onnx_pdist

April 5, 2022

1 Pairwise distances with ONNX (pdist)

Function pdist computes pairwise distances between observations in n-dimensional space. It is not that difficult to convert that into *ONNX* when the dimension of the input is always the same. What if not?

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

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

[2]:
```
%load_ext mlprodict
```

```
The mlprodict extension is already loaded. To reload it, use:
  %reload_ext mlprodict
```

1.1 Function pdist

The function pdist distances. Let's denote a list of vectors $(X_1, ..., X_n)$, function pdist returns the matrix $D = (d_{ij})$ where $d_{ij} = dist(X_i, X_j) = \|X_i - X_j\|^2$.

[3]:
```
import numpy
from scipy.spatial.distance import pdist, squareform

M = numpy.array([[0, 1],
                 [1, 2],
                 [0.1, 1.1],
                 [2, 2]], dtype=float)

d1 = squareform(pdist(M, metric='sqeuclidean'))
d1
```

[3]:
```
array([[0.  , 2.  , 0.02, 5.  ],
       [2.  , 0.  , 1.62, 1.  ],
       [0.02, 1.62, 0.  , 4.42],
       [5.  , 1.  , 4.42, 0.  ]])
```

The two following functions are implemented to reduce the number of allocations the algorithm requires.

[4]:
```
def custom_pdist(M):
    n = M.shape[0]
    res = numpy.zeros((n, n))
    buffer = numpy.empty(M.shape)
    for i in range(n):
```

```
        numpy.subtract(M, M[i], out=buffer)  # broadcasted substraction
        numpy.square(buffer, out=buffer)
        res[i, :] = numpy.sum(buffer, axis=1)
    return res

d2 = custom_pdist(M)
d2
```

[4]:
```
array([[0.  , 2.  , 0.02, 5.  ],
       [2.  , 0.  , 1.62, 1.  ],
       [0.02, 1.62, 0.  , 4.42],
       [5.  , 1.  , 4.42, 0.  ]])
```

This function computes n^2 distances wheres only $\frac{n(n-1)}{2}$ are necessary since the final matrix is symmetric. Let's change the implementation to reflect that.

[5]:
```
def custom_pdist_lower(M):
    n = M.shape[0]
    res = numpy.zeros((n, n))
    buffer = numpy.empty((M.shape[0]-1, M.shape[1]))
    a = numpy.empty(M.shape[0])
    for i in range(1, n):
        numpy.subtract(M[:i], M[i], out=buffer[:i])  # broadcasted substraction
        numpy.square(buffer[:i], out=buffer[:i])
        numpy.sum(buffer[:i], axis=1, out=a[:i])
        res[:i, i] = a[:i]
        res[i, :i] = a[:i]
    return res

d3 = custom_pdist_lower(M)
d3
```

[5]:
```
array([[0.  , 2.  , 0.02, 5.  ],
       [2.  , 0.  , 1.62, 1.  ],
       [0.02, 1.62, 0.  , 4.42],
       [5.  , 1.  , 4.42, 0.  ]])
```

1.2 Loop mechanism in ONNX

Operator Loop seems appropriate but it is just a loop wheras Scan holds accumulator. The first graph is what is repeated inside the loop.

[6]:
```
from skl2onnx.algebra.onnx_ops import OnnxAdd, OnnxIdentity, OnnxScan
from skl2onnx.common.data_types import FloatTensorType

initial = numpy.array([0, 0]).astype(numpy.float32).reshape((2,))
x = numpy.array([1, 2, 3, 4, 5, 6]).astype(numpy.float32).reshape((3, 2))

add_node = OnnxAdd('sum_in', 'next', output_names=['sum_out'], op_version=12)
id_node = OnnxIdentity(add_node, output_names=['scan_out'], op_version=12)

scan_body = id_node.to_onnx(
    {'sum_in': initial, 'next': initial},
    outputs=[('sum_out', FloatTensorType()),
```

```
             ('scan_out', FloatTensorType())])

# add -l 1 if nothing shows up
%onnxview scan_body
```

[6]: <jyquickhelper.jspy.render_nb_js_dot.RenderJsDot at 0x234da711a90>

The operator Scan repeats this graph a couple of times. *sum_in* is an accumulator, *next* is the iterated row from the input matrix.

