Python for High Performance Data Analytics

—— (2) Data Arrays ——

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Questions from last talk

- Q: Do you recommend a class or course for a beginner?
  - Python for Beginners - Learn Python in 1 Hour (Youtube)
  - Software Carpentries workshops in the UC System (Programming in Python)
- Q: Share a link or site of basic python information for visual designers?
  - GUI: PyQt, Kivy Designer, PyGTK
  - Visualization: Software Carpentries Worshops at UCLA
  - Animations: PyGame, Blender, …
- Q: Would love a basic link / reference for python for statistics
  - Python build-in module: statistics
  - Third-party libraries: Numpy, Scipy, Statsmodels, Scikit-learn
- Q: Would it be possible to get this slide deck
  - Github Repo:

COMPUTATION

Single Node/GPU, SIMD

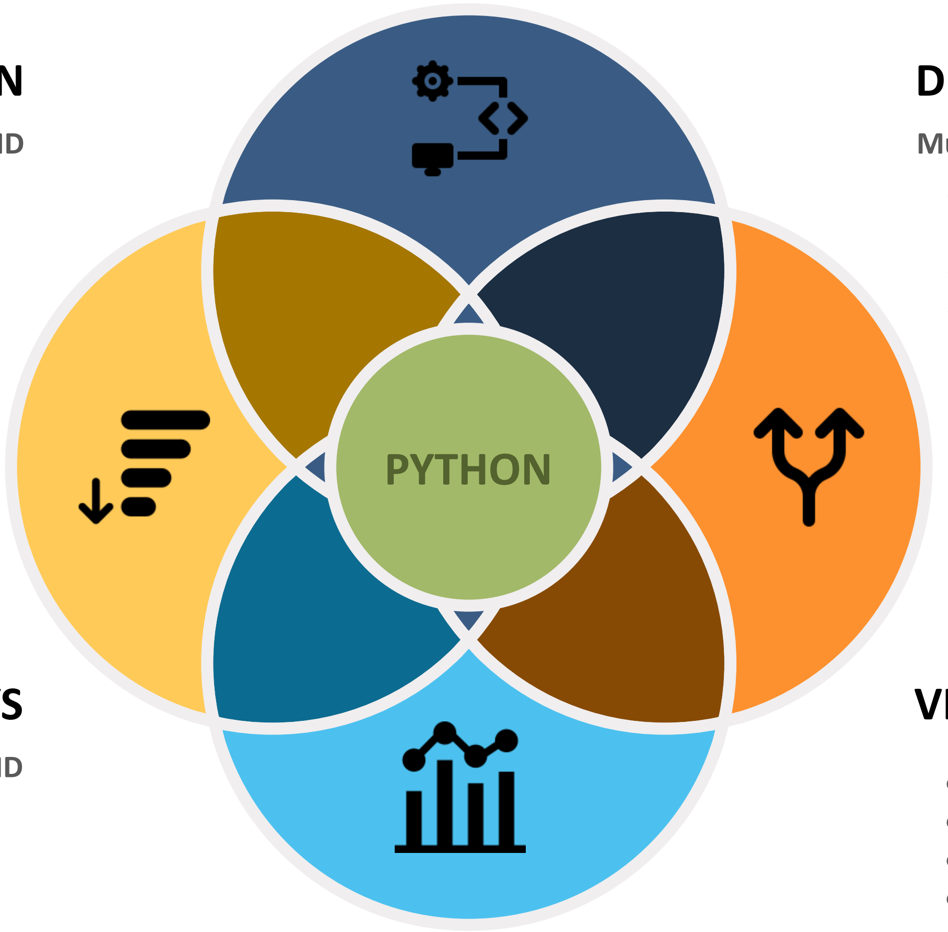
- Pypy, Numba, NumExpr
- Pythran, Cython
- F2py, ctypes

Mojo

DISTRIBUTED

Multiple Nodes/Machines

- MapReduce-based: **PySpark**, PyFlink
- MPI-based: mpi4py, Horovod
- Joblib, Dask, Ray



