Scalable Machine Learning in Python with Dask

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

Gedion Teklemariam, HPCMP PET

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Light Review of terms covered during intro course

- **Dask.array**
  - cuts up large arrays into many small ones.
- **Dask.dataframe**
  - Cuts up large dataframes into many pieces.
- **Dask.Delay**
  - Puts off bringing data into memory, until after task graph is developed.
- **Dask.bag**
  - Used to parallelize computation on unstructured or semi-structured data, like text data.
- **Trask Graphs**

Intro Course on Dask available

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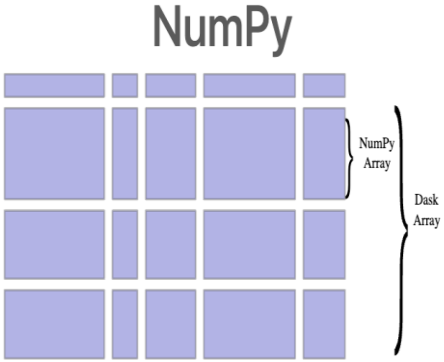
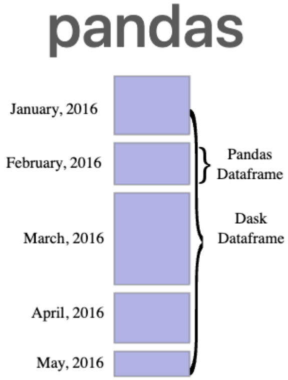
The Dask Benefits

Scale Numpy Workflows



Scale Pandas workflows

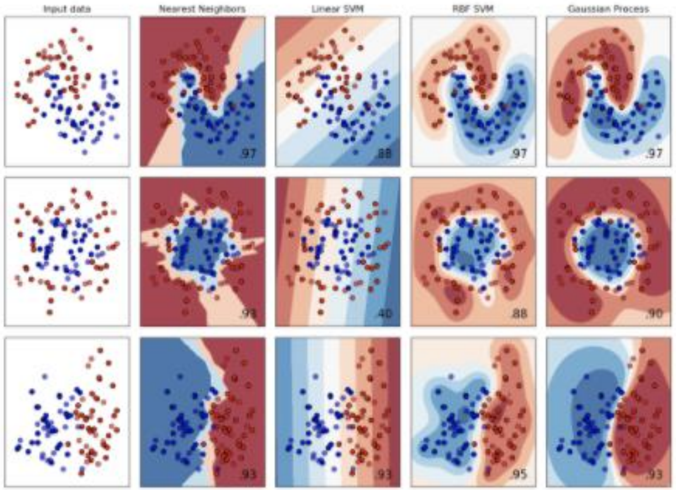


- **Parallel computing / multiprocessing :**
  - Use all cores on system (even on laptops).
- **Larger-than-memory problems:**
  - Not limited by large datasets, if using Dask.
  - work on datasets that are larger than your available memory can handle.
  - Chunk/break up your array into many small pieces, and compute on the chunks in parallel.
  - Only stream chunk data from disk when needed for computation.
- **Blocked Algorithms:**
  - Fracture large computations to many smaller computations, and execute on the smaller computations.

