

Distributed computing and Big Data with Dask

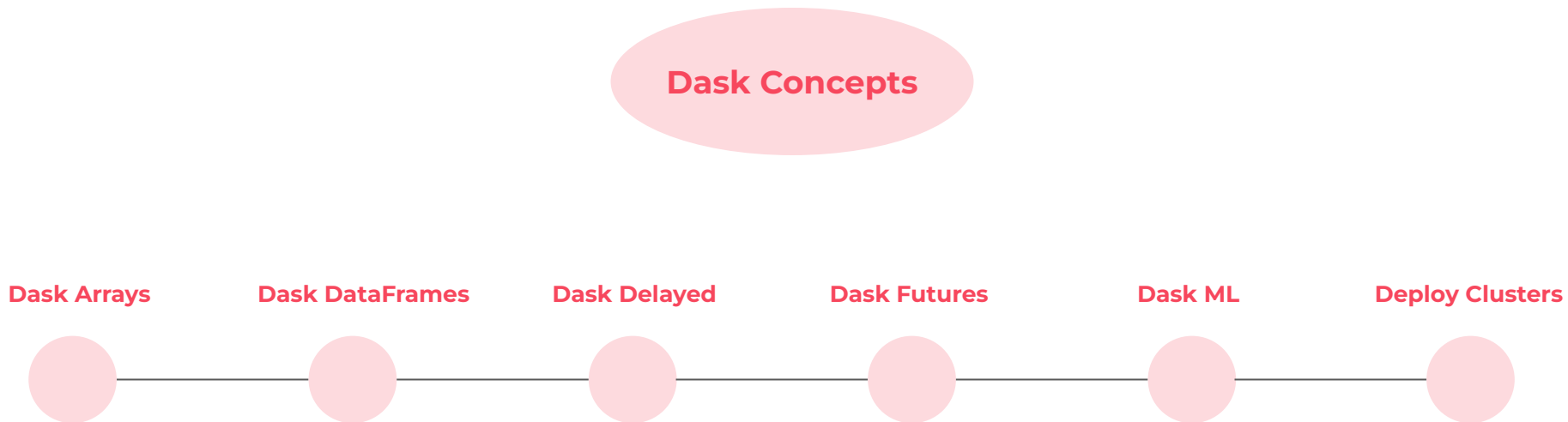


What is Dask?

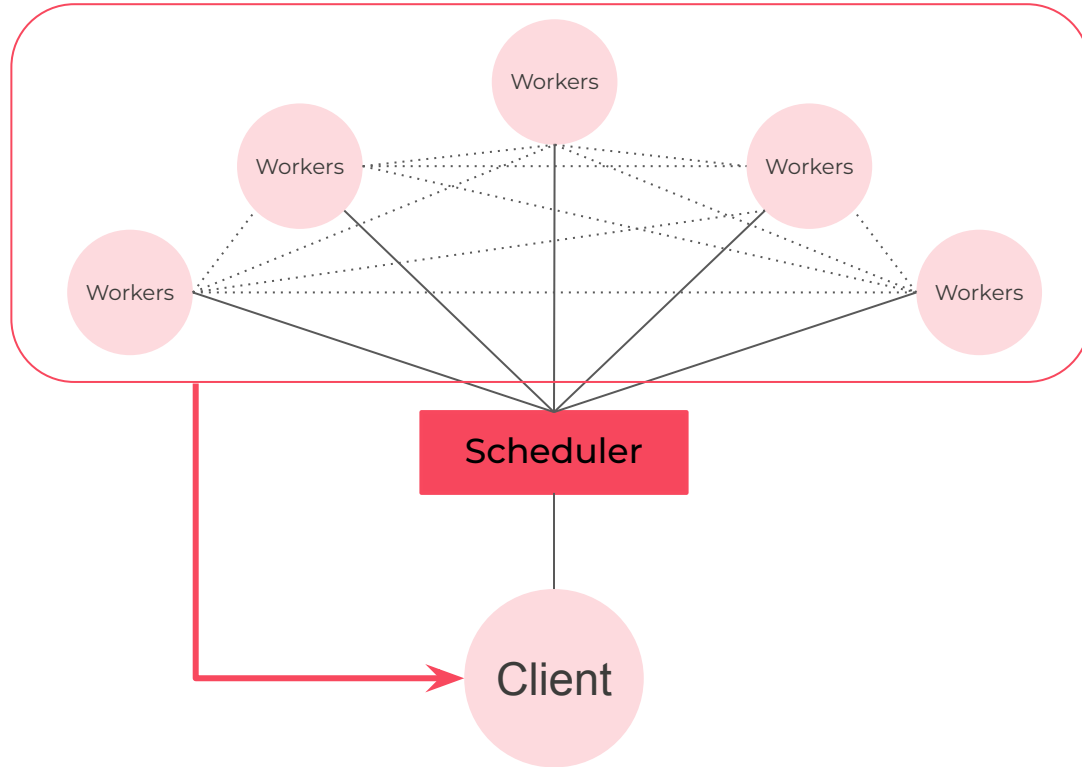
- Flexible open-source Python library for parallel computing (2015);
- Built by the NumPy, Pandas, Jupyter, Scikit-Learn developer community;
- Lightweight and easily installed library;
- Ability to scale by deploying clusters (from single to thousand nodes);
- Handles out-of-memory data for big data analysis.