DATA ARRAYS

Single Node/GPU, SIMD

- Numpy
- Pandas, Polars
- Modin, Pandarallel, Swifter
- Dask DataFrame, Vaex

VISUALIZATION

- Viz process for big data
- Matplotlib, Bokeh, Plotly
- Holoview and Datashader
- Traited VTK, Mayavi, Paraview

Key Issues in Array-Type Data

Data Types

- Fixed-vs.variable-width: numericals, strings
- Nullable/masked: can/cannot be None
- Heterogeneous: different types in array
- Nested records with named (dict) or unnamed (tuple) fields

Data Storage

- Memory & Disk format
- Row-based vs Columnar format
- Sparseness: dense vs sparse
- Chunking and partitioning: for parallel processing

Data Structures

- Structured: **numpy**, pandas, ...
- Unstructured:
  - nD-Panel data structure: xarray, TensorStore
  - Tree structures: datrie, treelib, awkward arrays, ...
  - Graph structures: networkx, stellar graph, …

Data Processing

- Virtualness: lazy load/evaluation
- Subclassing arrays with high level specialized methods

Backends

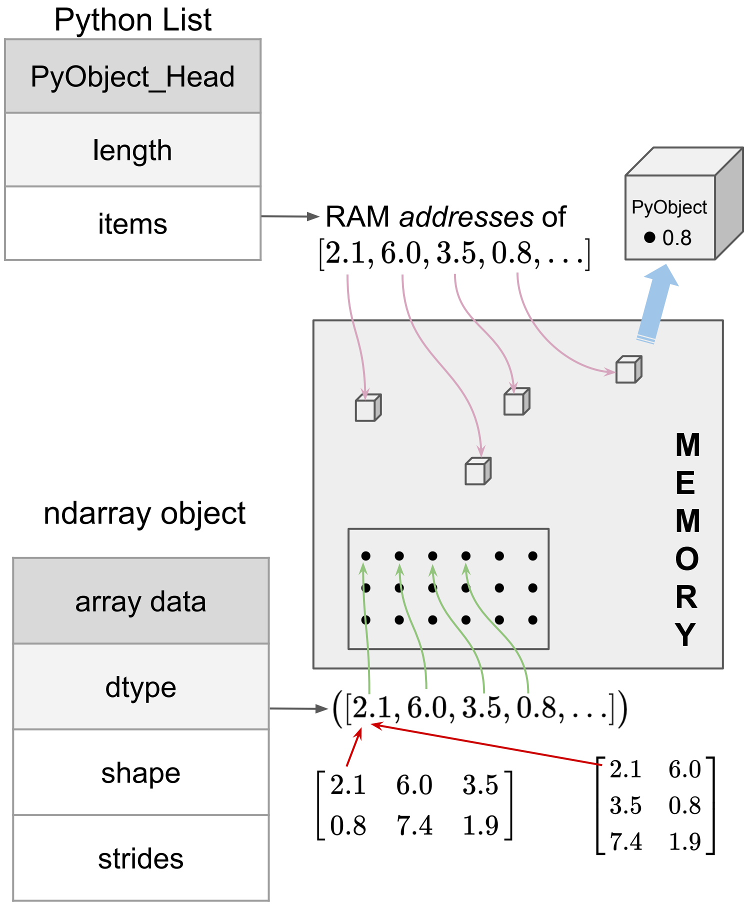
- Engines for storage, processing
- Two choices:
  - Numpy
  - Arrow

Outline for today

- Key issues in array-type data
- Using single thread, single cpu
  - Numpy and Pandas 1.x
- Using multithread, multiple cpus
  - Pandarallel, Modin, Swifter
- When data is too large to fit the memory
  - Polars, Pandas 2.0, Dask, Vaex
- Colab demos