Intro Course on Dask available

Parallelize Scikit-learn / Joblib

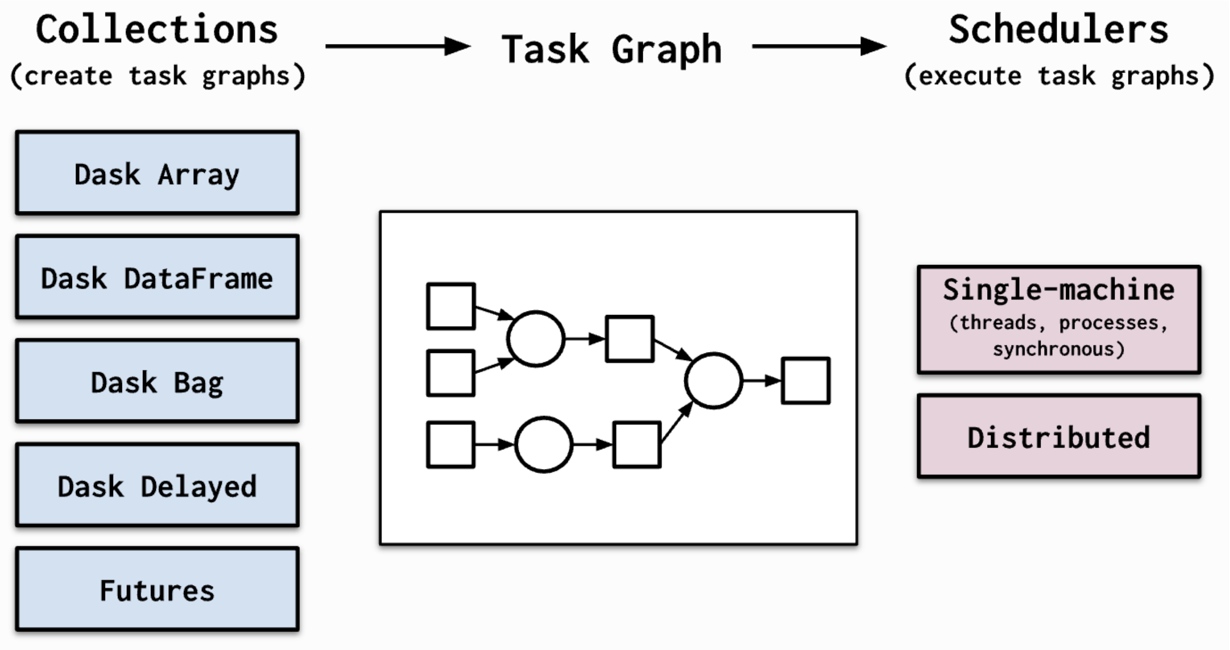
scikit-learn



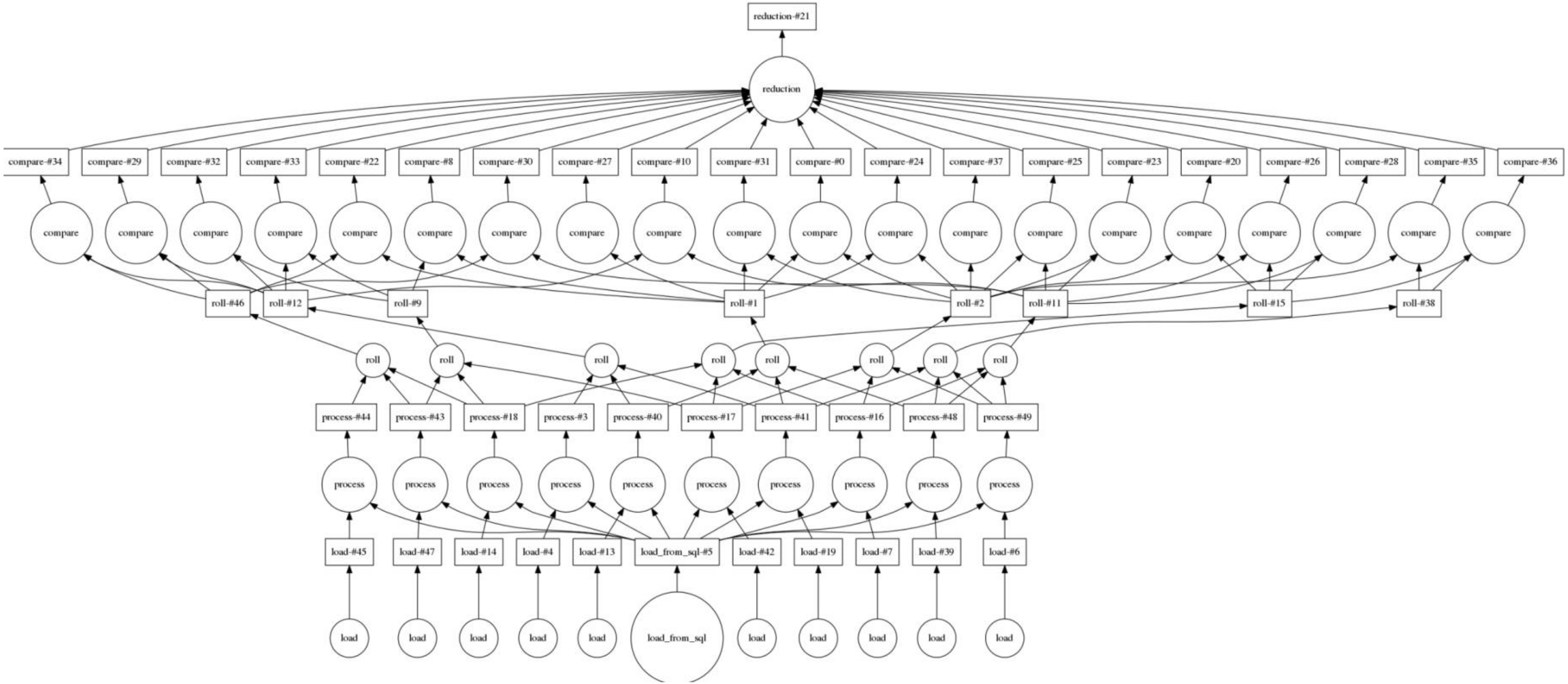
- **Scale Machine Learning APIs**
  - Scikit-learn
  - XGBoost
- **Enable scalable training and predictions on large models & large datasets.**
- **With use of wrappers for Tensorflow & Pytorch Models, integrate Dask with Neural Network models.**
  - We will be proving the concepts with light models.

Use of Task Graphs

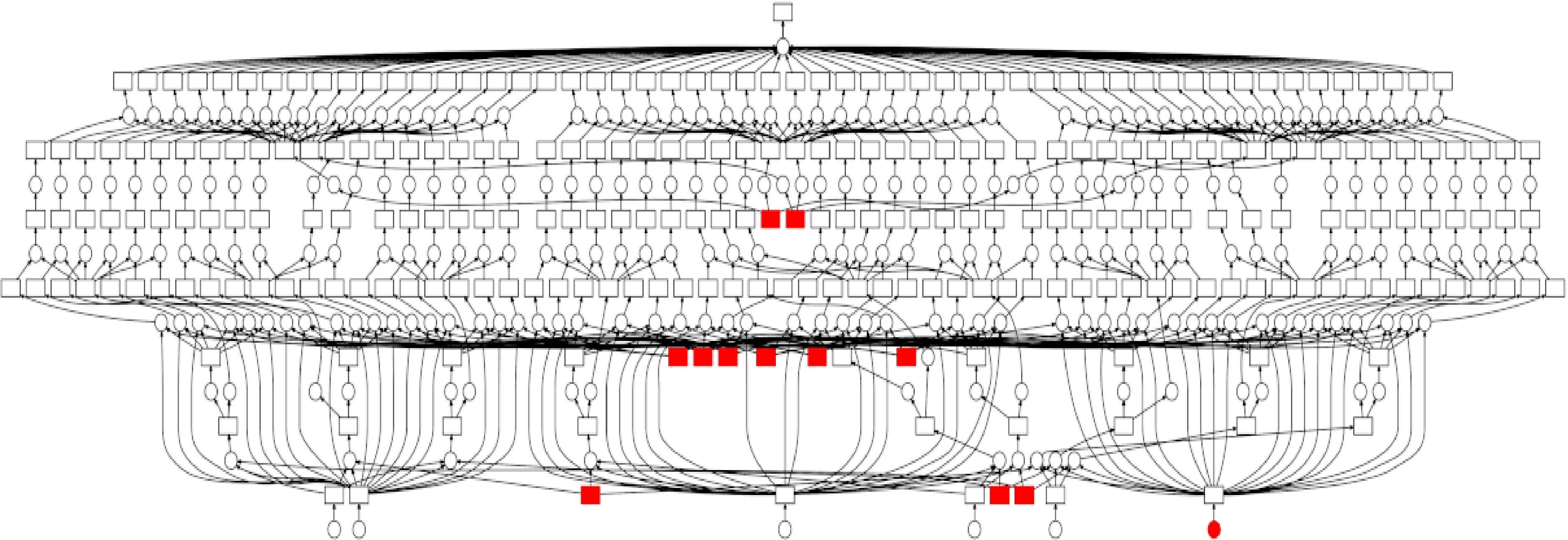
- **First Generates Task Graph.**
- **Execute them on parallel nodes.**