Main source : <https://docs.dask.org/>

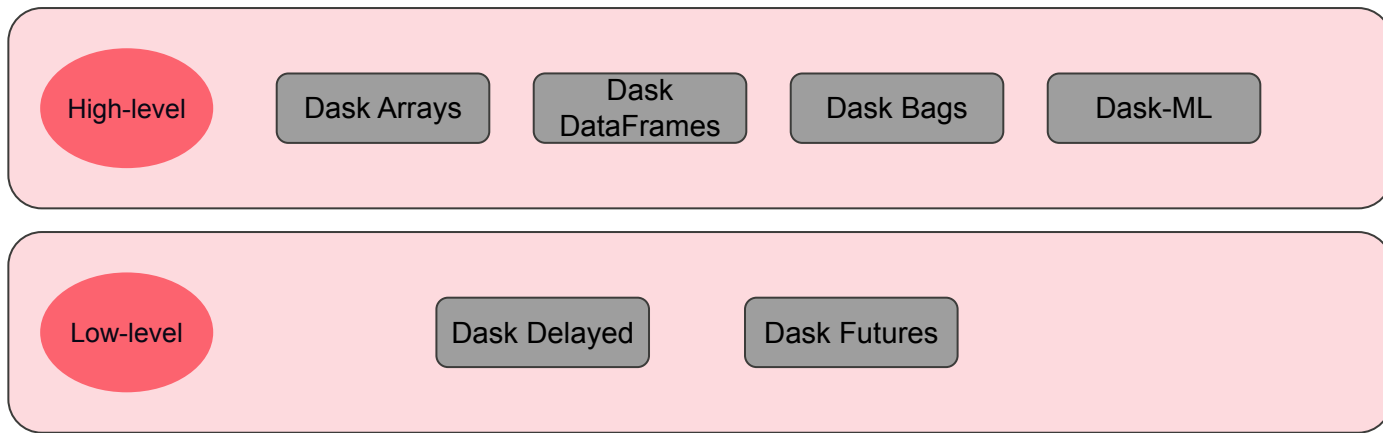
Roadmap



Dask concept: Architecture



Dask concept: Collections



Dask concept: Scheduler

Collections

(create task graphs)

Dask Array

Dask DataFrame

Dask Bag

Dask Delayed

Futures

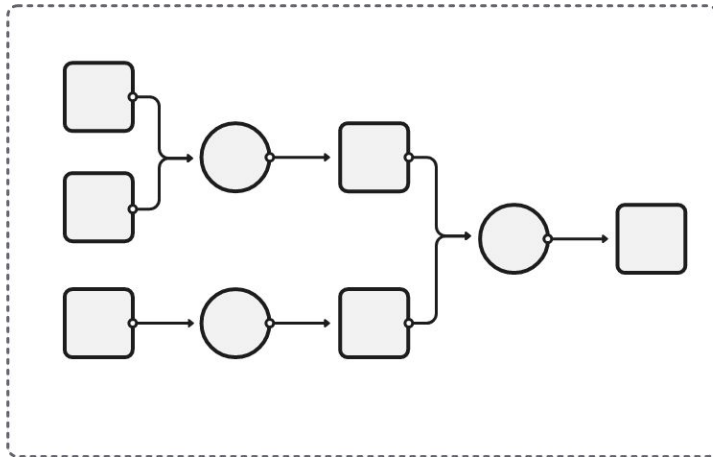


Task Graph



Schedulers

(execute task graphs)



Single-machine
(threads, processes,
synchronous)

Distributed



Notebooks

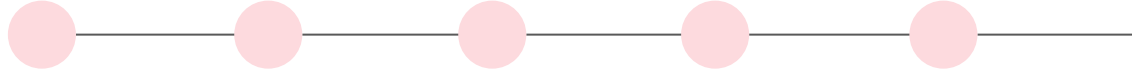
Dask Arrays

Dask DataFrames

Dask Delayed

Dask Futures

Dask ML



Dask Arrays

Dask DataFrames

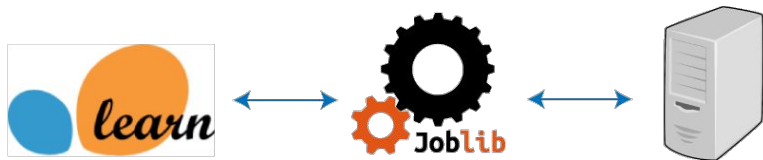
Dask Delayed

Dask Futures

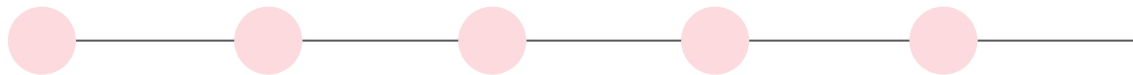
Dask ML



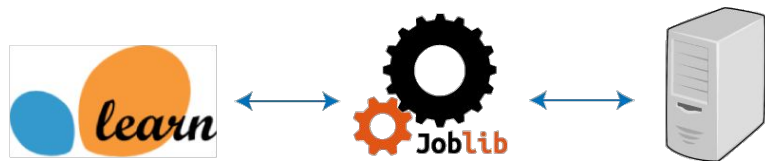
Provides scalable machine learning algorithms compatible with
scikit-learn



Scikit-learn



Provides scalable machine learning algorithms compatible with
scikit-learn

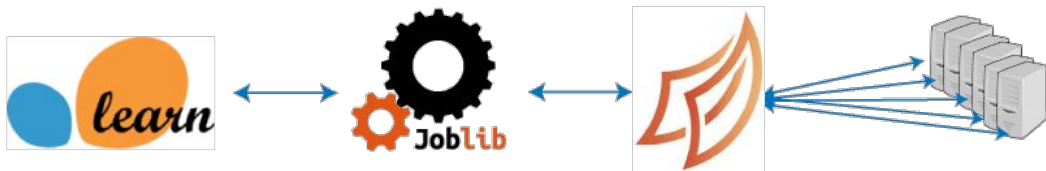


Scikit-learn

```
from dask.distributed import Client
import joblib

client = Client() # create local cluster
# client = Client("scheduler-address") # or remote cluster

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



Scikit-learn + Dask



Use cases

- Pre-processing (`dask_ml.preprocessing`):
 - *MinMaxScaler, LabelEncoder, OneHotEncoder, PolynomialFeatures ...*
- Cross Validation (for instance extension to dask arrays):
 - *`dask_ml.model_selection.train_test_split()`*
- Hyper Parameter Search optimization.
- Generalized Linear Models:
 - *Linear Regression, Logistic Regression, Poisson Regression ...*
- Clustering:
 - *KMeans, Spectral Clustering ...*

Dask Arrays

Dask DataFrames

Dask Delayed

Dask Futures

Dask ML

Deploy Clusters



Dask Arrays

Dask DataFrames

Dask Delayed

Dask Futures

Dask ML

Deploy Clusters



Deploy Clusters anywhere!

- Locally (`dask.distributed.Client()`);



Deploy Clusters anywhere!

- Locally (`dask.distributed.Client()`);
- High Performance Computers (HPC) with job schedulers (SGE, SLURM, PBS);

