topk_cpp

April 5, 2022

1 Fast TopK elements

Looking for the top k elements is something needed to implement a simple k nearest neighbors. The implementation *scikit-learn* is using relies on *numpy*: _kneighbors_reduce_func. *mlprodict* also contains a C++ implementation of the same function. Let's compare them.

[1]:
```
from jyquickhelper import add_notebook_menu
add_notebook_menu()
```

[1]:
```
<IPython.core.display.HTML object>
```

[2]:
```
%matplotlib inline
```

1.1 Two implementations

We assume we are looking for the `k` nearest elements of every row of matrix `X` which is a dense matrix of doubles.

[3]:
```
import numpy.random as rnd
from sklearn.neighbors._base import KNeighborsMixin

mixin = KNeighborsMixin()
```

[4]:
```
def topk_sklearn(X, k):
    return mixin._kneighbors_reduce_func(X, 0, k, False)

X = rnd.randn(5, 10)
ind = topk_sklearn(X, 3)
ind
```

[4]:
```
array([[2, 7, 3],
       [7, 0, 8],
       [1, 5, 6],
       [8, 9, 3],
       [4, 6, 5]], dtype=int64)
```

Now the implementation with *mlprodict* (C++) available at topk_element_min. It uses heap.

[5]:
```
from mlprodict.onnxrt.ops_cpu._op_onnx_numpy import topk_element_min_double
```

[6]:
```
def topk_cpp(X, k):
    return topk_element_min_double(X, k, True, 50)
```

```
ind = topk_cpp(X, 3)
ind
```

[6]:
```
array([[2, 7, 3],
       [7, 0, 8],
       [1, 5, 6],
       [8, 9, 3],
       [4, 6, 5]], dtype=int64)
```

1.2 Speed comparison by size

[7]:
```
%timeit topk_sklearn(X, 3)
```

```
21.7 µs ± 4.19 µs per loop (mean ± std. dev. of 7 runs, 100000 loops each)
```

[8]:
```
%timeit topk_cpp(X, 3)
```

```
4.1 µs ± 435 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
```

Quite a lot faster on this simple example. Let's look for bigger matrices.

[9]:
```
X = rnd.randn(1000, 100)
```

[10]:
```
%timeit topk_sklearn(X, 10)
```

```
1.8 ms ± 102 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

[11]:
```
%timeit topk_cpp(X, 10)
```

```
786 µs ± 116 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

[12]:
```
from cpyquickhelper.numbers import measure_time
from tqdm import tqdm
from pandas import DataFrame

rows = []
for n in tqdm(range(1000, 10001, 1000)):
    X = rnd.randn(n, 1000)
    res = measure_time('topk_sklearn(X, 20)',
                       {'X': X, 'topk_sklearn': topk_sklearn},
                       div_by_number=True,
                       number=2, repeat=2)
    res["N"] = n
    res["name"] = 'topk_sklearn'
    rows.append(res)
    res = measure_time('topk_cpp(X, 20)',
                       {'X': X, 'topk_cpp': topk_cpp},
                       div_by_number=True,
                       number=4, repeat=4)
    res["N"] = n
```

```
    res["name"] = 'topk_cpp'
    rows.append(res)

df = DataFrame(rows)
df.head()
```

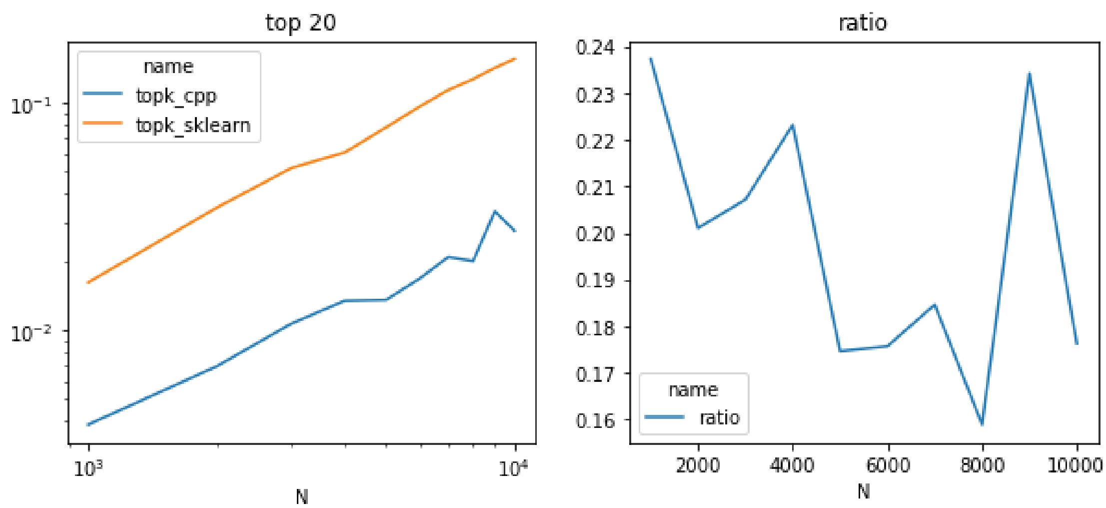
```
100%|¿ ¿ ¿ ¿ ¿ ¿ ¿ ¿ ¿ ¿ | 10/10 [00:08<00:00,  1.16it/s]
```

