Rapids

Sadržaj

Dostupne verzije

Verzija	Modul	Paralelna okolina
22.04	rapids/22.04	gpusingle

Korištenje

Dva su načina korištenja dostupna:

1. jedan GPU
2. više GPU-ova na jednom čvoru

U prvom slučaju nisu potrebne dodatne postavke, već se rapids knjižnice zovu direktno.

U drugom slučaju je potrebno instancirati lokalni klaster putem LocalCUDACluster naredbe iz knjižnice dask-cuda (primjer se nalazi ispod).

LocalCUDACluster_primjer.py

```
from dask.distributed import Client
from dask_cuda import LocalCUDACluster

# pokreni klaster i spoji se klijentom
cluster = LocalCUDACluster(
    interface="ib0",
    protocol="ucx",
)
client = Client(cluster)

# izradi proraun
...

# ugasi workere i zatvori klijenta
workers = client.get_scheduler_info()['workers']
client.retire_workers(workers=workers)
client.close()
```

Korištenje više GPU jezgri

Korištenjem LocalCUDACluster se **NE OSIGURAVA** automatsko raspodjeljivanje memorije ili izračuna

Pri razvoju multi-GPU aplikacija, treba pripaziti kako je svaka od funkcija implementirana (detalji u tablici ispod):

Knjižnica	multi-GPU	Poveznice
cuPY	x	poveznica
cuDF	x	poveznica
cuML	x	poveznica
cuGraph	x	poveznica
cuSignal	-	-
cuSpatial	-	-
CLX	-	-
cuCIM	-	-

Performanse

Postavke

Ispod se nalazi rezultati nekih tipičnih aplikacija na jednoj GPU jezgri:

1. Matrične operacije - cuPy vs. NumPy
2. DataFrame operacije - cuDF vs. pandas
3. K-means clustering - cuML vs. sklearn

U slučaju cuPy-a, matrične operacije su se testirale na matricama veličina:

- 100 x 100 - 80 Kb
- 1000 x 1000 - 8 Mb
- 10000 x 10000 - 0.8 Gb

U slučaju cuDF-a, dataframe operacije su se testirale na podacima strukture:

- 10 kategorija
- 10 varijabli
- 10**3, 10**5 i 10**7 opažanja

U slučaju cuML-a, klasteriranje se testiralo na podacima strukture:

- 2 varijable
- 5 klastera
- 10**8 opažanja

Kod

cuPy

cupy_test.sge

```
#$ -cwd
#$ -o output/
#$ -e output/
#$ -pe gpu 1

# module
module load rapids/22.04

# python
cuda-wrapper.sh python cupy_test.py
```

cupy_test.py

```
import timeit
import cupy as cp
import numpy as np

def print_time(function, message):
    n = 10
    t = timeit.timeit( lambda: function(), number=n )
    print( '%s %0.10f' % ( message, t/n ) )

if __name__ == '__main__':

    # define matrix sizes
    sizes = [ 100, 1000, 10000 ]

    # create matrices
    np_matrices = [ np.random.random((size, size)) for size in sizes ]
    cp_matrices = [ cp.random.random((size, size)) for size in sizes ]


    for i, (np_matrix, cp_matrix) in enumerate(zip(np_matrices, cp_matrices)):

        # print nbytes
        print( 'np %i nbytes %s' % ( np_matrix.shape[0], np_matrix.nbytes ) )
        print( 'cp %i nbytes %s' % ( cp_matrix.shape[0], cp_matrix.nbytes ) )

        # fft
        print_time( lambda: np.fft.fft2(np_matrix),  'np %s fft' % np_matrix.shape[0] )
        print_time( lambda: cp.fft.fft2(cp_matrix),  'cp %s fft' % cp_matrix.shape[0] )

        # sum
        print_time( lambda: np_matrix.sum(),  'np %s sum' % np_matrix.shape[0] )
        print_time( lambda: cp_matrix.sum(),  'cp %s sum' % cp_matrix.shape[0] )

        # std
        print_time( lambda: np_matrix.std(),  'np %s std' % np_matrix.shape[0] )
        print_time( lambda: cp_matrix.std(),  'cp %s std' % cp_matrix.shape[0] )

        # elementwise
        print_time( lambda: np.multiply(np_matrix, np_matrix),  'np %s multiply' % np_matrix.shape[0] )
        print_time( lambda: cp.multiply(cp_matrix, cp_matrix),  'cp %s multiply' % cp_matrix.shape[0] )

        # dot
        print_time( lambda: np_matrix.dot(np_matrix),  'np %s dot' % np_matrix.shape[0] )
        print_time( lambda: cp_matrix.dot(cp_matrix),  'cp %s dot' % cp_matrix.shape[0] )

        # slice
        print_time( lambda: np_matrix[::10],  'np %s slice' % np_matrix.shape[0] )
        print_time( lambda: cp_matrix[::10],  'cp %s slice' % cp_matrix.shape[0] )

        # svd
        print_time( lambda: np.linalg.svd(np_matrix),  'np %s svd' % np_matrix.shape[0] )
        print_time( lambda: np.linalg.svd(cp_matrix),  'cp %s svd' % cp_matrix.shape[0] )
```