NumPy

- First choice for numerical arrays
  - ndarray
  - Functions/tools for fast math and data ops
  - C APIs for C/C++, Fortran libs
- Internals of numpy vs. Python list
  - Python list: scattered across the system mem
  - Numpy data: stored in a continuous block mem
- Performance tips
  - Use *view*, avoid *copy*
    - watch out for implicit-copy!
  - Take advantage of vectorization
    - Try binary ufunc methods
    - Use broadcasting if possible
    - Explicitly define a vectorized function



pandas DataFrame v1.x

bit.ly/hpdspy_02

- NumPy and Pandas
  - Pandas built on top of numpy
  - Numpy: for homogeneously-typed numerical array data
    Pandas: for tabular or heterogeneous data
  - Pandas provides more domain-specific functions
- Under the hood
  - Column grouping
  - Numeric values as NumPy ndarrays
  - Object type values as Python string objects
- Optimize the numeric data
  - int64 and float64 are default and expensive
  - Subtypes can save RAM and a bit faster
- Optimize the object data
  - Strings are expensive and slow
  - Categoricals: 10x to save RAM & speedup

DataFrame

	date	number_of_game	day_of_week	v_name	v_league	v_game_number	h_name	h_league	length_outs
0	01871054	0	Thu	CL1	na	1	FW1	na	54.0
1	18710505	0	Fri	BS1	na	1	WS3	na	54.0
2	18710506	0	Sat	CL1	na	2	RC1	na	54.0

IntBlock

	0	1	2	3	4	5
0	01871054	0	1	1	0	2
1	18710505	0	1	1	20	18
2	18710506	0	2	1	12	4

ObjectBlock

	0	1	2	3	4
0	Thu	CL1	na	FW1	na
1	Fri	BS1	na	WS3	na
2	Sat	CL1	na	RC1	na

FloatBlock

	0
0	54.0
1	54.0
2	54.0

Try “dtype_diet” package to get help.

Optimize your pandas dataframe with its advice.

+

Drop to Numpy whenever you can.

Take advantage of vectorization in loops.

Pandaral·lel

- Numpy and Pandas: using single core
  - Workaround is possible, but very complicated
- Pandarallel: using multiple cores
  - Instantiates a Pyarrow Plasma shared memory
  - Creates one sub processes for each CPU to work on a sub part of the DataFrame
  - Combine all the results in the parent process

- A drop-in replacement:

```
from pandarallel import pandarallel
pandarallel.initialize()
df/series.apply -> df/series.parallel_apply
df/series.map -> df/series.parallel_map
df/series.applymap -> df/series.parallel_applymap
```

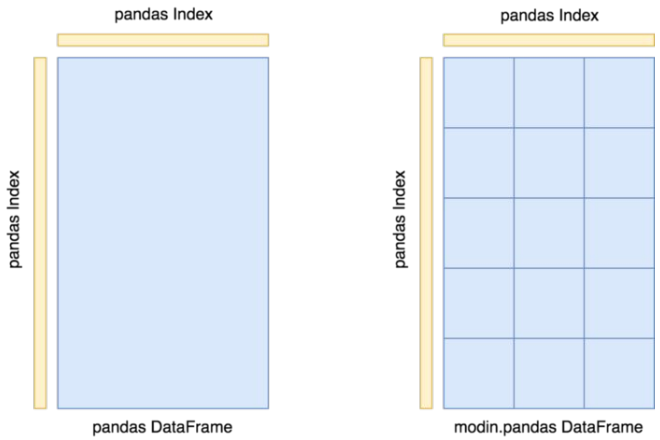
Watch out for the overhead!

