CV] … n_neighbors=20, total=   0.0s
[CV] n_neighbors=20 …
[CV] … n_neighbors=20, total=   0.0s
[CV] n_neighbors=20 …
[CV] … n_neighbors=20, total=   0.0s
[CV] n_neighbors=25 …
[CV] … n_neighbors=25, total=   0.0s
[CV] n_neighbors=25 …
[CV] … n_neighbors=25, total=   0.0s
[CV] n_neighbors=25 …
[CV] … n_neighbors=25, total=   0.0s
[CV] n_neighbors=30 …
[CV] … n_neighbors=30, total=   0.0s
[CV] n_neighbors=30 …
[CV] … n_neighbors=30, total=   0.0s
[CV] n_neighbors=30 …
[CV] … n_neighbors=30, total=   0.0s
[CV] n_neighbors=35 …
[CV] … n_neighbors=35, total=   0.0s
[CV] n_neighbors=35 …
[CV] … n_neighbors=35, total=   0.0s
[CV] n_neighbors=35 …
[CV] … n_neighbors=35, total=   0.0s
[CV] n_neighbors=40 …
[CV] … n_neighbors=40, total=   0.0s
[CV] n_neighbors=40 …
[CV] … n_neighbors=40, total=   0.0s
[CV] n_neighbors=40 …
[CV] … n_neighbors=40, total=   0.0s
[CV] n_neighbors=45 …
[CV] … n_neighbors=45, total=   0.0s
[CV] n_neighbors=45 …
[CV] … n_neighbors=45, total=   0.0s
[CV] n_neighbors=45 …
[CV] … n_neighbors=45, total=   0.1s
[CV] n_neighbors=50 …
[CV] … n_neighbors=50, total=   0.0s
[CV] n_neighbors=50 …
[CV] … n_neighbors=50, total=   0.0s
[CV] n_neighbors=50 …
```

```
[CV] … n_neighbors=50, total=   0.0s
[CV] n_neighbors=50 …
[CV] … n_neighbors=50, total=   0.0s
[CV] n_neighbors=50 …
[CV] … n_neighbors=50, total=   0.1s
[CV] n_neighbors=50 …
[CV] … n_neighbors=50, total=   0.0s
[CV] n_neighbors=70 …
[CV] … n_neighbors=70, total=   0.0s
[CV] n_neighbors=70 …
[CV] … n_neighbors=70, total=   0.0s
[CV] n_neighbors=70 …
[CV] … n_neighbors=70, total=   0.0s
[CV] n_neighbors=90 …
[CV] … n_neighbors=90, total=   0.0s
[CV] n_neighbors=90 …
[CV] … n_neighbors=90, total=   0.0s
[CV] n_neighbors=90 …
[CV] … n_neighbors=90, total=   0.0s
[CV] n_neighbors=110 …
[CV] … n_neighbors=110, total=   0.1s
[CV] n_neighbors=110 …
[CV] … n_neighbors=110, total=   0.1s
[CV] n_neighbors=110 …
[CV] … n_neighbors=110, total=   0.1s
[CV] n_neighbors=130 …
[CV] … n_neighbors=130, total=   0.1s
[CV] n_neighbors=130 …
[CV] … n_neighbors=130, total=   0.1s
[CV] n_neighbors=130 …
[CV] … n_neighbors=130, total=   0.1s
[CV] n_neighbors=150 …
[CV] … n_neighbors=150, total=   0.1s
[CV] n_neighbors=150 …
[CV] … n_neighbors=150, total=   0.1s
[CV] n_neighbors=150 …
[CV] … n_neighbors=150, total=   0.1s
[CV] n_neighbors=170 …
[CV] … n_neighbors=170, total=   0.1s
[CV] n_neighbors=170 …
[CV] … n_neighbors=170, total=   0.1s
[CV] n_neighbors=170 …
[CV] … n_neighbors=170, total=   0.1s
[CV] n_neighbors=190 …
[CV] … n_neighbors=190, total=   0.1s
[CV] n_neighbors=190 …
[CV] … n_neighbors=190, total=   0.1s
[CV] n_neighbors=190 …
[CV] … n_neighbors=190, total=   0.1s

[Parallel(n_jobs=1)]: Done  54 out of  54 | elapsed:   18.0s finished
```

[12]:
```
GridSearchCV(cv=None, error_score='raise',
       estimator=KNeighborsRegressor(algorithm='auto', leaf_size=30,
```

```
metric='minkowski',
          metric_params=None, n_jobs=1, n_neighbors=5, p=2,
          weights='uniform'),
       fit_params=None, iid=True, n_jobs=1,
       param_grid={'n_neighbors': [5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 50,
70, 90, 110, 130, 150, 170, 190]},
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring=None, verbose=2)
```

[13]:
```
res = grid.cv_results_
k = res['param_n_neighbors']
train_score = res['mean_train_score']
test_score = res['mean_test_score']

import pandas
df_score = pandas.DataFrame(dict(k=k, test=test_score, train=train_score))
ax = df_score.plot(x='k', y='train', figsize=(6, 4))
df_score.plot(x='k', y='test', ax=ax, grid=True)
ax.set_title("Evolution de la performance sur\nles bases d'apprentissage et de test" +
             "\nen fonction du nombre de voisins")
ax.set_ylabel("r2");
```



Après 25 voisins, la pertinence du modèle décroît fortement, ce qui paraît normal car plus il y a de voisins, moins la prédiction est locale en quelque sorte.

[14]: