PHYS4038/MLiS and AS1/MPAGS

Scientific Programming in python™

mpags-python.github.io

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An introduction to scientific programming with

python™

Session 6:
Data handling

Databases

- Python has tools for accessing most (all?) databases
    - e.g. MySQL, SQLite, MongoDB, Postgres, …

- Allow one to work with huge datasets
- Data can be at remote locations
- Robust and fast

- May require knowledge of DB-specific language
- But often provide Pythonic interface

Databases

- SQLite
  - Lightweight
  - No server
  - Just uses files (convenient, but less powerful)
  - Standard python module: `sqlite3`

Databases

- MariaDB (MySQL)
  - Widely used
  - Need MySQL server installed
  - Official: `mariadb`
  - `SQLAlchemy, mysqlclient, pymysql, MySQLdb`

Databases

- MongoDB
  - NoSQL database
  - Documents rather than tables
  - Need Mongo database server
  - Official: `pymongo`

Databases

- Python has tools for accessing most (all?) databases
  - e.g. MySQL, SQLite, MongoDB, Postgres, …

- Allow one to work with huge datasets
- Data can be at remote locations
- Fast random read and write
- Atomic transactions
- Concurrent connections

Databases

- **DB pros and cons**

- Allow one to work with huge datasets
- Data can be at remote locations
- Fast random read and write
- Concurrent, atomic transactions

- However, most databases are designed for webserver use
  - typically not optimised for data analysis
  - write once, multiple sequential reads

pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$

- Python Data Analysis Library
  - http://pandas.pydata.org
- Easy-to-use data structures
  - DataFrame (more friendly recarray)
  - Handles missing data (more friendly masked array)
  - read and write various data formats
  - data-alignment
    - tries to be helpful, though not always intuitive
  - Easy to combine data tables
  - Surprisingly fast!

Notebook demo…

Dask

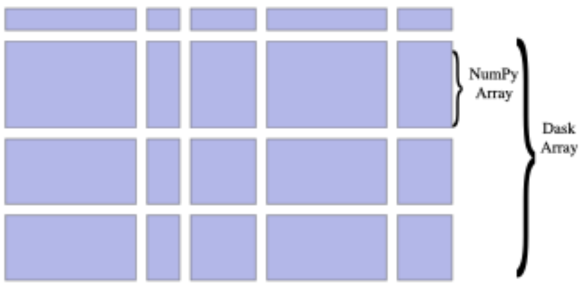
Dask natively scales Python

```python
# 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)
```

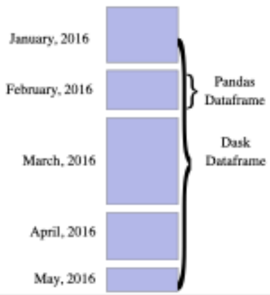
```python
# Dataframes implement the Pandas API
import dask.dataframe as dd
df = dd.read_csv('s3://.../2018-*-*.csv')
df.groupby(df.account_id).balance.sum()
```

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

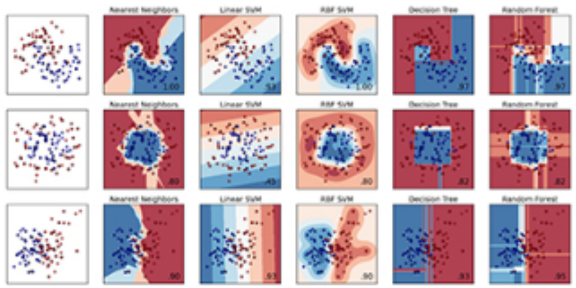
Numpy



Pandas



Scikit-Learn



PySpark

- typically for dealing with very large datasets
- distributed computing on a cluster
- need to setup infrastructure

PyTables / h5py

- http://pytables.github.io
- For creating, storing and analysing datasets
  - from simple, small tables to complex, huge datasets
  - standard HDF5 file format
  - incredibly fast – even faster with indexing
  - uses on the fly block compression
  - designed for modern systems
    - fast multi-code CPU; large, slow memory

  - "in-kernel" – data and algorithm are sent to CPU in optimal way
  - "out-of-core" – avoids loading whole dataset into memory

PyTables / h5py

- Can store many things in one HDF5 file (like FITS)
- Tree structure
- Everything in a group (starting with root group, '/')
- Data stored in leaves
- Arrays (e.g. n-dimensional images)

```
>>> from tables import *

>>> h5file = openFile("test.h5", mode = "w")
>>> x = h5file.createArray("/", "x", arange(1000))
>>> y = h5file.createArray("/", "y", sqrt(arange(1000)))
>>> h5file.close()
```

PyTables

- Tables (columns with different formats) – *better to use Pandas!*
  - described by a class
  - accessed by a row iterator

```
>>> class MyTable(IsDescription):
        z = Float32Col()
>>> table = h5file.createTable("/", "mytable", MyTable)
>>> row = table.row
>>> for i in xrange(1000):
        row["z"] = i**(3.0/2.0)
        row.append()
>>> table.flush()
>>> z = table.cols.z
```

PyTables Expr

- **Expr** enables in-kernel & out-of-core operations

```
>>> r = h5file.createArray("/", "r", np.zeros(1000))
>>> xyz = Expr("x*y*z")
>>> xyz.setOutput(r)
>>> xyz.eval()
/r (Array(1000,)) ''
  atom := Float64Atom(shape=(), dflt=0.0)
  maindim := 0
  flavor := 'numpy'
  byteorder := 'little'
  chunkshape := None
>>> r.read(0, 10)
array([   0.        ,    1.        ,    7.99999986,   26.9999989 ,
         64.        ,  124.99999917,  216.00000085,  343.00001259,
        511.99999124,  729.        ])
```