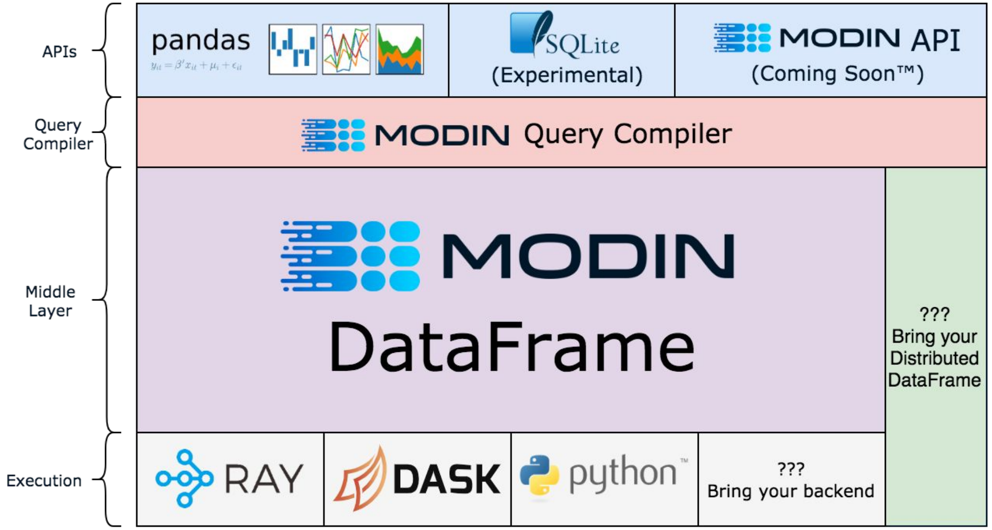
MODIN

- Multiprocess dataframe
  - Project from UCB's RISELab
  - Have identical APIs to Pandas
- Internals of Modin
  - 2-dimensional partitioning
  - Re-implementing Pandas APIs
  - 4-layer architectures
- Installation & Usage

```
pip install modin[dask/ray/all]
import os
os.environ["MODIN_ENGINE"]="dask"
```

```
import pandas as pd
```



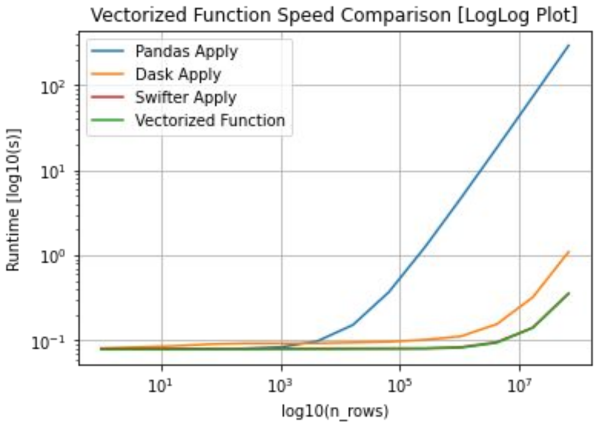


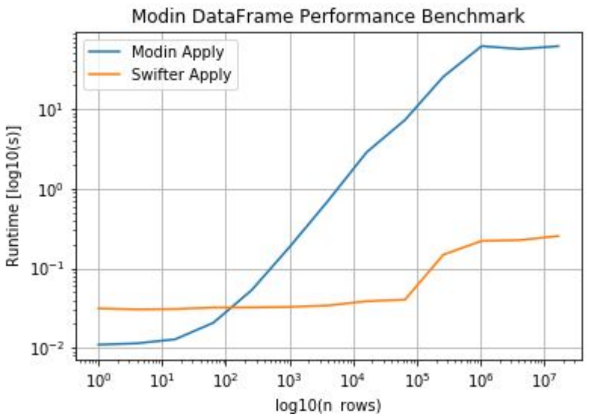
Swifter

- A booster to Pandas and/or Modins
  - A project developed by Jason Carpenter
- Basic idea:
  - Try vectorization first
  - If not succeeded, automatically decides whether it is faster to perform dask parallel processing or use a simple pandas apply.
- Installation and usage