[7]:
```
node = OnnxScan('initial', 'x', output_names=['y', 'z'],
                num_scan_inputs=1, body=scan_body.graph)

model_def = node.to_onnx(
    {'initial': initial, 'x': x},
    outputs=[('y', FloatTensorType()),
             ('z', FloatTensorType())])

# add -l 1 if nothing shows up
%onnxview model_def
```

[7]: <jyquickhelper.jspy.render_nb_js_dot.RenderJsDot at 0x234da3810a0>

All together in the same graph.

[8]:
```
# add -l 1 if nothing shows up
%onnxview model_def -r 1
```

[8]: <jyquickhelper.jspy.render_nb_js_dot.RenderJsDot at 0x234dc1e7880>

[9]:
```
from mlprodict.onnxrt import OnnxInference
oinf = OnnxInference(model_def)
res = oinf.run({'initial': initial, 'x': x})
res['y']
```

[9]:
```
array([ 9., 12.], dtype=float32)
```

[10]:
```
res['z']
```

[10]:
```
array([[ 1.,  2.],
       [ 4.,  6.],
       [ 9., 12.]], dtype=float32)
```

1.3 Back to pdist

sklearn-onnx implements function *pdist* with *ONNX* operators. The parameter `inputs=[('x', FloatTensorType())` tels the method `to_onnx` that the dimension of the inputs is not fixed and should not be checked.

[11]:
```
# from skl2onnx.algebra.complex_functions import squareform_pdist_

from collections import OrderedDict
from skl2onnx.algebra.onnx_ops import (
    OnnxSub, OnnxReduceSumSquare, OnnxSqueeze,
    OnnxIdentity, OnnxScan)
```

```python
from skl2onnx.common.data_types import FloatTensorType
from mlprodict.tools import get_opset_number_from_onnx


def squareform_pdist(X, **kwargs):
    """Returns the ONNX graph which computes
    ``squareform(pdist(X, metric='sqeuclidean')``."""

    # The subgraph executed at every iteration.
    opv = get_opset_number_from_onnx()
    diff = OnnxSub('next_in', 'next', output_names=['diff'], op_version=opv)
    id_next = OnnxIdentity('next_in', output_names=['next_out'], op_version=opv)
    norm = OnnxReduceSumSquare(diff, output_names=['norm'], axes=[1], op_version=opv)
    flat = OnnxSqueeze(norm, numpy.array([1], dtype=numpy.int64),
                       output_names=['scan_out'], op_version=opv)
    scan_body = id_next.to_onnx(
        OrderedDict([('next_in', FloatTensorType()),
                     ('next', FloatTensorType())]),
        # Size must be empty otherwise onnxruntime fails
        # at execution time if it receives a matrix
        # with a different shape. With 'None', the same ONNX graph
        # can compute pairwise distance for any shape.
        outputs=[('next_out', FloatTensorType([None, None])),
                 ('scan_out', FloatTensorType([None]))],
        other_outputs=[flat])

    # The loop.
    # 'scan0_{idself}' means the variable name will include
    # id(OnnxScan), this is needed if squareform_pdist is used
    # twice in the same graph.
    node = OnnxScan(X, X, output_names=['scan0_{idself}', 'scan1_{idself}'],
                    num_scan_inputs=1, body=scan_body.graph, op_version=opv,
                    **kwargs)
    return node[1]

opv = get_opset_number_from_onnx()
onnx_fct = OnnxIdentity(squareform_pdist('x'), output_names='Y', op_version=opv)
model_def = onnx_fct.to_onnx(inputs=[('x', FloatTensorType())])

# add -l 1 if nothing shows up
%onnxview model_def
```