cuDF

cudf_test.sge

```
#$ -cwd
#$ -o output/
#$ -e output/
#$ -pe gpu 1

# module
module load rapids/22.04

# run python
cuda-wrapper.sh python cudf_test.py
```

cudf_test.py

```
import time
import cudf
import cupy as cp
import numpy as np
import pandas as pd
import random

def print_time(function, message):
    start = time.time()
    out = function()
    end = time.time()
    print( '%s %0.4e' % ( message, end-start ) )
    return out

if __name__ == '__main__':

    # change number of rows
    ncat = 10
    nobs = 10
    rows = [ 10**n for n in range(3, 8, 2) ]
    for nrows in rows:

        # fake dataset
        cdf = cudf.DataFrame()

        cats = cudf.DataFrame(
            data = cp.random.randint(0, ncat, (nrows, ncat)),
            columns = [ 'c%i' % i for i in range(ncat) ],
        )
        cdf = cudf.concat([ cdf, cats ], axis=1)
        del cats

        obs = cudf.DataFrame(
            data = cp.random.random(size=(nrows, nobs)),
            columns = [ 'o%i' % i for i in range(nobs) ],
        )
        cdf = cudf.concat([ cdf, obs ], axis=1)
        del obs

        pdf = cdf.to_pandas()

        print('cdf %i nbytes %i' % (nrows, cdf.memory_usage().sum()))
        print('pdf %i nbytes %i' % (nrows, pdf.memory_usage().sum()))

        # groupby
        cats = [ column for column in cdf.columns if 'c' in column ]

        print_time( lambda: cdf.groupby(cats).sum(), 'cdf %i groupby_sum' % nrows )
        print_time( lambda: pdf.groupby(cats).sum(), 'pdf %i groupby_sum' % nrows )

        print_time( lambda: cdf.groupby(cats).count(), 'cdf %i groupby_count' % nrows )
        print_time( lambda: pdf.groupby(cats).count(), 'pdf %i groupby_count' % nrows )
```

```
        print_time( lambda: cdf.groupby(cats).nunique(), 'cdf %i groupby_nunique' % nrows )
        print_time( lambda: pdf.groupby(cats).nunique(), 'pdf %i groupby_nunique' % nrows )

        # describe
        print_time( lambda: cdf.describe(), 'cdf %i describe' % nrows )
        print_time( lambda: pdf.describe(), 'pdf %i describe' % nrows )

        # sort
        print_time( lambda: cdf.sort_values(by=list(cdf.columns), axis=0), 'cdf %i sort_values' % nrows )
        print_time( lambda: pdf.sort_values(by=list(pdf.columns), axis=0), 'pdf %i sort_values' % nrows )

        # drop_duplicates
        print_time( lambda: cdf.drop_duplicates(), 'cdf %i drop_duplicates' % nrows )
        print_time( lambda: pdf.drop_duplicates(), 'pdf %i drop_duplicates' % nrows )

        # mask_where
        ind = [ 'o' in col for col in cdf.columns ]
        cdf = print_time( lambda: cdf.mask( (cdf > 0.05) & ind, np.nan ), 'cdf %i mask_where' % nrows )
        pdf = print_time( lambda: pdf.mask( (pdf > 0.05) & ind, np.nan ), 'pdf %i mask_where' % nrows )

        # query
        query = ' | '.join([ '( o%i > 0 )' % i for i in range(10) ])
        cdf = print_time( lambda: cdf.query( query ), 'cdf %i query' % nrows )
        pdf = print_time( lambda: pdf.query( query ), 'pdf %i query' % nrows )

        # fillna
        cdf = print_time( lambda: cdf.fillna(-1), 'cdf %i fillna' % nrows )
        pdf = print_time( lambda: pdf.fillna(-1), 'pdf %i fillna' % nrows )
```

