Introduction to Dask: Scalable Analytics in Python

DoD High Performance Computing and Modernization Program (HPCMP)
Productivity Enhancement and Training (PET)

USER PRODUCTIVITY ENHANCEMENT AND TRAINING

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GENERAL DYNAMICS
Information Technology

Overview

- What is Dask?
- Installation and setup
- The task graph
- Delayed and futures
- Bag, Array, Dataframe
- Distributed
- Machine Learning
- Dask Dashboard
- Jupyter Notebook demo

What is Dask?

- Dask is defined as a parallel computing library that scales the existing Python ecosystem
- Operates by constructing and executing a task graph
- Very good at scaling to different hardware
- It provides multi-core and distributed parallel execution on larger-than-memory datasets

Installation

- **Dask is easily installed via conda or pip and can be built from source**
- **Included in the default Anaconda distribution**
- **More details: https://docs.dask.org/en/latest/install.html**
- **Single machine and distributed schedulers**

Dependency	Version	Description
bokeh	>=1.0.0	Visualizing dask diagnostics
cloudpickle	>=0.2.2	Pickling support for Python objects
cityhash		Faster hashing of arrays
distributed	>=2.0	Distributed computing in Python
fastparquet		Storing and reading data from parquet files
fsspec	>=0.6.0	Used for local, cluster and remote data IO
gcsfs	>=0.4.0	File-system interface to Google Cloud Storage
murmurhash		Faster hashing of arrays
numpy	>=1.13.0	Required for dask.array
pandas	>=0.23.0	Required for dask.dataframe
partd	>=0.3.10	Concurrent appendable key-value storage
psutil		Enables a more accurate CPU count
pyarrow	>=0.14.0	Python library for Apache Arrow
s3fs	>=0.4.0	Reading from Amazon S3
sqlalchemy		Writing and reading from SQL databases
cytoolz/toolz	>=0.8.2	Utility functions for iterators, functions, and dictionaries
xxhash		Faster hashing of arrays

Task Graph

- Dask encodes algorithms in a simple format involving Python dicts, tuples, and functions

```
{'x': 1,
 'y': 2,
 'z': (add, 'x', 'y'),
 'w': (sum, ['x', 'y', 'z']),
 'v': [(sum, ['w', 'z']), 2]}
```

- Task scheduling is often used as a means to parallelize a program by breaking the work into smaller tasks
- Dask represents these tasks as nodes in a graph with edges between nodes if one task depends on data produced by another
- A task scheduler executes this graph in a way that respects data dependencies and leverages parallelism where possible

Delayed

- **Delayed allows developers to parallelize their own algorithms**
- **Decorating functions with delayed will allow Dask to parallelize any portion of your problem that can be run in parallel**
- **Decorated (wrapped) functions will return a Delayed object and perform no computations**

```python
from dask import delayed

@delayed
def inc(x):
    return x + 1
```

```python
import dask

def inc(x):
    return x + 1

inc_delayed = dask.delayed(inc)
```

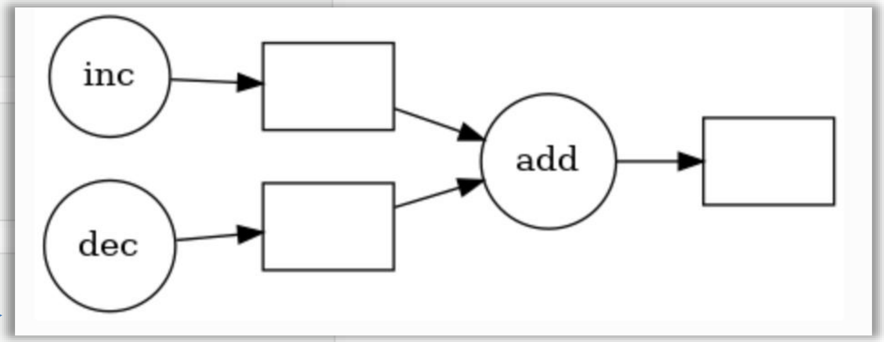
Delayed

```python
import time
import random

def inc(x):
    time.sleep(random.random())
    return x + 1

def dec(x):
    time.sleep(random.random())
    return x - 1

def add(x, y):
    time.sleep(random.random())
    return x + y
```

```python
import dask
inc = dask.delayed(inc)
dec = dask.delayed(dec)
add = dask.delayed(add)
```

```python
%%time
x = inc(1)
y = dec(2)
z = add(x, y)
z
```

- **Here z is a Delayed object**
- **The only work that has been done is the construction of the task graph**



Questions?