[11]: <jyquickhelper.jspy.render_nb_js_dot.RenderJsDot at 0x234da7785e0>

[12]:
```python
from collections import OrderedDict
from skl2onnx.algebra.onnx_ops import (
    OnnxSub, OnnxReduceSumSquare, OnnxSqueeze,
    OnnxIdentity, OnnxScan)
from skl2onnx.common.data_types import FloatTensorType
from mlprodict.tools import get_opset_number_from_onnx


def squareform_pdist(X, **kwargs):
```

```
    # The subgraph executed at every iteration.
    opv = get_opset_number_from_onnx()
    diff = OnnxSub('next_in', 'next', output_names=['diff'], op_version=opv)
    id_next = OnnxIdentity('next_in', output_names=['next_out'], op_version=opv)
    norm = OnnxReduceSumSquare(diff, output_names=['norm'], axes=[1], op_version=opv)
    flat = OnnxSqueeze(norm, numpy.array([1], dtype=numpy.int64),
                       output_names=['scan_out'], op_version=opv)
    scan_body = id_next.to_onnx(
        OrderedDict([('next_in', FloatTensorType()),
                     ('next', FloatTensorType())]),
        outputs=[('next_out', FloatTensorType([None, None])),
                 ('scan_out', FloatTensorType([None]))],
        other_outputs=[flat])

    # The loop.
    node = OnnxScan(X, X, output_names=['scan0_{idself}', 'scan1_{idself}'],
                    num_scan_inputs=1, body=scan_body.graph, op_version=opv,
                    **kwargs)
    return node[1]

opv = get_opset_number_from_onnx()
onnx_fct = OnnxIdentity(squareform_pdist('x'), output_names='Y', op_version=opv)
model_def = onnx_fct.to_onnx(inputs=[('x', FloatTensorType())])
```

Notice the double arrow. Input x is used twice, once as an permanent state involved in broacasted substract, another time to iterator rows. On the other side, the first output of operator *Scan* is a permanent state equal to the input, the second one is an aggregation of results produced at each iteration. Each of those produces a row of a final matrix.

[13]:
```
oinf = OnnxInference(model_def)
body = oinf['Sc_Scan', 'body']

# add -l 1 if nothing shows up
%onnxview body.g
```

[13]: <jyquickhelper.jspy.render_nb_js_dot.RenderJsDot at 0x234dc3b2a00>

All together.

[14]:
```
# add -l 1 if nothing shows up
%onnxview model_def -r 1
```

[14]: <jyquickhelper.jspy.render_nb_js_dot.RenderJsDot at 0x234dc3b23d0>

Let's now execute the graph and compare it with the original graph.

[15]:
```
d1 = squareform(pdist(M, metric='sqeuclidean'))
d1
```

[15]:
```
array([[0.  , 2.  , 0.02, 5.  ],
       [2.  , 0.  , 1.62, 1.  ],
       [0.02, 1.62, 0.  , 4.42],
       [5.  , 1.  , 4.42, 0.  ]])
```

[16]:
```
oinf.run({'x': M})['Y']
```

[16]:
```
array([[0.  , 2.  , 0.02, 5.  ],
       [2.  , 0.  , 1.62, 1.  ],
       [0.02, 1.62, 0.  , 4.42],
       [5.  , 1.  , 4.42, 0.  ]])
```

[17]:
```
%timeit squareform(pdist(M, metric='sqeuclidean'))
```

```
9.31 µs ± 423 ns per loop (mean ± std. dev. of 7 runs, 100,000 loops each)
```

[18]:
```
%timeit custom_pdist(M)
```

```
35.1 µs ± 1.52 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

[19]:
```
%timeit custom_pdist_lower(M)
```

```
34.2 µs ± 2.18 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

[20]:
```
%timeit oinf.run({'x': M})['Y']
```

```
177 µs ± 11.3 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

[21]:
```
M32 = M.astype(numpy.float32)
```

[22]:
```
from mlprodict.tools import get_ir_version_from_onnx
model_def.ir_version = get_ir_version_from_onnx()
```

[23]:
```
oinfrt = OnnxInference(model_def, runtime="onnxruntime1")
oinfrt.run({'x': M32})['Y']
```

```
No CUDA runtime is found, using CUDA_HOME='C:\Program Files\NVIDIA GPU Computing
Toolkit\CUDA\v11.5'
```

[23]:
```
array([[0.        , 2.        , 0.02000001, 5.        ],
       [2.        , 0.        , 1.6199999 , 1.        ],
       [0.02000001, 1.6199999 , 0.        , 4.42      ],
       [5.        , 1.        , 4.42      , 0.        ]], dtype=float32)
```

[24]:
```
%timeit oinfrt.run({'x': M32})['Y']
```

```
43.1 µs ± 4.32 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
```

1.4 Benchmark

[25]:
```
from timeit import Timer


def measure_time(name, stmt, context, repeat=10, number=10):
    tim = Timer(stmt, globals=context)
```

```python
    res = numpy.array(tim.repeat(repeat=repeat, number=number))
    res /= number
    mean = numpy.mean(res)
    dev = numpy.mean(res ** 2)
    dev = (dev - mean**2) ** 0.5
    return dict(average=mean, deviation=dev, min_exec=numpy.min(res),
                max_exec=numpy.max(res), repeat=repeat, number=number,
                nrows=context['M'].shape[0], ncols=context['M'].shape[1],
                name=name)

measure_time("scipy", "squareform(pdist(M, metric='sqeuclidean'))",
             context={'squareform': squareform, 'M': M,
                      'pdist': pdist})
```

[25]:

