# Dask-ML and Dask-distributed

Joseph John

National Computational Infrastructure, Australia

# Cluster Support

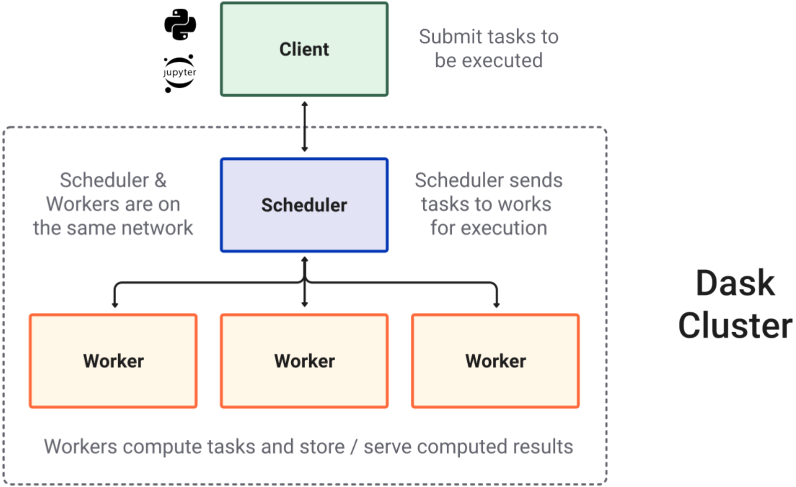
- **project**: vp91
- **modules**: python3/3.8.5 cuda/12.0.0
- **venv**: /scratch/vp91/AAPP2023/dask-python3.9-venv
- **repo**: https://github.com/nci900/AAPP-Distributed-Dask.git

dask

This session will cover:

1. Machine learning in Dask.
2. How to scale machine learning using Dask.
3. How to use Dask together with PBS.

# Dash Cluster



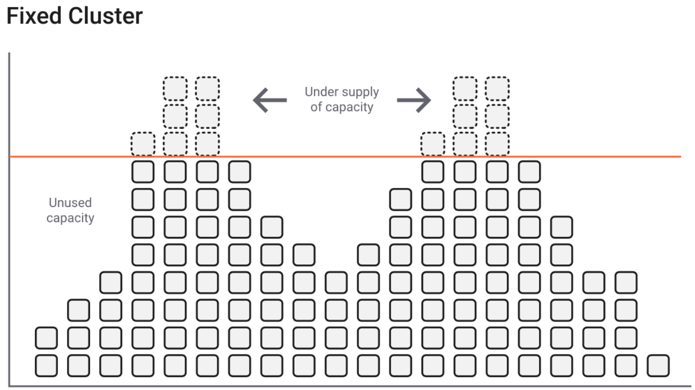
# Dask Cluster

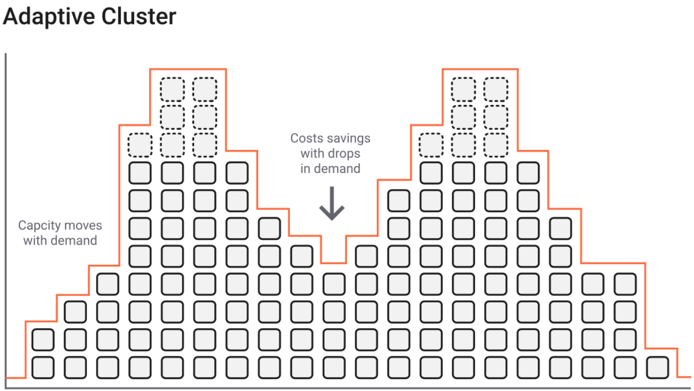
1. A cluster managers deploy a scheduler and the necessary workers.
2. Dask by default use single-machine scheduler.

# Dask Cluster Components

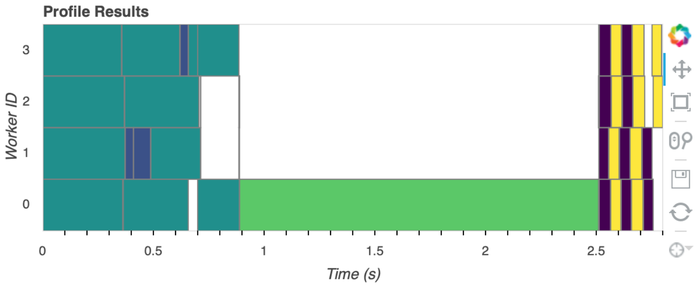
1. **Clients**: Sends instructions to the scheduler and collects results from the workers. Programmers usually interacts with the client.
2. **Scheduler**: It tracks metrics, and allows the workers and clients to coordinate.
3. **Workers**: Threads, processes, or separate machines in a cluster. They execute the computations from the computation graph.