K-means

kmeans_demo.sge

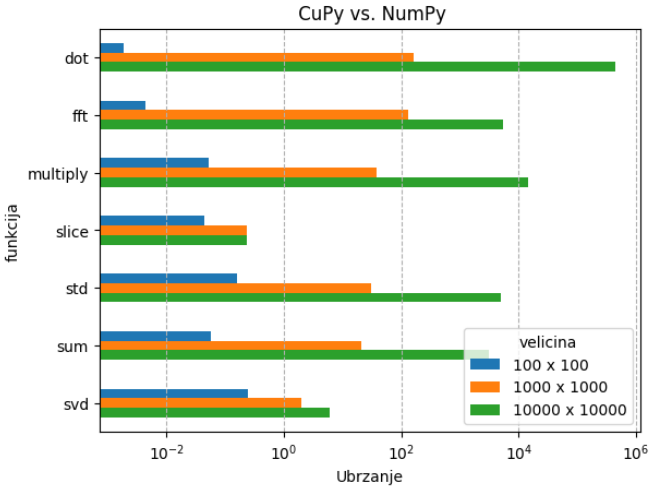
```
#$ -cwd
#$ -o output/
#$ -e output/
#$ -pe gpu 1

# module
module load rapids/22.04

# run python
cuda-wrapper.sh python kmeans_demo.py
```

kmeans_demo.py

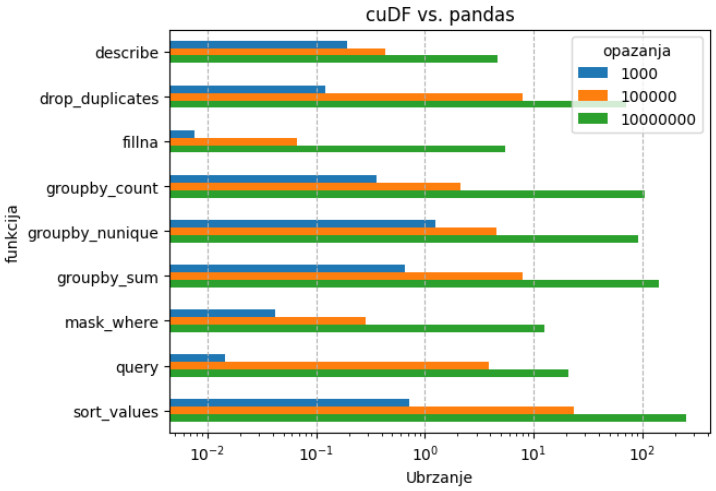
```
#
# https://github.com/rapidsai/cuml/blob/branch-21.12/notebooks/kmeans_demo.ipynb
#

import sys
import cudf
import cupy
import time
import matplotlib.pyplot as plt

from cuml.cluster import KMeans as cuKMeans
from cuml.datasets import make_blobs

from sklearn.cluster import KMeans as skKMeans
from sklearn.metrics import adjusted_rand_score

# time_it
def time_it(command, message):
    start = time.time()
    out = command()
    end = time.time()
    print('%-20s %s' % ( message, end-start ))
    return out

if __name__ == '__main__':

    # parameters
    n_samples = 10**8
    n_features = 2
    n_clusters = 5
    random_state = 0

    # generate data
    device_data, device_labels = make_blobs(
        n_samples=n_samples,
        n_features=n_features,
        centers=n_clusters,
        cluster_std=0.1,
    )
    device_data = cudf.DataFrame(device_data)
    device_labels = cudf.Series(device_labels)

    host_data = device_data.to_pandas()
    host_labels = device_labels.to_pandas()

    # scikit
    kmeans_sk = skKMeans(
        init="k-means++",
        n_clusters=n_clusters,
        random_state=random_state,
    )
    time_it( lambda: kmeans_sk.fit(host_data), 'sklearn fit' )

    # cuml
    kmeans_cuml = cuKMeans(
        init="k-means||",
        n_clusters=n_clusters,
        oversampling_factor=40,
        random_state=random_state,
    )
    time_it( lambda: kmeans_cuml.fit(device_data), 'cuml fit' )

    # compare
    cuml_score = adjusted_rand_score(host_labels, kmeans_cuml.labels_.to_numpy())
    sk_score = adjusted_rand_score(host_labels, kmeans_sk.labels_)
    threshold = 1e-4
    passed = ( cuml_score - sk_score ) < threshold
    print('compare kmeans: cuml vs sklearn labels_ are ' + ('equal' if passed else 'not equal'))
```

Rezultati

cuPy



cuDF



K-means

knjižnica	funkcija	Vrijeme [s]
sklearn	sklearn.cluster.KMeans.fit	1702.17
	sklearn.cluster.KMeans.predict	55.73
cuML	cuML.cluster.KMeans.fit	7.43
	cuML.cluster.KMeans.predict	1.58