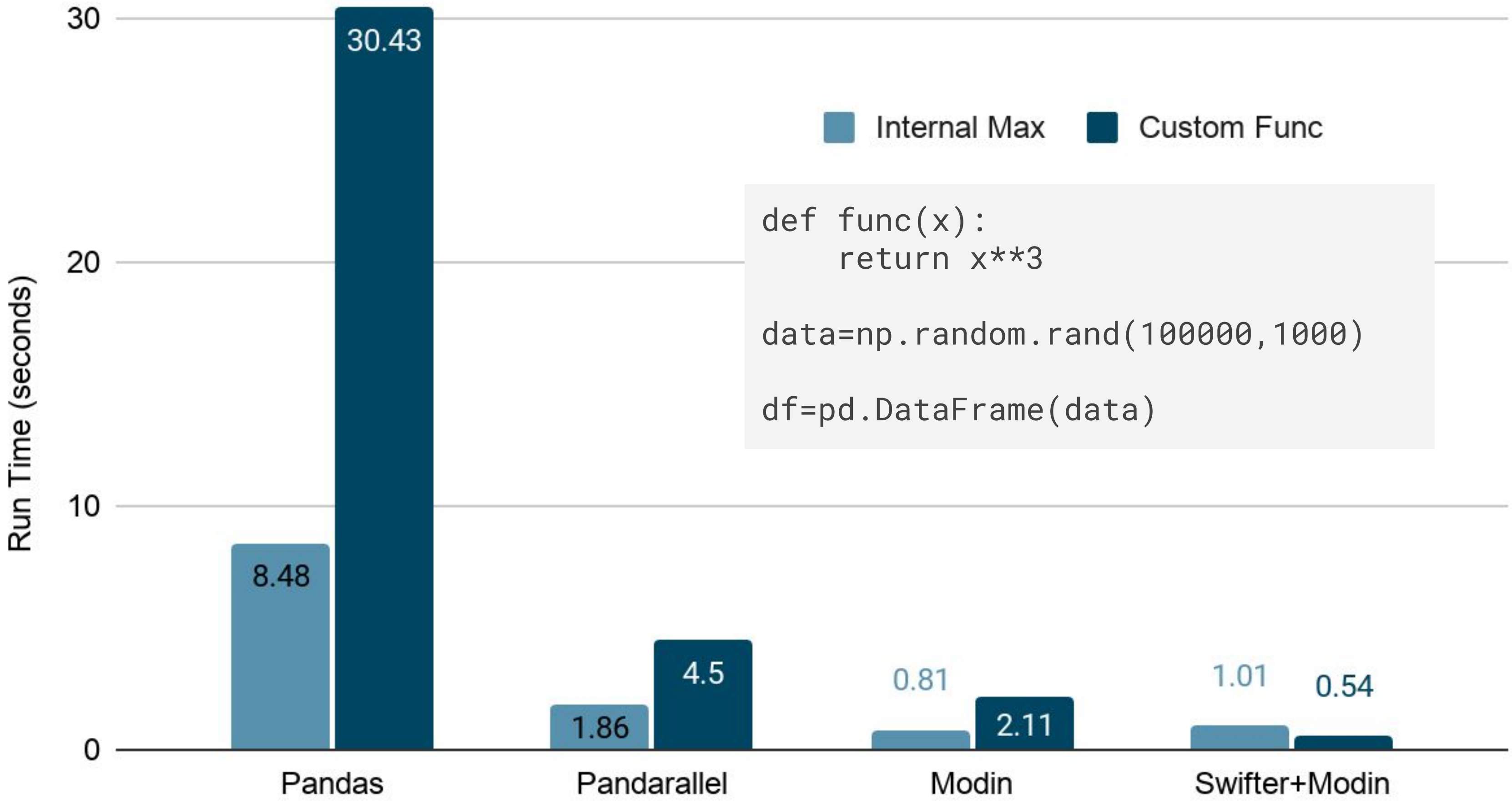
```
pip install swifter
import modin.pandas as pd
import swifter

df=pd.DataFrame(data)
df.swifter.apply(func, axis=1)
```