```
{'average': 4.233300000009876e-05,
 'deviation': 2.7235873787981297e-05,
 'min_exec': 1.8629999999575375e-05,
 'max_exec': 0.00010153999999999997,
 'repeat': 10,
 'number': 10,
 'nrows': 4,
 'ncols': 2,
 'name': 'scipy'}
```

[26]:

```python
from tqdm import trange

def generator():
    for feat in [5, 10, 50, 100]:
        for n in [5, 10, 20, 50, 100, 400, 1000]:
            if n <= 500 or feat <= 10:
                yield feat, n

all_values = list(generator())

rows = []

with trange(len(all_values)) as t:
    for i in t:
        feat, n = all_values[i]
        t.set_description("feat=%d n=%d" % (feat, n))
        M = numpy.random.rand(n, feat)

        context = {'squareform': squareform, 'M': M, 'pdist': pdist}
        res = measure_time("scipy", "squareform(pdist(M, metric='sqeuclidean'))",
 ↪context=context)
        res['dimres'] = squareform(pdist(M, metric='sqeuclidean')).shape[0]
        rows.append(res)

        context = {'M': M, 'custom_pdist': custom_pdist}
        res = measure_time("numpy", "custom_pdist(M)", context=context)
        res['dimres'] = custom_pdist(M).shape[0]
        rows.append(res)
```

```
        context = {'M': M, 'custom_pdist_lower': custom_pdist_lower}
        res = measure_time("numpy-lower", "custom_pdist_lower(M)", context=context)
        res['dimres'] = custom_pdist_lower(M).shape[0]
        rows.append(res)

        context = {'oinf': oinf, 'M': M}
        res = measure_time("onnx-py", "oinf.run({'x': M})['Y']", context=context)
        res['dimres'] = oinf.run({'x': M})['Y'].shape[0]
        rows.append(res)

        M32 = M.astype(numpy.float32)
        context = {'oinfrt': oinfrt, 'M': M32}
        res = measure_time("onnx-rt", "oinfrt.run({'x': M})['Y']", context=context)
        res['dimres'] = oinfrt.run({'x': M32})['Y'].shape[0]
        rows.append(res)


from pandas import DataFrame
df = DataFrame(rows)
df.head()
```

```
feat=100 n=400: 100%|¿ ¿ ¿ ¿ ¿ ¿ ¿ ¿ ¿ ¿ | 26/26 [01:20<00:00,  3.10s/it]
```

[26]:

```
    average  deviation  min_exec  max_exec  repeat  number  nrows  ncols  \
0  0.000015   0.000005  0.000010  0.000025      10      10      5      5
1  0.000106   0.000023  0.000065  0.000138      10      10      5      5
2  0.000053   0.000005  0.000048  0.000064      10      10      5      5
3  0.000240   0.000017  0.000219  0.000273      10      10      5      5
4  0.000053   0.000008  0.000046  0.000072      10      10      5      5

          name  dimres
0        scipy       5
1        numpy       5
2  numpy-lower       5
3      onnx-py       5
4      onnx-rt       5
```

[27]:

```
from pandas import pivot_table
piv = pivot_table(df, index=["nrows"], columns= ['ncols', 'name'], values='average')
piv.head().T
```

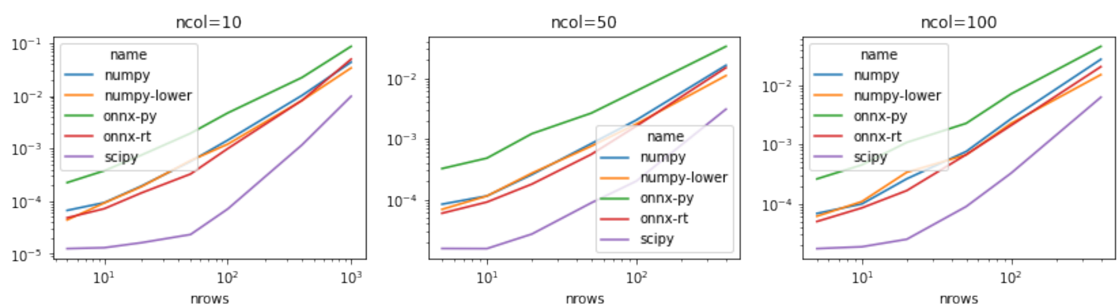
[27]:

```
nrows                     5         10        20        50        100
ncols name
5     numpy         0.000106  0.000108  0.000193  0.000464  0.001121
      numpy-lower   0.000053  0.000099  0.000225  0.000520  0.001190
      onnx-py       0.000240  0.000407  0.000797  0.002581  0.003790
      onnx-rt       0.000053  0.000071  0.000118  0.000306  0.000766
      scipy         0.000015  0.000011  0.000014  0.000020  0.000044
10    numpy         0.000067  0.000094  0.000194  0.000569  0.001441
      numpy-lower   0.000044  0.000093  0.000189  0.000591  0.001209
      onnx-py       0.000226  0.000379  0.000751  0.001945  0.004731
      onnx-rt       0.000048  0.000072  0.000144  0.000329  0.000995
      scipy         0.000013  0.000013  0.000016  0.000023  0.000071
```

50	numpy	0.000084	0.000114	0.000257	0.000833	0.002031
	numpy-lower	0.000069	0.000114	0.000272	0.000757	0.001749
	onnx-py	0.000323	0.000480	0.001214	0.002648	0.006138
	onnx-rt	0.000059	0.000091	0.000179	0.000554	0.001614
	scipy	0.000016	0.000016	0.000027	0.000088	0.000200
100	numpy	0.000068	0.000098	0.000262	0.000759	0.002712
	numpy-lower	0.000061	0.000108	0.000338	0.000666	0.002270
	onnx-py	0.000261	0.000451	0.001082	0.002272	0.007142
	onnx-rt	0.000050	0.000084	0.000166	0.000672	0.002097
	scipy	0.000017	0.000019	0.000025	0.000089	0.000327

[28]:
```
%matplotlib inline
```

[29]:
```
import matplotlib.pyplot as plt
fig, ax = plt.subplots(1, 3, figsize=(14, 3))
for i, ncol in enumerate([10, 50, 100]):
    piv = df[df.ncols==ncol].pivot("nrows", "name", "average")
    piv.plot(ax=ax[i], logy=True, logx=True)
    ax[i].set_title("ncol=%d" % ncol)
ax;
```

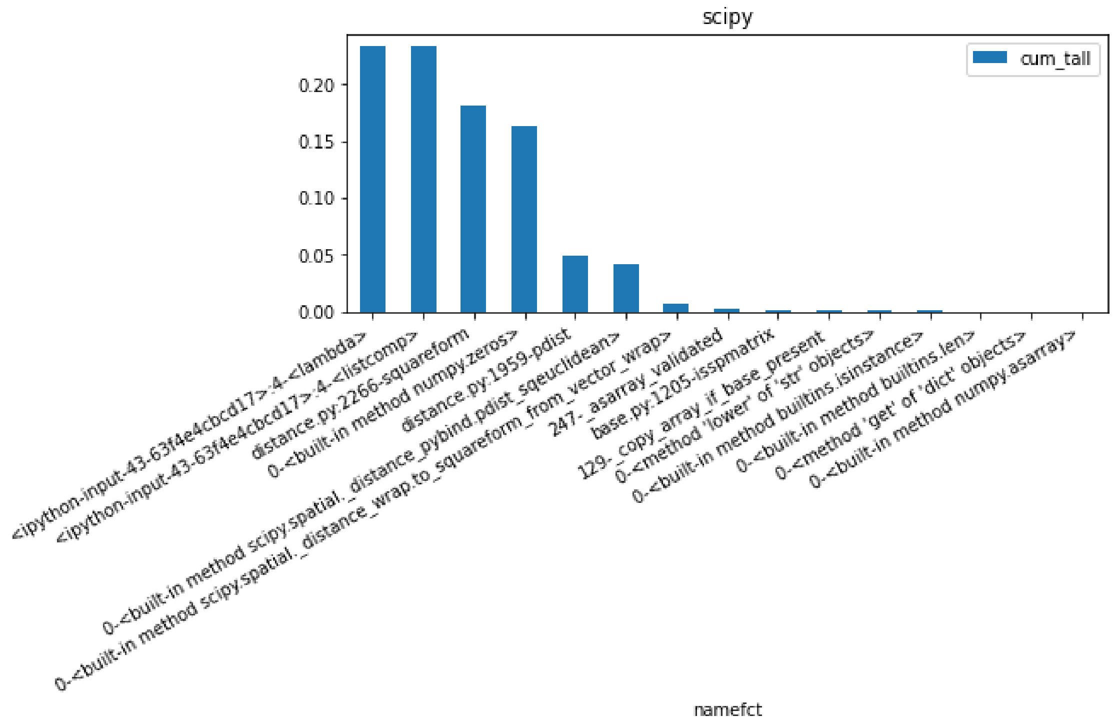


Curves are not linear and rather difficult to interpret. The algorithm *numpy-lower* and *scipy* should be close as the cost of both algorithm are similar. However, *scipy* reduces the number of trips between C and python. The C implementation of the distance is here: sqeuclidean_distance_double. The final cost is a combination of computation, multithreading, allocations…

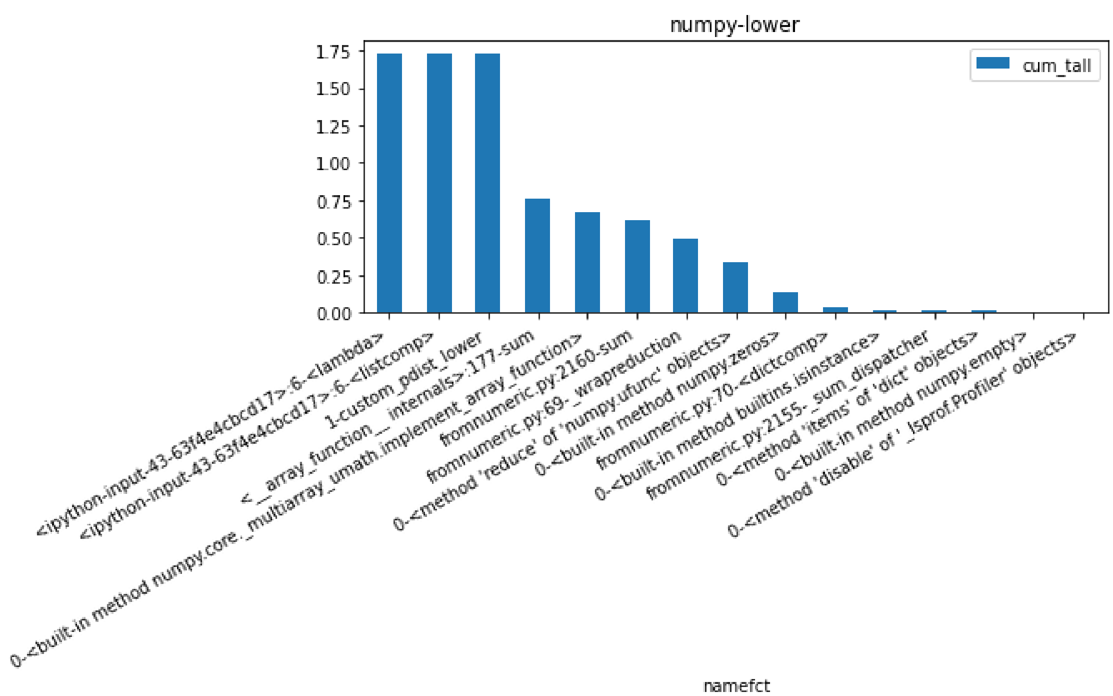
[30]:
```
from pyquickhelper.pycode.profiling import profile
M = numpy.random.rand(100, 10)