```
# SGE cluster
from dask.distributed import Client
from dask_jobqueue import SGECluster

cluster = SGECluster(name="dask-worker", walltime="12:00:00",
                    memory="4GB", death_timeout=240, project="P_ztf",
                    resource_spec="sps=1", local_directory="$TMPDIR",
                    cores=1, processes=1)

cluster.scale(10) # How many workers?
client = Client(cluster)
```

Deploy Clusters anywhere!

- Locally (`dask.distributed.Client()`);
- High Performance Computers (HPC) with job schedulers (SGE, SLURM, PBS);
- Kubernetes (Native, Helm);

```
from dask_kubernetes.operator import KubeCluster, make_cluster_spec

config = {
    "name": "foo",
    "n_workers": 2,
    "resources": {"requests": {"memory": "2Gi"}, "limits": {"memory": "64Gi"}}
}

cluster = KubeCluster(**config)
# is equivalent to
cluster = KubeCluster(custom_cluster_spec=make_cluster_spec(**config))
```



Deploy Clusters anywhere!

- Locally (`dask.distributed.Client()`);
- High Performance Computers (HPC) with job schedulers (SGE, SLURM, PBS);
- Kubernetes (Native, Helm);
- Cloud providers (AWS, GCP, Azure, ...)

```
from dask_cloudprovider.azure import AzureVMCluster
cluster = AzureVMCluster(resource_group="<resource group>",
                        vnet="<vnet>",
                        security_group="<security group>",
                        n_workers=1)

from dask.distributed import Client
client = Client(cluster)
```


Conclusion

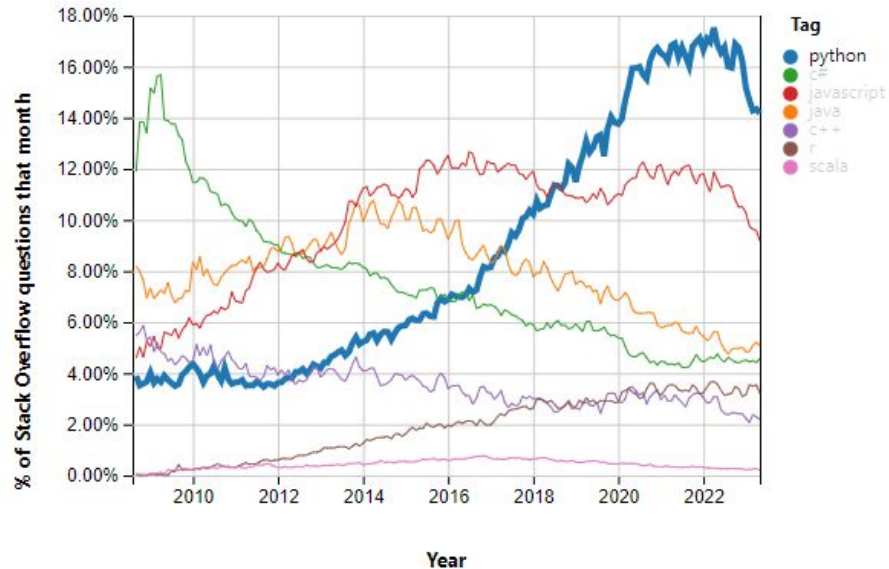
- Pure Python library;
- Numpy and Pandas APIs, familiar for Python users;
- Distributed computing (locally and on clusters);
- Allowing Big Data analysis;
- Highly flexible use thanks to Delayed and Futures;

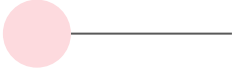


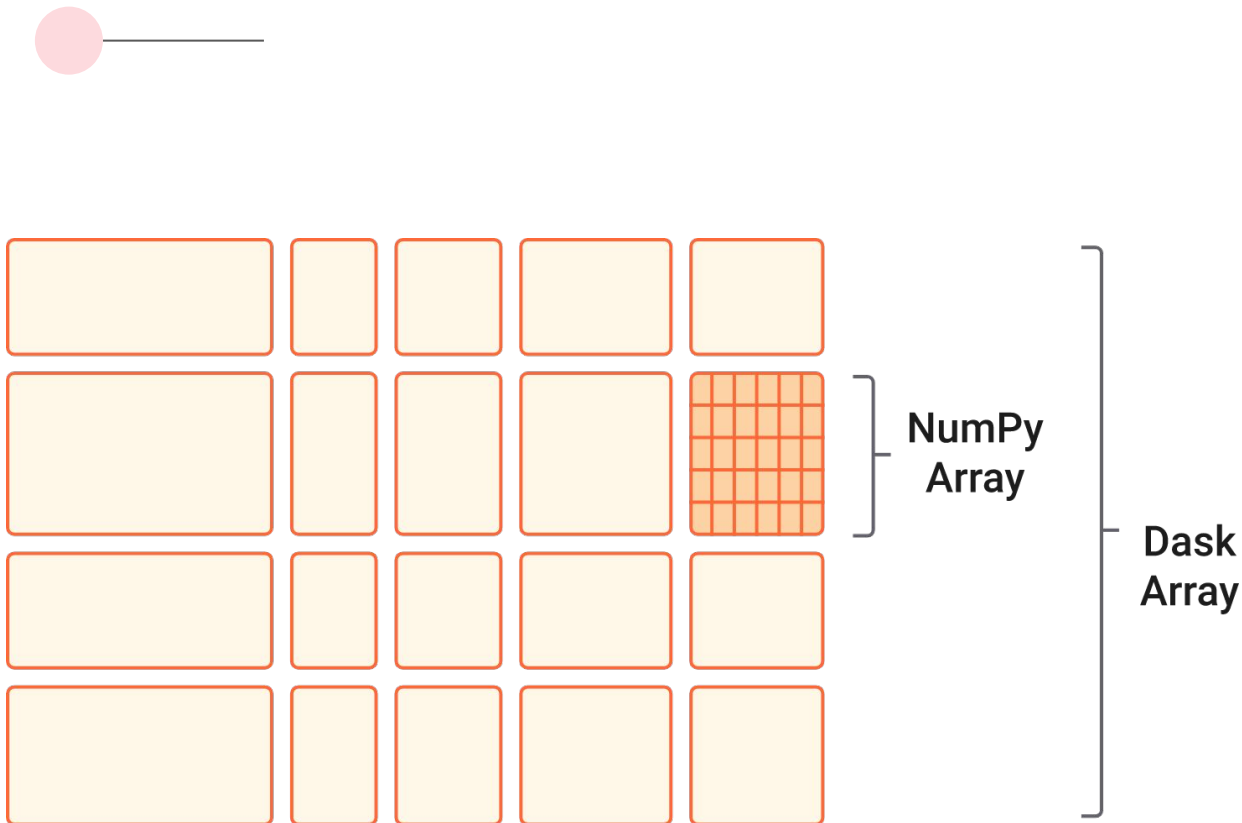
No Notebooks Version

What is Dask?

- Flexible open-source Python library for parallel computing (2015);







Parallel Numpy:

- Single array chunked into smaller ones;
- Load of array larger than RAM;
- Computation optimization.

Highly use in:

- Science (astronomy, oceanography...);
- Large scale imaging;
- Numerical algorithms
- ...