# Fixed Cluster




Adaptive Cluster
Capcity moves
with demand
Costs savings
with drops
in demand

# Profiling



# Dask ML

1. Dask-ML provides scalable machine learning in Python.
2. Works with ML libraries like Scikit-Learn, XGBoost.
3. Dask-ML API is similar to Scikit-Learn API.

# Data Prepossessing

The first process step in building a machine learning model is data cleaning.
Data cleaning mainly involves:

1. Remove any unnecessary observations from your dataset
2. Remove redundant information
3. Remove duplicate information
4. Remove structural errors in data collection
5. Remove unwanted outliers - outliers can result in overfitting
6. Handle missing data:
    1. Remove observations with values missing
    2. Infer the missing values

# Data Prepossessing

We are taking the easiest method to address missing values. We are removing any dataframe row that has missing values. , we end up not getting the entire picture. Inferring data is also not always a good idea as we may add some bias to the inference.

1. This is not always advisable as we are losing a lot of information and in the end.
2. Inferring data is also not always a good idea as we may add some bias to the inference.

.

# Drop Missing Data

```
import dask.dataframe as dd

ddf = dd.read_csv("weatherAUS.csv",
    dtype={'Humidity3pm': 'float64',
    'Humidity9am': 'float64',
    'WindGustSpeed': 'float64',
    'WindSpeed3pm': 'float64',
    'WindSpeed9am': 'float64'})

ddf_clean = ddf.dropna()
    ...
```

# Types of data

Data cleaning mainly involves:

1. Categorical data groups information (usually text) with similar characteristics.
2. Numerical data expresses information in the form of numbers

Most machine learning algorithms cannot handle categorical variables unless it is converted to numerical data. This process is called **encoding**.

# Encoding

Data cleaning mainly involves:

1. One-hot encoding
2. Label encoding
3. Target encoding
4. Frequency
5. Binary encoding
6. Feature Hashing

We will be using **One-hot** encoding (also called Dummy encoding).

# One-hot Encoding

| Team | Colour |
|---|---|
| 1 | Red |
| 2 | Blue |
| 3 | Green |

# One-hot Encoding

| Team | Red_colour | Blue_colour | Green_colour |
|---|---|---|---|
| 1 | 1 | 0 | 0 |
| 2 | 0 | 1 | 0 |
| 3 | 0 | 0 | 1 |

# Categorical data in Dask

There are two types of categorical data in Dask

1. Known: categories are known statically (from the metadata).
2. Unknown: categories are not known statically (from the metadata).

# One-hot Encoder

```
from dask_ml.preprocessing import Categorizer, DummyEncoder

de = DummyEncoder()
ddf_features_preproc = de.fit_transform(ddf_features.categorize())
    ...
```

# Normalization

1. Normalization is the process of translating data into the range.
2. It is a good practice to normalize the data - especially useful when different features have different value ranges.
3. Normalization ensures that one feature does not overtly influence the model.

# Normalization

```
from dask_ml.preprocessing import StandardScaler

scaler = StandardScaler()
scalar_norm = scaler.fit(ddf_features_preproc)
ddf_features_norm = scaler.fit_transform(ddf_features_preproc)
    ...
```

# Correlation matrix

Correlation is often used in machine learning to identify multi-collinearity.

1. Two or more predictor variables are highly correlated with each other.
2. Multicollinearity can adversely affect the accuracy of predictive models.
3. The coefficients become very sensitive to small changes in the model.
4. Multicollinearity reduces the precision of the estimated coefficients, which weakens the statistical power of your regression model.
5. Multicollinearity can be addressed by removing one of the correlated variables.

# Correlation matrix

1. Pearson's correlation
2. Spearman's correlation
3. Kendall's Tau correlation

We will me using **Pearson's correlation.**

# Correlation matrix

```
corr_matrix = ddf_features_norm.corr(method='pearson',
    min_periods=None, numeric_only='__no_default__',
    split_every=False)
    ...
```

# Principal Component Analysis

Principal component analysis, or PCA, is a that is often used to reduce the dimensionality of large data sets, by that .