Dask Futures

- **Futures extends the concurrent.futures interface of Python and is very similar to the ThreadPoolExecutor (or ProcessPoolExecutor) that is in the standard library**
- **The major difference from Delayed is that futures starts the computation immediately**

```python
from dask.distributed import Client

client = Client()  # by default workers are processes - pass processes=False for threads
```

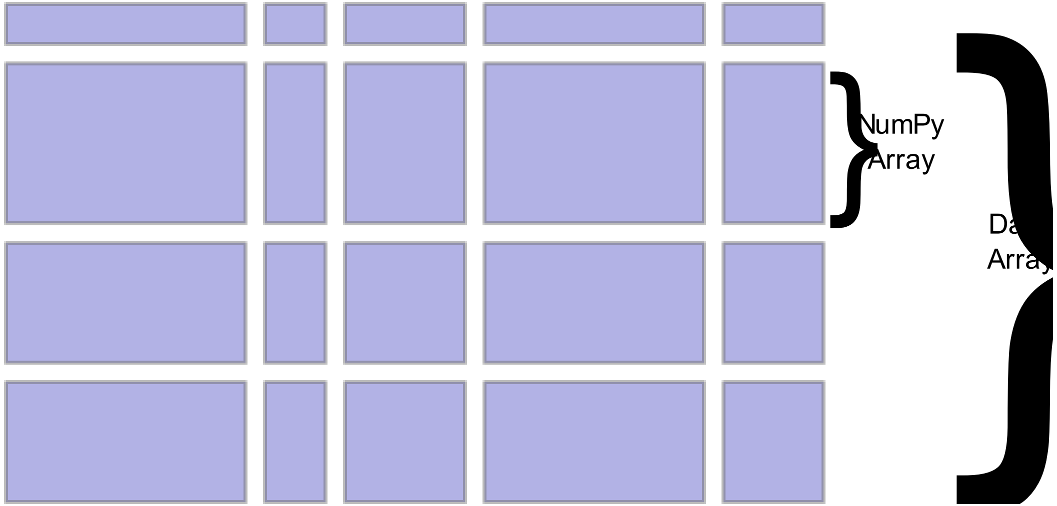
```python
def inc(x):
    return x + 1

futures = client.map(inc, range(1000))

results = [future.result() for future in futures]
results = client.gather(futures)  # may be faster
```

Dask Array

- **Dask arrays use Numpy under the hood and many of the numpy functionalities are supported**
- **Dask arrays are simply chunked numpy arrays**

In [4]:
```python
import numpy as np

arr = np.arange(50)
arr.shape
```
Out[4]: (50,)

In [5]:
```python
import dask.array as da

arr = da.arange(50)
arr.shape
```
Out[5]: (50,)

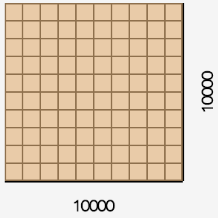


Dask Array

- **Dask provides some nice visualization of arrays in Jupyter Notebooks**

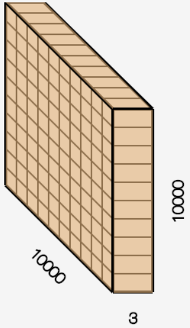
```python
import dask.array as da

arr = da.random.random((10000, 10000), chunks=(1000, 1000))
arr
```

	Array	Chunk
Bytes	800.00 MB	8.00 MB
Shape	(10000, 10000)	(1000, 1000)
Count	100 Tasks	100 Chunks
Type	float64	numpy.ndarray




```python
import dask.array as da

arr = da.random.random((10000, 10000, 3), chunks=(1000, 1000, 3))
arr
```

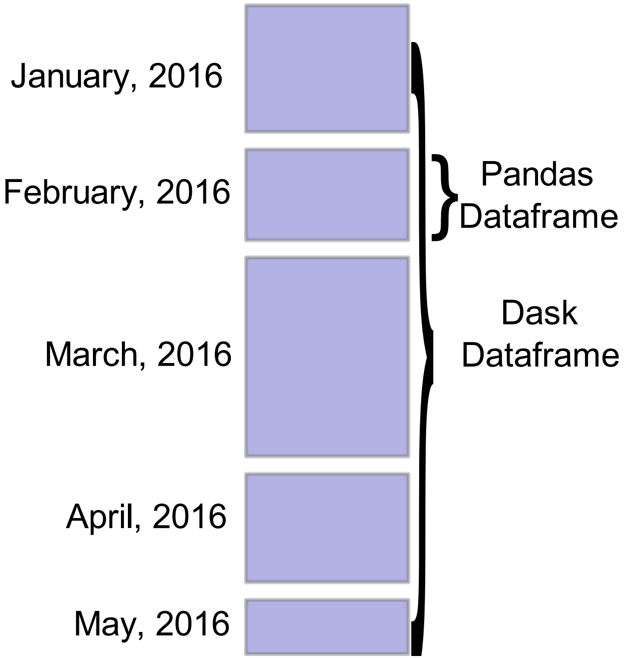
	Array	Chunk
Bytes	2.40 GB	24.00 MB
Shape	(10000, 10000, 3)	(1000, 1000, 3)
Count	100 Tasks	100 Chunks
Type	float64	numpy.ndarray



Dask Dataframe

- **Dask DataFrames coordinate many Pandas DataFrames/Series arranged along the index**
- **A Dask DataFrame is partitioned row-wise, grouping rows by index value for efficiency**

```python
import pandas as pd
df = pd.read_csv('some data')

import dask.dataframe as dd
df = dd.read_csv('some data')
```