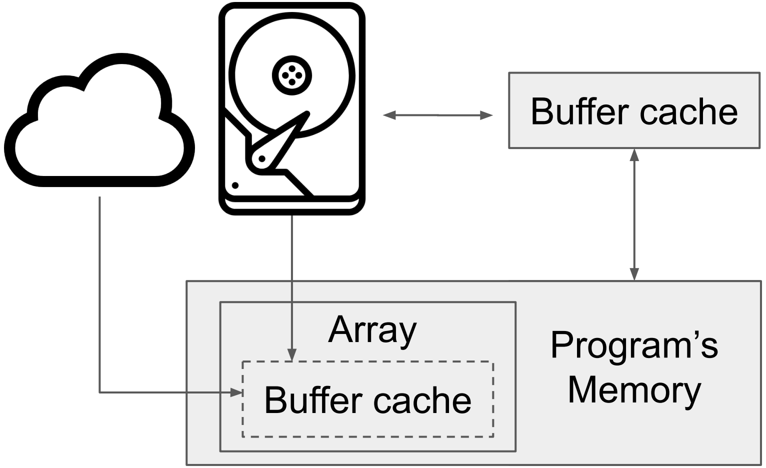


Dataframe's apply method speed test on Hoffman2



When Data > RAM

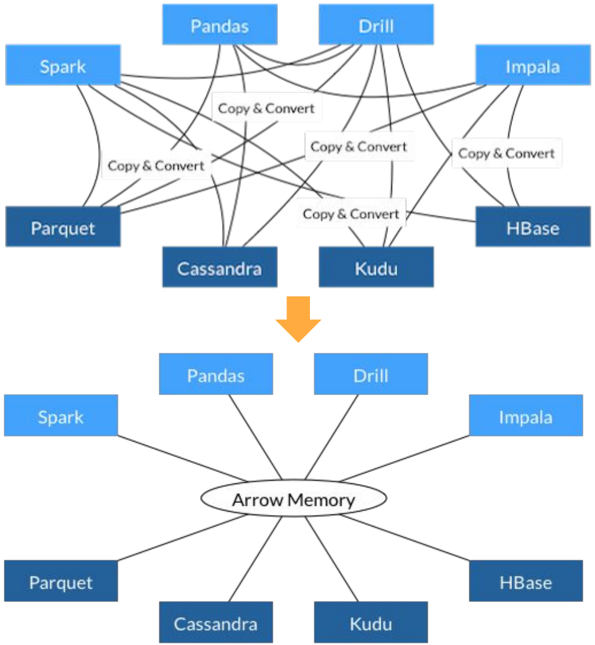
- Numpy Arrays
  - Using smaller subtypes
  - Compressing sparse arrays
  - Chunking the data for *on-demand* reads
    - Using `np.mmap()`
    - Using `Zarr` and/or `HDF5` format



- Pandas Dataframes (v1.x)
  - Using Categorical dtypes and smaller subtypes
  - Loading columns selectively: `pd.read_csv(file, usecols=[...])`
  - Sampling rows: `pd.read_csv(file, skiprows=samplingFunc)`
  - Reading in chunks: `for df in pd.read_csv(file, chunksize=1000):`
  - Using SQLite as data storage for Pandas: 50x faster lookups

Arrow comes to the rescue!

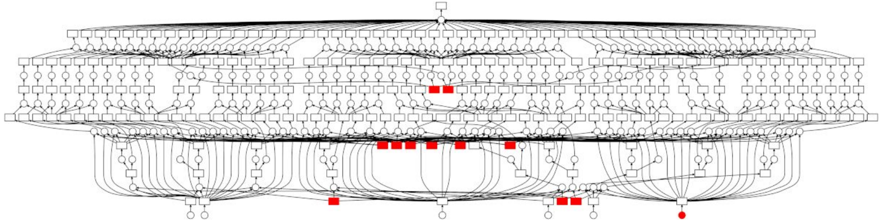
- Apache Arrow: a competitor to Numpy
  - An open standard for processing and transporting large data
  - Using in-memory columnar format
  - Zero-copy data access
- Polars: a superfast dataframe library
  - Written in Rust, internally using Arrow2 object
  - Support multi-threaded and SIMD
  - Lazy evaluation with query optimization and streaming data
- pandas v2.x: published in March 2023
  - Add arrow as backend, perfect for data ETL
  - Internally using PyArrow object, slower than Polars, but with lighter cpu load
  - Numpy backend also got improved