PyTables Expr

- **where** enables in-kernel selections

```
>>> r_bigish = [ row['z'] for row in
                 table.where('(z > 1000) & (z <= 2000)' ]

>>> for big in table.where('z > 10000;'):
...       print('A big z is {}'.format(big['z'])
```

- There is also a **where** in **Expr**

Multiprocessing

- Python includes modules for writing "parallel" programs:
  - threaded – limited by the Global Interpreter Lock
  - multiprocessing – generally more useful

```
from multiprocessing import Pool

def f(x):
   return x*x

pool = Pool(processes=4)      # start 4 worker processes

z = range(10)
print pool.map(f, z)   # apply f to each element of z in parallel
```

Multiprocessing

```
from multiprocessing import Process
from time import sleep

def f(name):
    print('Hello {}, I am going to sleep now'.format(name))
    sleep(3)
    print('OK, finished sleeping')

if __name__ == '__main__':
    p = Process(target=f, args=(lock, 'Steven'))
    p.start()           # start additional process
    sleep(1)            # carry on doing stuff
    print 'Wow, how lazy is that function!'
    p.join()            # wait for process to complete
```

(Really, should use a lock
to avoid writing output
to screen at same time)

```
$  python thinking.py
Hello Steven, I am going to sleep now
Wow, how lazy is that function!
OK, finished sleeping
```

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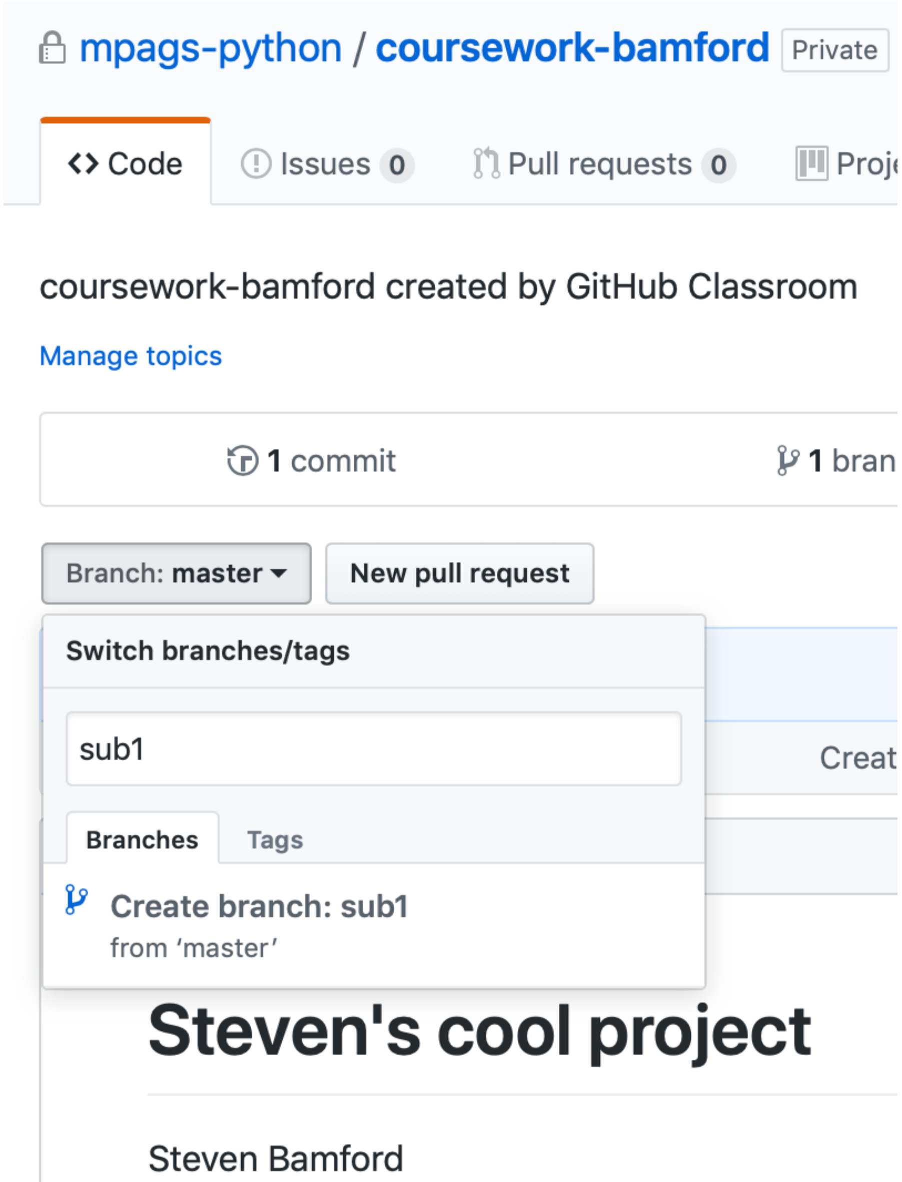
Coursework submission

- Ongoing work
  - preliminary version
  - Incomplete / with bugs
  - roughly working
  - understandable
  - problems to be solved
  - questions

- Submission and feedback via your GitHub repository
- Mandatory for MLiS, optional for MPAGS

- Create a branch called `sub2`



Questions and exercises

Any questions?

- ask on the Slack channel (@Steven Bamford)
- email steven.bamford@nottingham.ac.uk
- ask in the next synchronous session