Dask Task Graph - Example



Parallel Computing on Chunks



Familiar to Python Users

- Designed for Python Ecosystem
- Familiar APIs for Python Users
- Scales upto 1000 node clusters

```
# Arrays implement the NumPy API
import dask.array as da
x = da.random.random(size=(10000, 10000),
                     chunks=(1000, 1000))
x + x.T - x.mean(axis=0)
```

```
# Dataframes implement the pandas API
import dask.dataframe as dd
df = dd.read_csv('s3://.../2018-*-*.csv')
df.groupby(df.account_id).balance.sum()
```

```
# Dask-ML implements the scikit-learn API
from dask_ml.linear_model \
  import LogisticRegression
lr = LogisticRegression()
lr.fit(train, test)
```

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Easily Parallelize existing codebases

- **Example of using existing codes:**
  - Easily apply lazy function dask.delayed() to existing functions to improve computational speeds.
  - Computation would not occur until the dask.compute() function is executed.
- **Dask is flexible**
  - Supports current scikit-learn workflows
  - You may also develop your own new scalable algorithms.

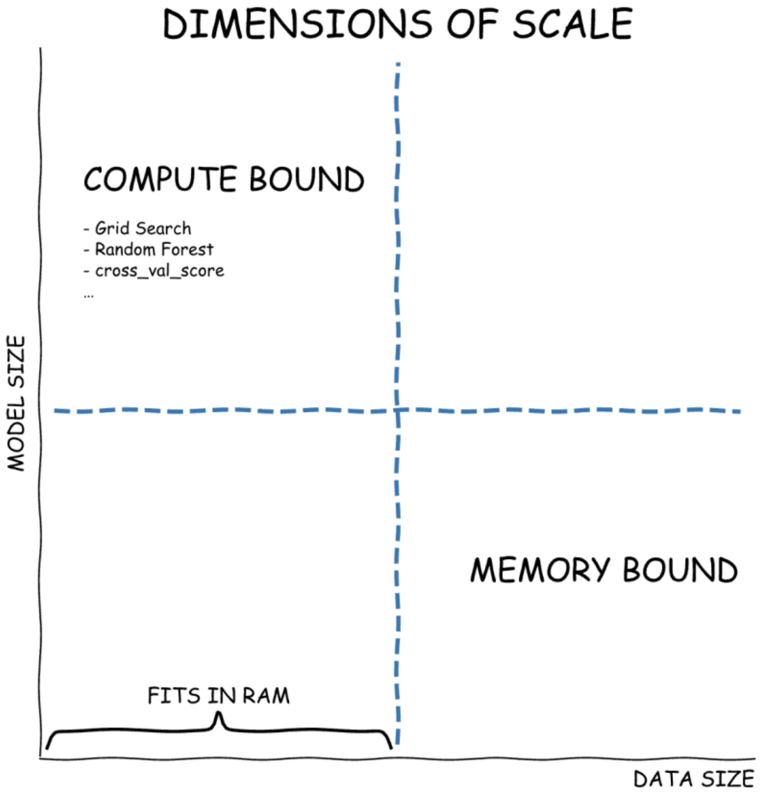
```
func1 = dask.delayed(func1)
func2 = dask.delayed(func2)

for i in X_list:
    for j in Y_list:
        if i > j:
            c = func1(i,j)
        else:
            c = func2(i,j)

        results.append(c)

final = dask.compute(results)
```

```
grid_search.fit(data.data, data.target)
```

```
with joblib.parallel_backend('dask'):
    grid_search.fit(data.data, data.target)
```

Challenges with Large ML models

- **Large Memory Problem:**
  - Dask chunks the dataset into several pieces, so that only a fraction at a time comes into memory.
- **Large Model Problem:**
  - Dask distributes and trains sub-models onto available nodes.
  - Dask distributes batches onto multiple nodes.