[12]:

	average	deviation	min_exec	max_exec	repeat	number	context_size	N	name
0	0.016310	0.000260	0.016050	0.016571	2	2	240	1000	topk_sklearn
1	0.003872	0.000501	0.003335	0.004631	4	4	240	1000	topk_cpp
2	0.034684	0.001629	0.033055	0.036313	2	2	240	2000	topk_sklearn
3	0.006973	0.000558	0.006307	0.007756	4	4	240	2000	topk_cpp
4	0.051934	0.000851	0.051084	0.052785	2	2	240	3000	topk_sklearn

[13]:

```
import matplotlib.pyplot as plt

fig, ax = plt.subplots(1, 2, figsize=(10, 4))
piv = df.pivot("N", "name", "average")
piv.plot(ax=ax[0], logy=True, logx=True)
ax[0].set_title("top 20")
piv["ratio"] = piv["topk_cpp"] / piv["topk_sklearn"]
piv[["ratio"]].plot(ax=ax[1])
ax[1].set_title("ratio");
```



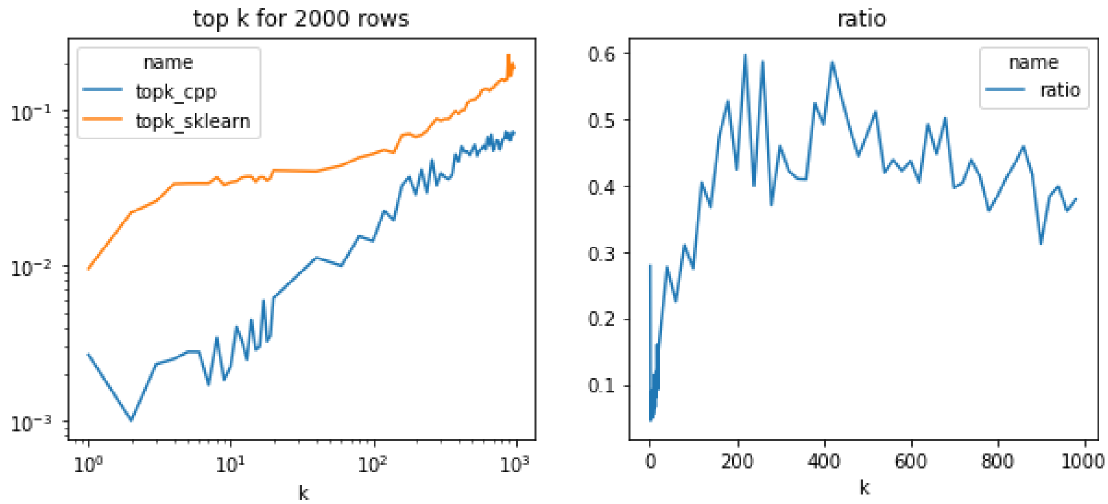
1.3 Speed comparison by k

[14]:
```
rows = []
X = rnd.randn(2000, 1000)
for k in tqdm(list(range(1, 20)) + list(range(20, 1000, 20))):
    res = measure_time('topk_sklearn(X, k)',
                       {'X': X, 'topk_sklearn': topk_sklearn, 'k': k},
                       div_by_number=True,
                       number=2, repeat=2)
    res["k"] = k
    res["name"] = 'topk_sklearn'
    rows.append(res)
    res = measure_time('topk_cpp(X, k)',
                       {'X': X, 'topk_cpp': topk_cpp, 'k': k},
                       div_by_number=True,
                       number=2, repeat=2)
    res["k"] = k
    res["name"] = 'topk_cpp'
    rows.append(res)

df = DataFrame(rows)
df.head()
```

```
100%|¿ ¿ ¿ ¿ ¿ ¿ ¿ ¿ ¿ ¿ | 68/68 [00:34<00:00,  1.95it/s]
```

[14]:
```
    average  deviation  min_exec  max_exec  repeat  number  context_size  k  \
0  0.009558   0.001392  0.008166  0.010949       2       2           240  1
1  0.002665   0.000571  0.002094  0.003236       2       2           240  1
2  0.021933   0.000575  0.021358  0.022508       2       2           240  2
3  0.001000   0.000084  0.000917  0.001084       2       2           240  2
4  0.025986   0.001411  0.024575  0.027398       2       2           240  3

           name
0  topk_sklearn
1      topk_cpp
2  topk_sklearn
3      topk_cpp
4  topk_sklearn
```

[15]:
```
fig, ax = plt.subplots(1, 2, figsize=(10, 4))
piv = df.pivot("k", "name", "average")
piv.plot(ax=ax[0], logy=True, logx=True)
ax[0].set_title("top k for 2000 rows")
piv["ratio"] = piv["topk_cpp"] / piv["topk_sklearn"]
piv[["ratio"]].plot(ax=ax[1])
ax[1].set_title("ratio")
ax[0].set_xlabel("k")
ax[1].set_xlabel("k");
```



The implementation is half faster in all cases and much more efficient for small values which is usually the case for the nearest neighbors. This implementation is using *openmp*, maybe that's why it gets 50% faster on this two cores machine.

[16]:

```

```