```
import numpy as np
```

```
size=2000
```

```
arr = np.random.random((size,size,size))
```

```
-----  
MemoryError                                Traceback (most recent call last)
```

```
~\AppData\Local\Temp\ipykernel_6680\925286073.py in <module>
```

```
----> 1 arr = np.random.random((size,size,size))
```

```
mtrand.pyx in numpy.random.mtrand.RandomState.random()
```

```
mtrand.pyx in numpy.random.mtrand.RandomState.random_sample()
```

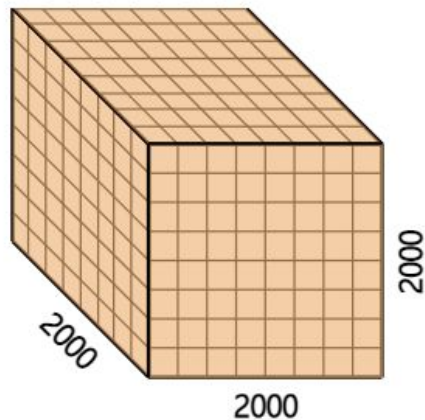
```
_common.pyx in numpy.random._common.double_fill()
```

```
MemoryError: Unable to allocate 59.6 GiB for an array with shape (2000, 2000, 2000) and data type float64
```

```
import dask.array as da
```

```
chunk = 'auto'  
x = da.random.random((size,size,size), chunks=(chunk,chunk,chunk))  
x
```

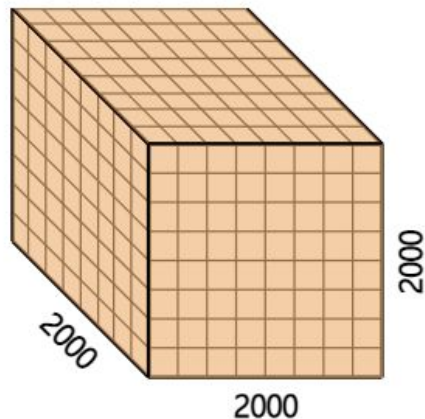
	Array	Chunk
Bytes	59.60 GiB	119.21 MiB
Shape	(2000, 2000, 2000)	(250, 250, 250)
Count	512 Tasks	512 Chunks
Type	float64	numpy.ndarray



```
import dask.array as da
```

```
chunk = 'auto'  
x = da.random.random((size,size,size), chunks=(chunk,chunk,chunk))  
x
```

	Array	Chunk
Bytes	59.60 GiB	119.21 MiB
Shape	(2000, 2000, 2000)	(250, 250, 250)
Count	512 Tasks	512 Chunks
Type	float64	numpy.ndarray



```
m = x.mean()
```

```
%%time  
m.compute()
```

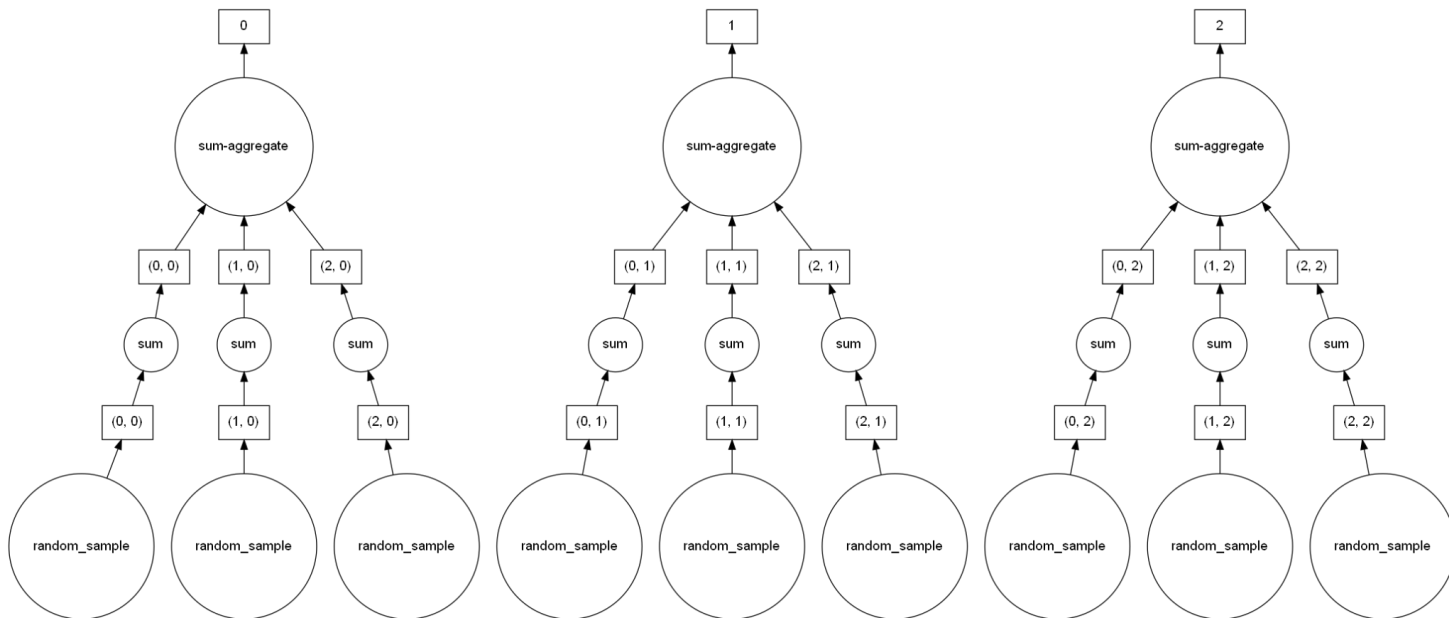
Wall time: 21.3 s

0.4999996563332088

Dask Arrays