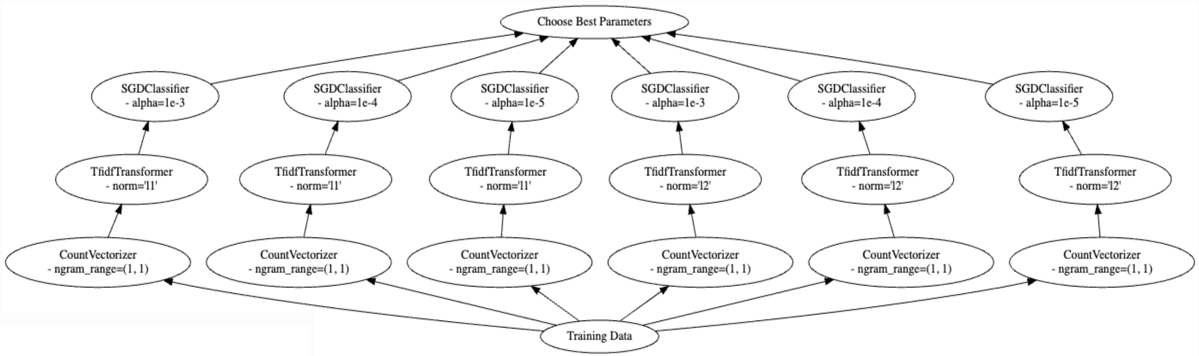
ML jobs where Dask can help

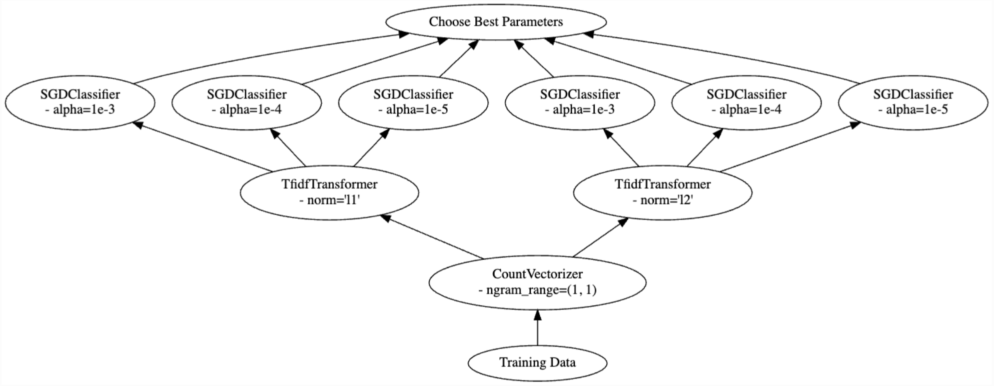
- HyperParameter Search
- Generalized Linear Models
- Parallel Meta-estimators
- Incremental Learning
- Text-Vectorization
- Automated Machine Learning (tpot)

- Use Dask for Batch Prediction with CNN models trained in PyTorch.
- Perform Hyperparameter search on tensorflow based Keras models Generalized Linear Models

Hyperparameter search – Impact of Dask

Dask (task-graph below) eliminates need to repeat redundant computational steps.





dask_ml.model_selection.IncrementalSearchCV(…)

Incrementally search for hyper-parameters on models that support partial_fit

dask_ml.model_selection.HyperbandSearchCV(…)

Find the best parameters for a particular model with an adaptive cross-validation algorithm.

dask_ml.model_selection.SuccessiveHalvingSearchCV(…)

Perform the successive halving algorithm [R424ea1a907b1-1].

dask_ml.model_selection.InverseDecaySearchCV(…)

Incrementally search for hyper-parameters on models that support partial_fit

Notes

- **During the next session, we will go through implementation examples.**
  - Demonstration will focus on utilization of Dask primarily.
  - Understanding and Developing ML models is not the primary objective of the training.
- **For additional information, links are embedded in the Jupyter Notebooks.**
- **If there are interests in some of the models discussed, a separate training will be prepared on those subject matters.**

Contact

Questions and Information

https://training.hpc.mil/

pet@hpc.mil

Gedion.R.Teklemariam.ctr@mail.nrl.navy.mil

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