1. Dimensionality reduction method.
2. Transform a large set of variables into a smaller one.
3. The reduced variable set will still contains most of the information in the large set.

# Correlation matrix

```
from dask_ml.decomposition import PCA

pca = PCA(n_components=3)
pca.fit(ddf_features_norm.to_dask_array(lengths=True))
PCA(copy=True, iterated_power='auto', n_components=3,
    random_state=None, svd_solver='auto', tol=0.0, whiten=False)
```

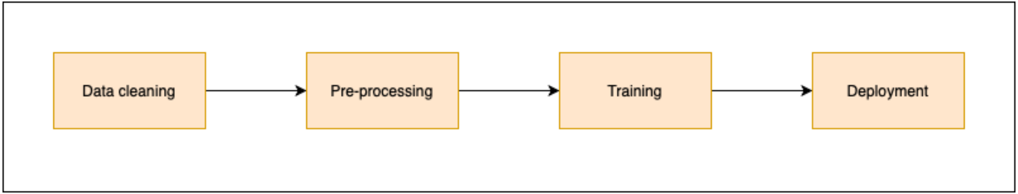
# Cross Validation

Cross-validation is a method for evaluating ML models by training several ML models on subsets of the data and evaluating another subset of the data.
The advantages of cross validation are :

1. Identify Overfitting
2. Comparison between different models
3. Hyperparameter tuning
4. Efficiency : Allows the use of data for both training and validation

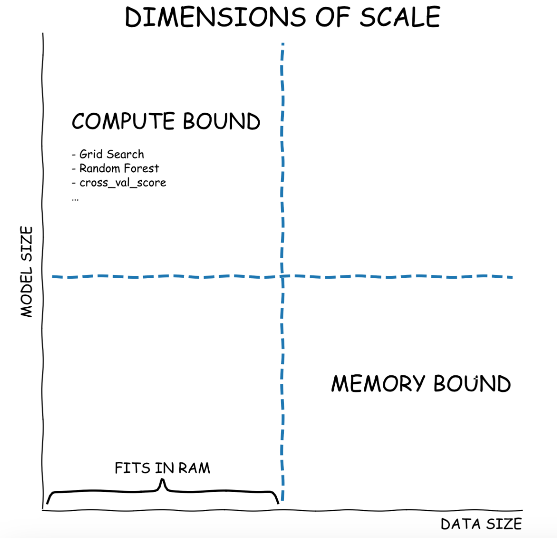
```
X_train, X_test, y_train, y_test=
    train_test_split(ddf_features_norm, ddf_target, shuffle=False)
```

# ML Pipelines




1. Automate the workflows.
2. Pipeline links all steps of data manipulation.
3. Shortens code.
4. Improves code quality.

# Scalability in ML



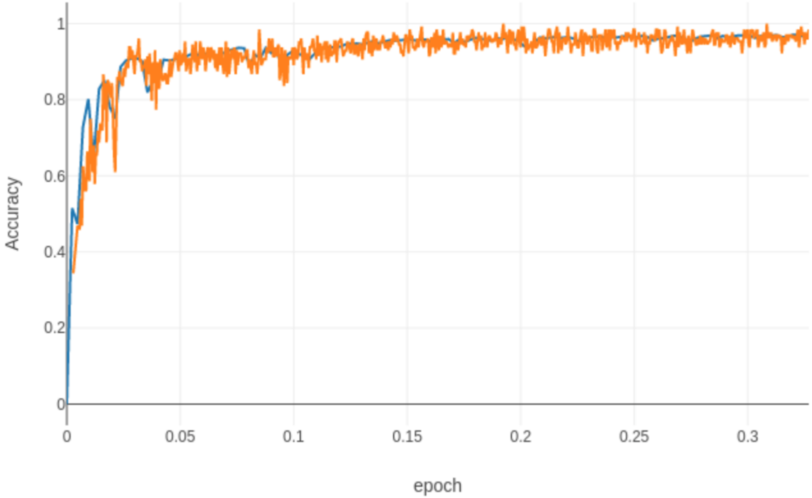
# Scaling Model Size

- Tasks like model training, prediction, or evaluation steps will (eventually) complete, but they just take too long.
- The model become compute bound.

# Data Size

- Datasets grow larger than RAM.

# When do you need scalability?



# Distributed Training

1. Scikit learn uses all the cores of your laptop or workstation.
2. Dask uses all the cores of your cluster without significantly changing your code.
3. This is most useful for training large models on medium-sized datasets.