```
x = da.random.random((15, 15), chunks=(5,5))  
comp = x.sum(axis=0)
```

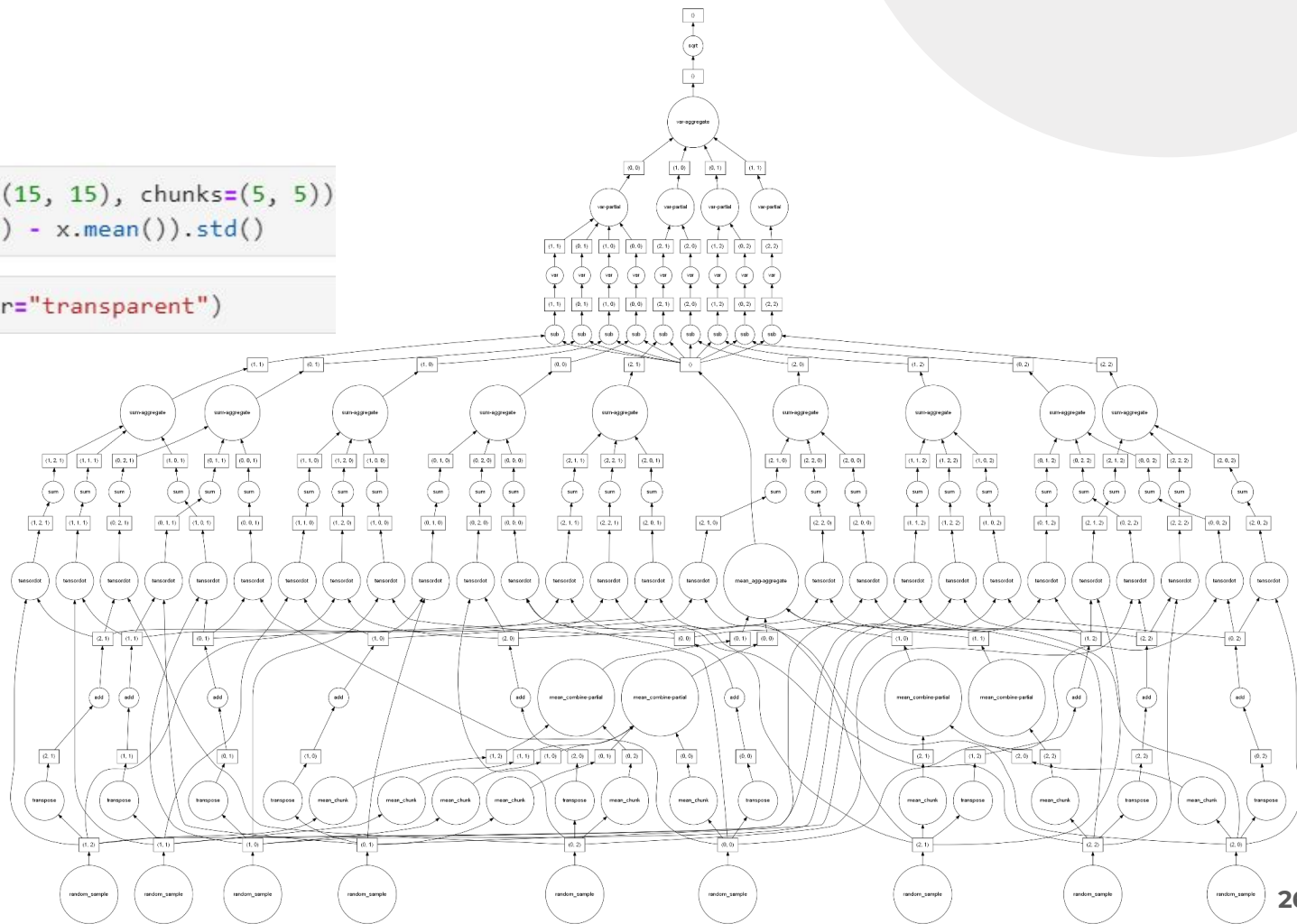
```
comp.visualize(bgcolor='transparent')
```



Note: needs **graphviz** engine

```
x = da.random.random((15, 15), chunks=(5, 5))
comp = (x.dot(x.T + 1) - x.mean()).std()
```

```
comp.visualize(bgcolor="transparent")
```



Note: needs **graphviz** engine

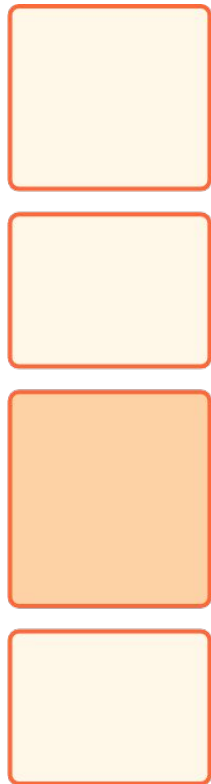
Dask Arrays

Dask DataFrames





**Pandas
DataFrame**



**Dask
DataFrame**

Parallel Pandas:

- Large dataframe chunked into smaller ones;
- As for dask arrays, allows load of DF larger than RAM;
- Speed up the computation;
- Allow big data visualization (hvplot, datashader...).



Taxi data on [Kaggle](#)

```
!ls -l --block-size=G "Data/"
```

total 7G

```
-rw-r--r-- 1 jlezmy Domain Users 2G Feb  2 14:56 yellow_tripdata_2015-01.csv  
-rw-r--r-- 1 jlezmy Domain Users 2G Feb  2 14:57 yellow_tripdata_2016-01.csv  
-rw-r--r-- 1 jlezmy Domain Users 2G Feb  2 14:57 yellow_tripdata_2016-02.csv  
-rw-r--r-- 1 jlezmy Domain Users 2G Feb  2 14:57 yellow_tripdata_2016-03.csv
```

```
import dask.dataframe as dd
```

```
%%time  
ddf = dd.read_csv( os.path.join("Data/*.csv"), blocksize="64MB" )
```

Wall time: 43.3 ms

```
len(ddf)
```

47248845

```
list(ddf.columns)
```

```
['VendorID',  
 'tpep_pickup_datetime',  
 'tpep_dropoff_datetime',  
 'passenger_count',  
 'trip_distance',  
 'pickup_longitude',  
 'pickup_latitude',  
 'RateCodeID',  
 'store_and_fwd_flag',  
 'dropoff_longitude',  
 'dropoff_latitude',  
 'payment_type',  
 'fare_amount',  
 'extra',  
 'mta_tax',  
 'tip_amount',  
 'tolls_amount',  
 'improvement_surcharge',  
 'total_amount']
```