pr1, df1 = profile(lambda: [squareform(pdist(M, metric='sqeuclidean')) for i in
  ↪range(0, 1000)],
                   as_df=True)
pr2, df2 = profile(lambda: [custom_pdist_lower(M) for i in range(0, 1000)], as_df=True)
```

[31]:
```
ax = df1[['namefct', 'cum_tall']].head(n=15).set_index('namefct').plot(
    kind='bar', figsize=(8, 3), rot=30)
ax.set_title("scipy")
for la in ax.get_xticklabels():
    la.set_horizontalalignment('right')
```

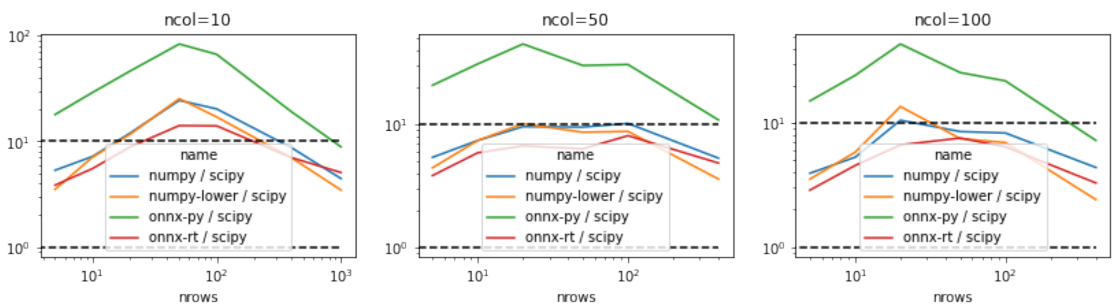


[32]:
```python
ax = df2[['namefct', 'cum_tall']].head(n=15).set_index('namefct').plot(
    kind='bar', figsize=(8, 3), rot=30)
ax.set_title("numpy-lower")
for la in ax.get_xticklabels():
    la.set_horizontalalignment('right');
```



[Universal function](#) do not seem to be very efficient in our case. The last graph shows time ratio between implementations of *pdist* and the baseline *scipy*.

[33]:
```
fig, ax = plt.subplots(1, 3, figsize=(14, 3))
for i, ncol in enumerate([10, 50, 100]):
    piv = df[df.ncols==ncol].pivot("nrows", "name", "average")
    piv['numpy / scipy'] = piv['numpy'] / piv['scipy']
    piv['numpy-lower / scipy'] = piv['numpy-lower'] / piv['scipy']
    piv['onnx-py / scipy'] = piv['onnx-py'] / piv['scipy']
    piv['onnx-rt / scipy'] = piv['onnx-rt'] / piv['scipy']
    piv = piv[['numpy / scipy', 'numpy-lower / scipy',
               'onnx-py / scipy', 'onnx-rt / scipy']]
    piv.plot(ax=ax[i], logy=True, logx=True)
    ax[i].plot([0, max(piv.index)], [1, 1], '--', color='black')
    ax[i].plot([0, max(piv.index)], [10, 10], '--', color='black')
    ax[i].set_title("ncol=%d" % ncol)
ax;
```



1.5 Test with a new operator CDist

The final question is: *should we introduce a new operator into [ONNX specifications](#)?* The function [pdist](#) is not necessarily often used for a big number of observations as the square matrix it produces will even bigger. It seems reasonable. We showed that a python runtime based on *numpy* would not help, the implementation must be done in C++ or directly used the *scipy* version. The experiment was done with a [GaussianProcessRegressor](#). The following section tests with and without a new operator `CDist` reusing *scipy* implementation.

[34]:
```
import numpy
from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import ExpSineSquared
from mlprodict.onnx_conv import to_onnx
from mlprodict.onnxrt import OnnxInference