# Hyper-parameters Search

1. Hyper-parameters are parameters that are not directly learnt within estimators.
2. Hyper-parameters are passed as arguments to the estimator.
3. **GridSearchCV** exhaustively generates candidates from a grid of parameter values.

# Hyper-parameters Search

```
pipeline = Pipeline([
        ('vect', HashingVectorizer()),
        ('tfidf', TfidfTransformer()),
        ('clf', SGDClassifier(max_iter=1000)),
        ])

parameters = {
    'tfidf__use_idf': (True, False),
    'tfidf__norm': ('l1', 'l2'),
    'clf__alpha': (0.00001, 0.000001),
}

grid_search = GridSearchCV(pipeline, parameters, n_jobs=-1,
verbose=1, cv=3, refit=False)
```

# Joblib

```
from math import sqrt
from joblib import Parallel, delayed
Parallel(n_jobs=2)(delayed(sqrt)(i ** 2) for i in range(10))
```

# Scaling Model Size

- Training, prediction, or evaluation steps take too long (compute bound).
- Dask can parallelize the workload on many machines.

# Predict Large Datasets

- Train on a smaller dataset that fits in memory, but predict for a much larger.
- We can use **ParallelPostFit** to parallelize and distribute the prediction steps.

# Scaling Data Size

NCI AUSTRALIA

- Most ML library estimators are designed to work on a single node.
- So the data must fit in the RAM on a single machine.
- Datasets grow larger than RAM and loading the data into NumPy or pandas becomes impossible.
- Use Dask's high-level collections combined with one of Dask-ML's estimators that are designed to work with Dask collections.
- Estimators implemented in Dask-ML work well with Dask Arrays and DataFrames.
- These can be distributed in memory on a cluster of machines.

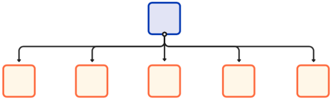
# Incremental Training

- We can train models on large datasets one batch at a time.
- Scikit-Learn handles all of the computation while Dask handles the data management.

# Dask Cluster & Resource Manager

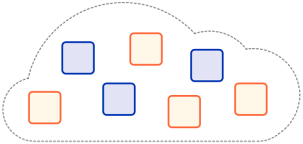
## Cluster Manager

Deploys one Scheduler and many Workers
by talking to the Resource Manager



## Resource Manager

Kubernetes/Yarn/SLURM/PBS/Abstract
pods/jobs on top of Physical Hardware



## Physical Hardware

Physical CPUs, GPUs, networking and
storage; either on-prem or on the cloud

# Dask Cluster & Resource Manager

1. Cluster manager communicate with the resource manager to determine where the workers are running.
2. In Gadi we use PBS as the resource manager.
3. Other popular resource managers are Slurm and SGE.
4. Dask also works with Kubernetes.

# Dask Jobqueue

1. Interfaces HPC resource manager with Dask Cluster manager.
2. Dask workers are automatically allocated physical hardware resources.

# Dask Jobqueue

```
os.environ['DASK_PYTHON'] =
    '/scratch/vp91/AAPP2023/dask-python3.9-venv/bin/python'
setup_commands =
    ["module load python3/3.9.2",
    "source /scratch/vp91/AAPP2023/dask-python3.9-venv/bin/activate"]
extra = ['-q normal',
 '-P vp91',
 '-l ncpus=48',
 '-l mem=192GB']
```

# Dask Jobqueue

```
cluster = PBSCluster(walltime="00:50:00",
             cores=48,
             memory="192GB",
             #processes=48,
             shebang='#!/usr/bin/env bash',
             job_extra=extra,
             local_directory='$TMPDIR',
             header_skip=["select"],
             interface="ib0",
             env_extra=setup_commands,
             python=os.environ["DASK_PYTHON"])
```

# Dask Jobqueue

```
#!/usr/bin/env bash

#PBS -N dask-worker
#PBS -l walltime=00:50:00
#PBS -q normal
#PBS -P vp91
#PBS -l ncpus=48
#PBS -l mem=192GB
module load python3/3.9.2
source /scratch/vp91/AAPP2023/dask-python3.9-venv/bin/activate
/scratch/vp91/Training/python3.9-venv/bin/python -m distributed.cli.dask_worker
tcp://10.6.41.71:36145 --nthreads 6 --nprocs 8 --memory-limit 22.35GiB
--name dummy-name --nanny --death-timeout 60 --local-directory $TMPDIR
--interface ib0 --protocol tcp://
```

**Thank You!**