Dask Bag

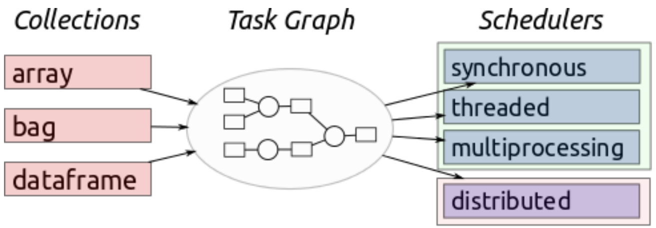
- Dask Bag implements operations like map, filter, fold, and groupby on collections of generic Python objects
- Typically used to parallelize simple computations on unstructured or semi-structured data like text data, log files, JSON records, or user defined Python objects

```
In [7]: import dask.bag as db

        bag = db.from_sequence([0,1,2,3,4,5,6,7,8,9], npartitions=4)
        bag.map(lambda x: x**2)

Out[7]: dask.bag<lambda, npartitions=4>

In [8]: bag.compute()

Out[8]: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

Questions?

Dask Distributed

- **Up to this point we have seen that Dask handles the computations for us**
- Dask has two families of task schedulers:
  - Single machine scheduler: This scheduler provides basic features on a local process or thread pool. This is the default scheduler
  - Distributed scheduler: This scheduler is more sophisticated, offers more features, but also requires a bit more effort to set up
- **Dask comes with four available schedulers:**
  - Threaded: a scheduler backed by a thread pool
  - Processes: a scheduler backed by a process pool
  - Single-threaded (aka "sync"): a synchronous scheduler, good for debugging
  - Distributed: a distributed scheduler for executing graphs on multiple machines



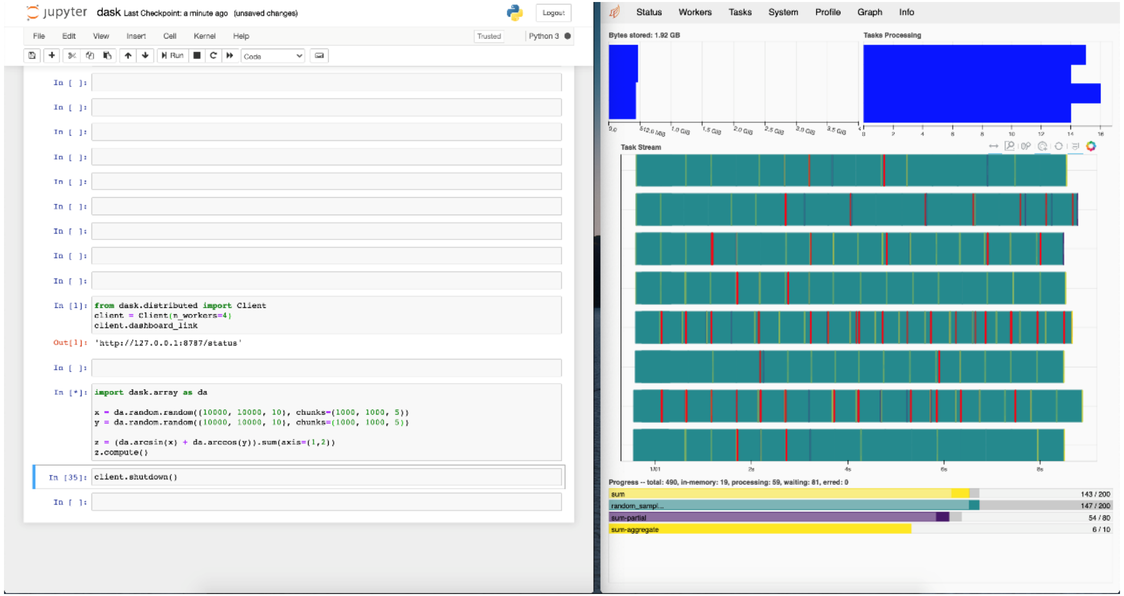
Dask for Machine Learning

- Dask-ML provides scalable machine learning in Python using Dask alongside popular machine learning libraries like scikit-learn
- Dask extends the parallelism in scikit-learn from a single machine to distributed resources
- Allows you to use some scikit-learn algorithms with larger-than-memory datasets
- Tips from Dask documentation:
  - For in-memory problems, use scikit-learn (or your favorite ML library).
  - For large models, use dask_ml.joblib and your favorite scikit-learn estimator
  - For large datasets, use dask_ml estimators

```python
from dask.distributed import Client
import joblib

client = Client()  # Connect to a Dask Cluster

with joblib.parallel_backend('dask'):
    # Your normal scikit-learn code here
```

Dask Dashboard

- **The Dashboard provides live information in the form of plots and tables**
- **Information on memory and CPU usage, task execution (progress, distribution), and detailed profiling information**



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Contact

Questions and Information

https://training.hpc.mil/

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References/Sources

1. Figures (Array, DataFrame, distributed, logo): https://docs.dask.org/en/latest/

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