```
from dask.distributed import Client, LocalCluster
```

```
# Let's create a local cluster:
```

```
cluster = LocalCluster()
client = Client(cluster)
```

```
### exactly the same than client = Client(), but more explicit.
```

```
client
```



Client

Client-d04b90bd-a6c8-11ed-bcd0-fcb3bce22673

Connection method: Cluster object

Cluster type: distributed.LocalCluster

Dashboard: <http://127.0.0.1:8787/status>

▼ Cluster Info



LocalCluster

4cbadea0

Dashboard: <http://127.0.0.1:8787/status>

Workers: 4

Total threads: 8

Total memory: 7.71 GiB

Status: running

Using processes: True

► Scheduler Info

Let's create a local cluster:

- Visibility on the task graph;
- “ task stream;
- “ workers status;
- ... through an awesome dashboard!

Note: a [dask extension](#) is available on jupyter-lab

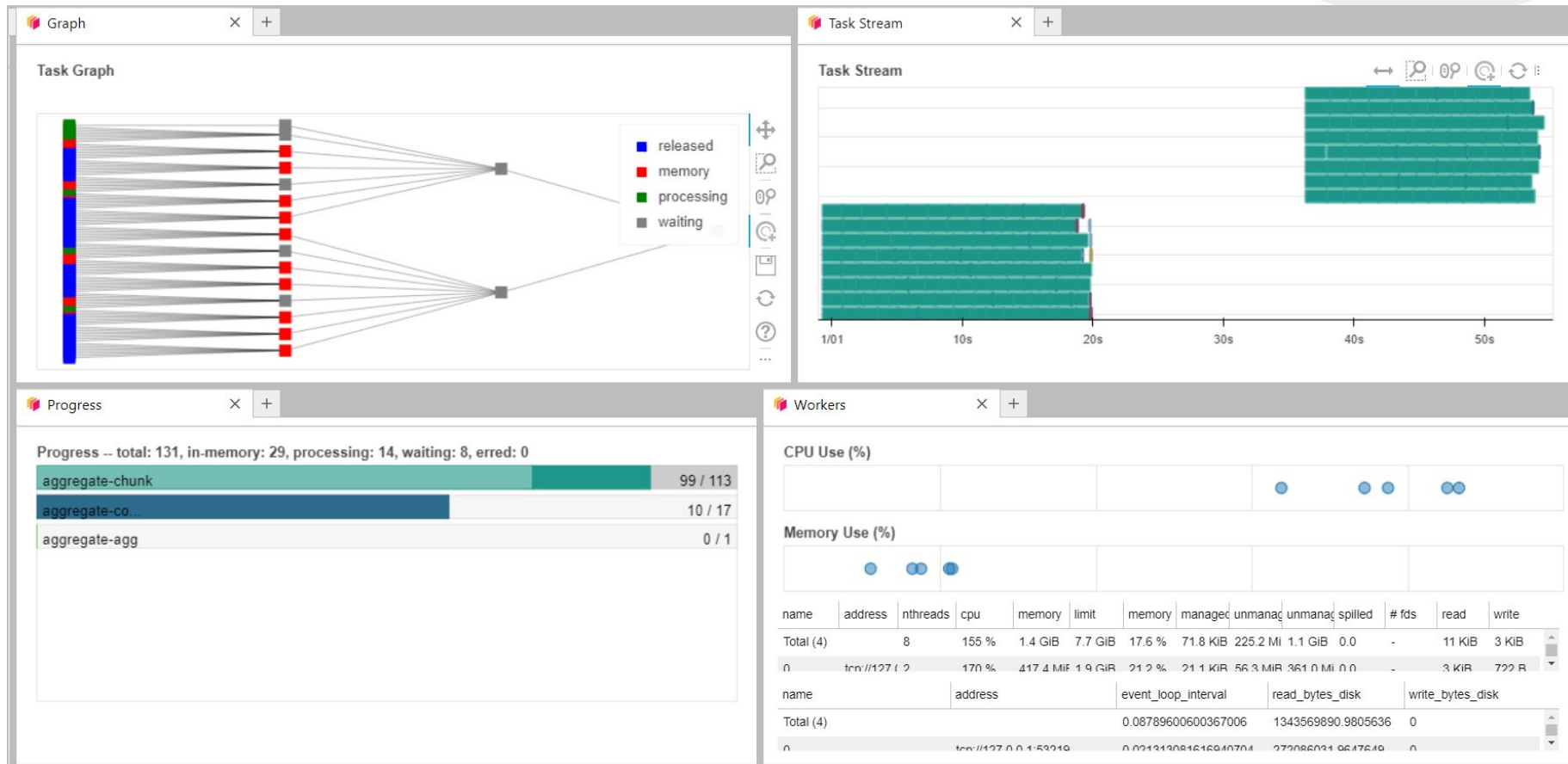
```
subdf = ddf[['payment_type', 'total_amount',  
            'trip_distance']]  
groupdf = subdf.groupby('payment_type').agg({'total_amount': "mean",  
                                             'trip_distance': "mean"})
```

```
%%time  
groupdf.compute()
```

Wall time: 19.6 s

	total_amount	trip_distance
payment_type		
1	17.109936	4.171999
2	12.711215	13.210922
3	15.030975	65.266945
4	12.290095	32.067464
5	6.200000	1.166667

Dask Arrays Dask DataFrames



Big Data visualization: Datashader

```
subdf = ddf[['pickup_longitude',  
            'pickup_latitude',  
            'passenger_count']]
```