iris = load_iris()
X, y = iris.data, iris.target
X_train, X_test, y_train, __ = train_test_split(X, y, random_state=12)
```

```
clr = GaussianProcessRegressor(ExpSineSquared(), alpha=20.)
clr.fit(X_train, y_train)

model_def = to_onnx(clr, X_train)

%onnxview model_def -r 1
```

[34]: <jyquickhelper.jspy.render_nb_js_dot.RenderJsDot at 0x234ede21a00>

[35]:
```
model_def_cdist = to_onnx(clr, X_train,
                          options={GaussianProcessRegressor: {'optim': 'cdist'}})
%onnxview model_def_cdist
```

[35]: <jyquickhelper.jspy.render_nb_js_dot.RenderJsDot at 0x234edc44fd0>

[36]:
```
oinf = OnnxInference(model_def)
oinf_cdist = OnnxInference(model_def_cdist)
```

[37]:
```
%timeit oinf.run({'X': X_test})
```

```
4.24 ms ± 274 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

[38]:
```
%timeit oinf_cdist.run({'X': X_test})
```

```
414 µs ± 15 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
```

[39]:
```
oinfrt = OnnxInference(model_def, runtime="onnxruntime1")
oinfrt_cdist = OnnxInference(model_def_cdist)
```

[40]:
```
%timeit oinfrt_cdist.run({'X': X_test})
```

```
345 µs ± 26.8 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
```

It is 10 times faster for this dataset so it is worth it. For bigger datasets, we should expect a lower gain but still significant.

[41]:
```

```