DASK Data Collections

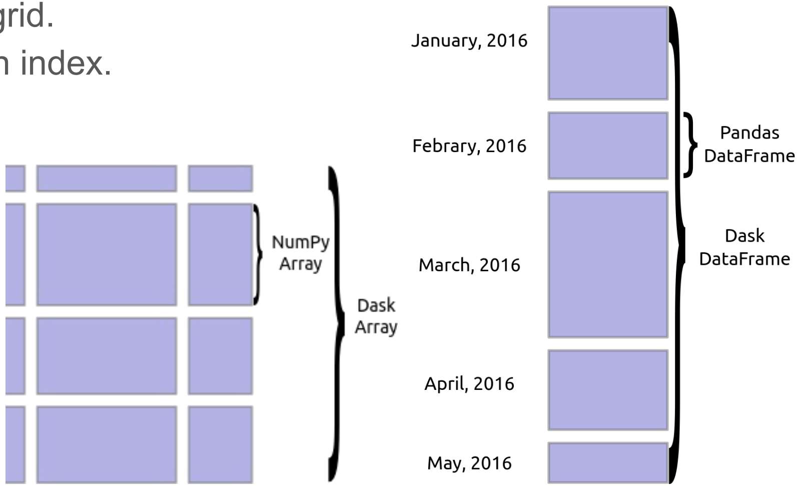
bit.ly/hpdspy_03

- A full parallel processing library *suite*
  - Parallel with ndarray and pd.DataFrame
  - Distributed computing w/ task schedulers
  - Real-time feedback and diagnostics



- Three parallel data collections:
  - Dask Arrays: arranging ndarrays into chunks within a grid.
  - Dask DataFrames: partitioning pd.DataFrame along an index.
  - Dask Bags: for unstructured or semi-structured data
- Dasks APIs to emulate Pandas:
  - Setting up a static graph of operations first
  - Running the computation on that graph

```
import dask.dataframe as dd
df = dd.read_csv(file)
df.groupby(df.user_id).value.mean().compute()
```



vaex

bit.ly/hpdspy_04

- A promising open-source DataFrame library in Python
  - APIs closely resemble that of Pandas.
  - Easy to work with very large (>100G+) datasets efficiently, 1000x faster than Pandas!
- Interesting features
  - Memory mapping
    - New string type (RAM efficient)
    - Support file formats of Apache Arrow, Apache Parquet, HDF5
    - Access from local disks and cloud storage
  - Dataframes are out-of-core
    - Lazy evaluations: compute only when needed (e.g. preview)
    - Lazy loading: data streaming only when needed to avoid memory copy
  - Parallelized and fast/efficient algorithms:
    - groupby, join, selection
    - JIT compilation: Numba, Pythran, CUDA
  - vaex.ml Package for *out-of-core* scikit-learn

When to use which?

		Multiple CPUs	Out-Of-Core	Pandas APIs	Keep-In-Mind Notes
1	Pandas 2.0	✗	✗	✓	• Always be the one if we can. • Lots of performance tricks!
2	Modin	✓	✗	✓	• Good for dataframes with many columns • Out-of-core is linked with parallel engines • Experimental distributed XG-Boost
3	Dask	✓	✓	✓	• Ultimate solution if distributed situations: ○ Data storage & computation. • Steep learning curve after a quick start
4	Vaex	✓	✓	✗	• Good for dataframes with many rows • HDF5 files work best so far. • Some APIs are different from Pandas

01

Use Pandas if possible

- Drop to numpy if you can.
- Try “dtype_diet” to save RAM for you.
- Use functions from well-established numpy-based libraries

02

When to consider Modin

- Your machine have many CPUs and a lot of RAM
- Your work depends on most Pandas operations.
- Your data needs “groupby” on many columns.

03

When to consider Dask

- Some machine learning tasks can get great performance boost in Dask.
- Your dataset has to be distributed stored and operated over a cluster.

04

When to consider Vaex

- Your data has about 10M to 1B rows, <100 columns (according to Ian Ozsvald)
- Your data is in HDF5 format on a single place (local or cloud).
- You only need a small set of Pandas functions.

What we didn’t talk about yet:

Spark DataFrame

Ray DataFrame

“Boosting Python for High Performance Data Analytics (3)”

RAPIDS cuDF

“Learning Scikit-Learn”

PyTorch Tensor

“Learning PyTorch”

OpenAI’s Triton Tensor

“Learning Convolutional Neural Networks” (?)