```
import datashader  
from datashader import transfer_functions as tf  
from datashader.colors import Hot  
  
def render(df, x_range=(-74.1, -73.7), y_range=(40.6, 40.9)):  
    canvas = datashader.Canvas(  
        x_range=x_range,  
        y_range=y_range,  
    )  
    agg = canvas.points(  
        source=df,  
        x="pickup_longitude",  
        y="pickup_latitude",  
        agg=datashader.count("passenger_count"),  
    )  
    return tf.shade(agg, cmap=Hot, how="eq_hist")
```

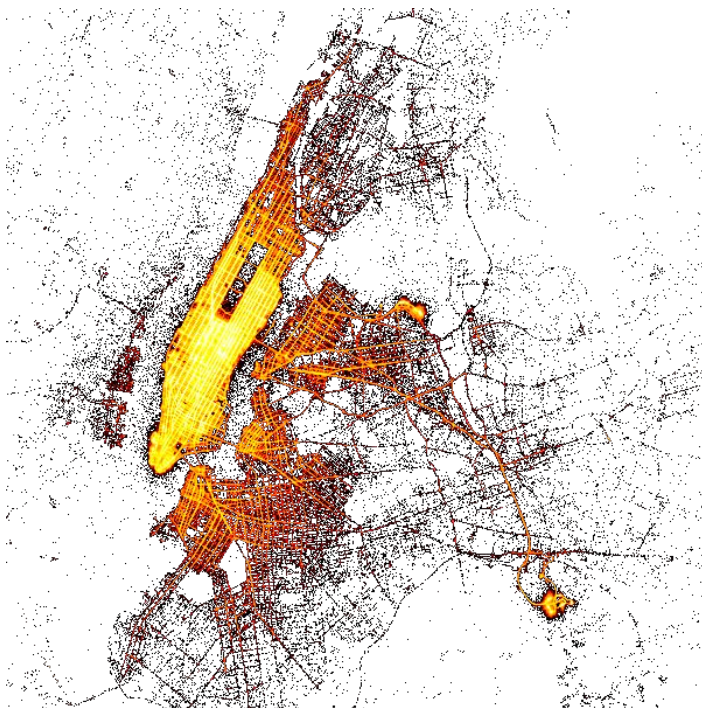
Big Data visualization: Datashader

```
subdf = ddf[['pickup_longitude',  
            'pickup_latitude',  
            'passenger_count']]
```

```
import datashader  
from datashader import transfer_functions as tf  
from datashader.colors import Hot  
  
def render(df, x_range=(-74.1, -73.7), y_range=(40.6, 40.9)):  
    canvas = datashader.Canvas(  
        x_range=x_range,  
        y_range=y_range,  
    )  
    agg = canvas.points(  
        source=df,  
        x="pickup_longitude",  
        y="pickup_latitude",  
        agg=datashader.count("passenger_count"),  
    )  
    return tf.shade(agg, cmap=Hot, how="eq_hist")
```

```
%time render(subdf) ## 48M points !!
```

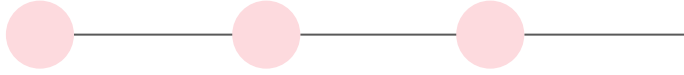
Wall time: 49.9 s



Dask Arrays

Dask DataFrames

Dask Delayed





Low-level API for **parallelizable problems** which don't fit into high-level abstractions (Dask Array / DataFrame)

- Lazy objects: computed only if explicitly asked to;
- Equivalent to DAG nodes;
- Dask creates an optimised graph, determining the dependencies between each delayed object;
- Doesn't need a *Client*.



```
from dask import delayed
def inc(x):
    return x + 1

def custom_op(x):
    return 2*x**2

def add(x, y):
    return x + y

data = np.arange(0,6,1)

a = [delayed(inc)(x) for x in data]
b = [delayed(custom_op)(x) for x in data]
output = [delayed(add)(i, j) for i,j in zip(a,b)]

total = delayed(sum)(output)
total
```

```
Delayed('sum-09ce14df-d4a1-4b0a-981e-e3a15f42bd9f')
```

```
total.compute()
```

```
Delayed('sum-09ce14df-d4a1-4b0a-981e-e3a15f42bd9f')
```

131



Dask Delayed as a *decorator*

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

@delayed
def custom_op(x):
    return 2*x**2

@delayed
def add(x, y):
    return x + y

data = np.arange(0,6,1)

a = [inc(x) for x in data]
b = [custom_op(x) for x in data]
output = [add(i, j) for i,j in zip(a,b)]

total = delayed(sum)(output)
print(inc(0))
```

```
Delayed('inc-789d1c17-df7b-4d14-954f-aab785f5fab5')
```



Dask Delayed as a *decorator*

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

@delayed
def custom_op(x):
    return 2*x**2

@delayed
def add(x, y):
    return x + y

data = np.arange(0,6,1)

a = [inc(x) for x in data]
b = [custom_op(x) for x in data]
output = [add(i, j) for i,j in zip(a,b)]

total = delayed(sum)(output)
print(inc(0))
```

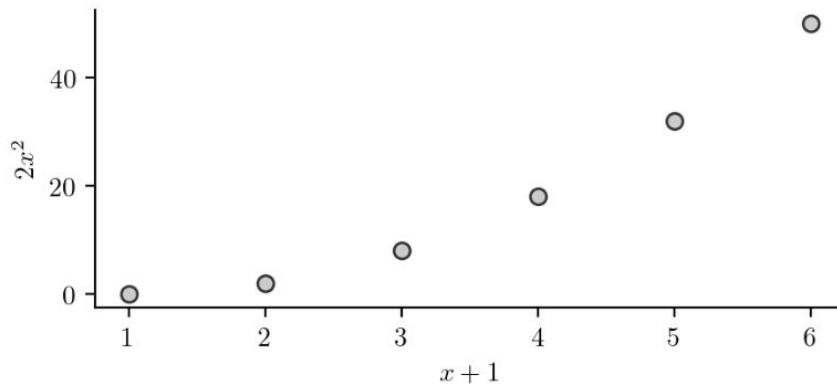
Delayed('inc-789d1c17-df7b-4d14-954f-aab785f5fab5')

```
@delayed
def plot(a,b):
    fig,ax = plt.subplots(figsize=(5,2), dpi=200)
    ax.scatter(a,b, marker='o', facecolor='0.8', edgecolor='0.2')
    ax.set_xlabel('$x+1$')
    ax.set_ylabel(r'$2x^2$')
    ax.spines[['right','top']].set_visible(False)
    return fig

plot(a,b)
```

Delayed('plot-65238b37-98a6-45b2-8cf5-f6b6a70ec463')

```
fig = plot(a,b).compute()
```



Dask Arrays

Dask DataFrames

Dask Delayed

Dask Futures





Low-level API : real-time task framework that extends Python's [concurrent.futures](#) interface

- ~~Lazy~~ Eager objects: computed **immediately**;
- Scale your Python futures workflow across a Dask cluster with minimal code changes;
- Add **flexibility**;
- *Dask client* is **needed** to use future interface.



Minimal example

```
from dask.distributed import Client, LocalCluster
import numpy as np
import time

cluster = LocalCluster()
client = Client(cluster) # Same as client=Client()
```

```
def load(x):
    time.sleep(0.2)
    return np.arange(10000) + x
```

```
def process1(x):
    return x**2
```

```
def process2(x,y):
    return 2*x + y
```

```
def save(x):
    time.sleep(0.2)
    return 'Saved'
```

```
inputs_1, inputs_2 = np.arange(0,50), np.arange(50,100)
futures = []

for i,j in zip(inputs_1,inputs_2):
    x = client.submit(load, i) #client.submit(fucn, *args)
    y = client.submit(load, j)
    xp = client.submit(process1, x)
    xyp = client.submit(process2, xp,y)
    z = client.submit(save, xyp)
    futures.append(z)

z
```

Future: save status: **pending**, type: NoneType, key: save-c6c436fe0ee6c4795657b742886162df

z

Future: save status: **finished**, type: str, key: save-c6c436fe0ee6c4795657b742886162df

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

Combining Futures and Delayed ?

```
from dask import delayed
@delayed
def inc(x):
    return x + 1
@delayed
def custom_op(x):
    return 2*x**2
@delayed
def add(x, y):
    return x + y
```

```
@delayed
def plot(a,b,savefile=None):
    fig,ax = plt.subplots(figsize=(5,2) )
    ax.scatter(a,b, marker='o', facecolor='0.8', edgecolor='0.2')
    ax.set_xlabel(r'$x+1$')
    ax.set_ylabel(r'$2x^{2}$')
    ax.spines[['right','top']].set_visible(False)
    fig.tight_layout()
    if savefile != None:
        fig.savefig(savefile,transparent=True)
    return fig
```

```
def compute_single(data, show=False, savefile=None):
    stored = []
    a = [inc(x) for x in data]
    b = [custom_op(x) for x in data]
    output = [add(i, j) for i,j in zip(a,b)]
    stored.append(delayed(sum)(output))
    if not show:
        return stored
    stored.append( plot(a,b,savefile) )
    return stored
```

```
stored = compute_single(data=np.arange(0,6,1),
                        show=True, savefile=None)
stored
```

```
[Delayed('sum-b6638107-bfe6-426a-90a9-4f33b2295286'),
 Delayed('plot-c30f1ea7-224c-420f-b8de-e24dbc69efb6')]
```

```
future = client.compute(stored)
results = client.gather(future);
results
```

```
[131, <Figure size 500x200 with 1 Axes>]
```

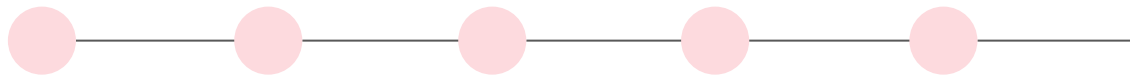


Use cases

- Pre-processing (`dask_ml.preprocessing`):
 - *MinMaxScaler, LabelEncoder, OneHotEncoder, PolynomialFeatures ...*
- Cross Validation (for instance extension to dask arrays):
 - *`dask_ml.model_selection.train_test_split()`*
- Hyper Parameter Search optimization.

Random forest algorithms with tunable parameters:

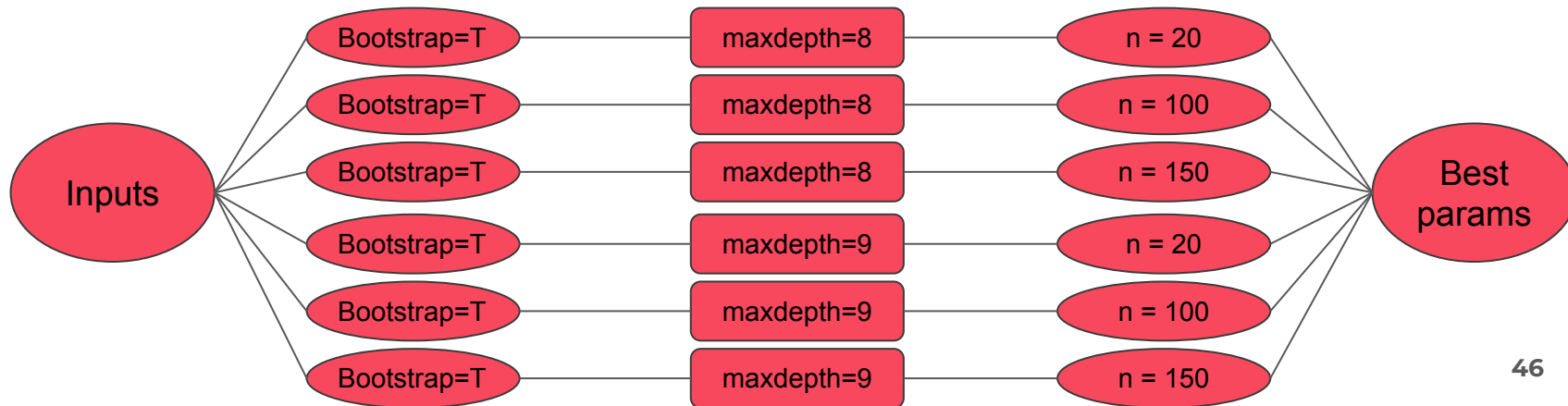
*Bootstrap = **True** max_depth = **[8, 10]** n_estimator = **[20, 100, 150]***

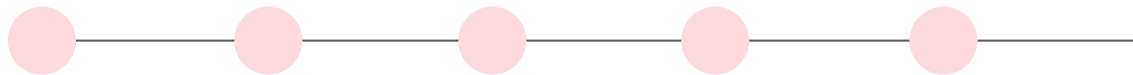


Use cases

- Pre-processing (`dask_ml.preprocessing`):
 - *MinMaxScaler, LabelEncoder, OneHotEncoder, PolynomialFeatures ...*
- Cross Validation (for instance extension to dask arrays):
 - *dask_ml.model_selection.train_test_split()*
- Hyper Parameter Search optimization.

SKlearn





Use cases

- Pre-processing (`dask_ml.preprocessing`):
 - *MinMaxScaler, LabelEncoder, OneHotEncoder, PolynomialFeatures ...*
- Cross Validation (for instance extension to dask arrays):
 - `dask_ml.model_selection.train_test_split()`
- Hyper Parameter Search optimization.

Dask

