Is your Python too slow?

Hardware and software for accelerating data science

Data Science Salon Virtual
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Hi!

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> *I work to make data scientists faster and happier*

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Bringing together the fastest hardware + OSS

DASK

- Pythonic parallelism
- Rapidly scale PyData

RAPIDS

- Multi-GPU computing
- The future of HPC

PREFECT

- Workflow orchestration
- Flow insight and mgmt

kubernetes

- Fast setup
- Enterprise secure

Data science with Python

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Data science with Python

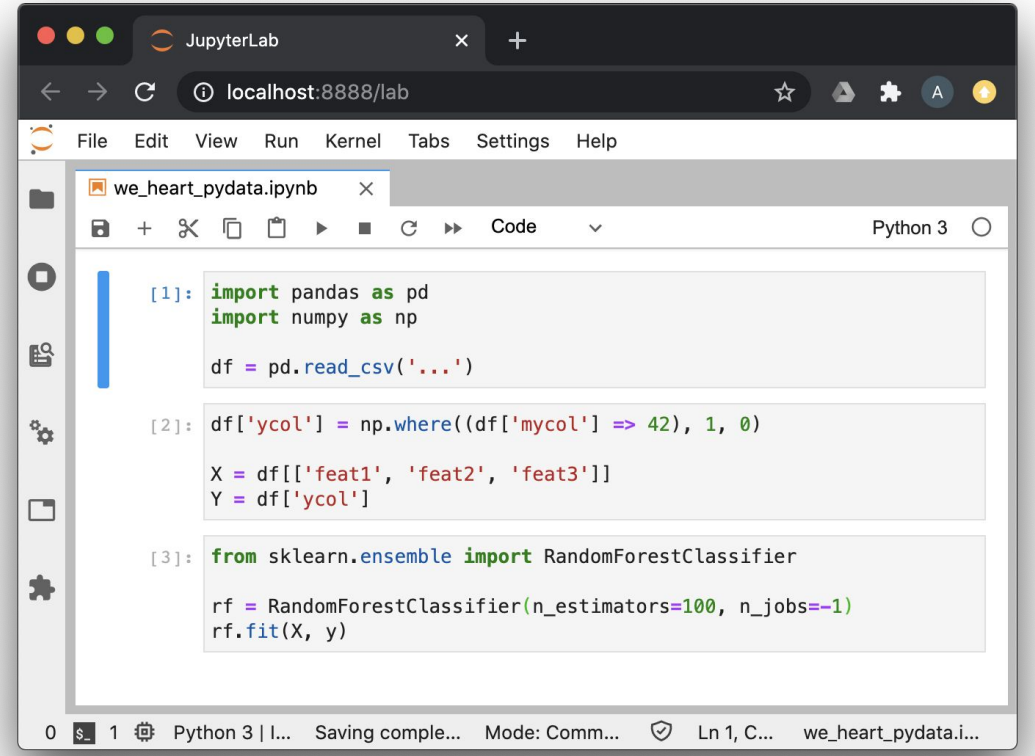
PyData

pandas

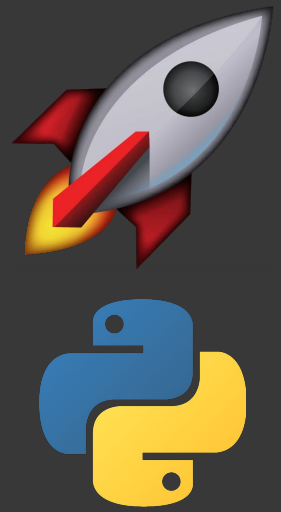
scikit learn

NumPy

jupyter



Accelerating data science in Python



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Hardware

Bigger data and compute requires more resources

Laptop / workstation
<64GB RAM
<12 cores
<1 GPU

Up-front cost
Expensive to upgrade

Cloud machine
1+ TB RAM
100+ cores
8+ GPUs

Pay per second
Switch machines easily

Cloud cluster
1000s of machines

Cloud machine, but lots of them!

Software

Considerations for adopting OSS data science tools

- Origin / maturity
- Community / usage
- Contributing
- “Native” support
- Ecosystem / compatibility
- Deployment / installation

Software

Data science workloads

- Arrays (multi-dim)
- DataFrames
- Machine learning
  - Classification & regression
  - Hyperparameter tuning
- Deep learning
- Arbitrary (custom) code

Software

PyData world

Software

Big data world

PyData world

Software

Big data world

PyData world

Python + big data!

Spark

- *Distributed computing based on MapReduce*
- U.C. Berkeley AMPLab ~2010
- Built in Scala; APIs for Java, SQL, R, Python
- Mature, big data / data eng communities
- Native DataFrames, streaming, ML, graph
- Integrates with Hadoop ecosystem
  - Python/Pandas limited with UDFs
- Cluster deployment is complex

http://spark.apache.org/

Dask

- *Distributed computing based on dynamic task scheduling*
- Anaconda, ~2015
- Built in Python; Python API
- Mature, scientific computing communities
- Low-level task library
- High-level libraries for DataFrames, arrays, ML
- Integrates with PyData ecosystem
- Runs on laptop, scales to clusters

https://dask.org/

Ray

- *Distributed computing: task/actor based*
- U.C. Berkeley RISELab, ~2016
- Built in Python/C++; APIs for Python, Java
- Low-level task library similar to Dask
- High-level libraries focused on reinforcement learning, hyperparameter tuning
- Runs on laptop, scales to clusters
  - Windows support in alpha

https://github.com/ray-project/ray

RAPIDS

- *GPU accelerated data science*
- NVIDIA, ~2018
- Built in C++(CUDA), Python; Python API
- Large dev team, support from NVIDIA
- Native DataFrames, arrays, ML, graph, streaming, spatial
- Integrates with PyData ecosystem
- Scales to clusters with Dask integration

https://rapids.ai/

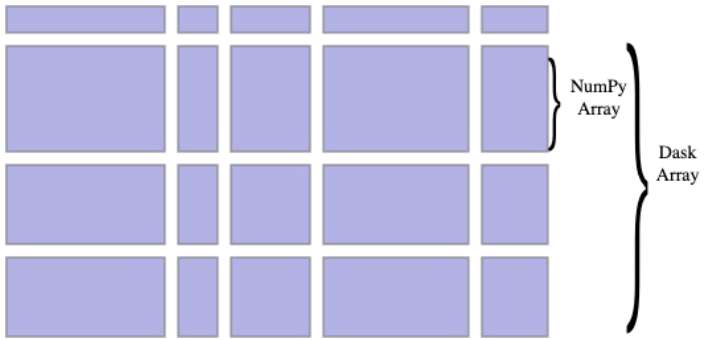
DataFrames

- PySpark DataFrame
- Dask DataFrame
- Koalas (Spark backend)
- Modin (Ray or Dask backend)
- Vaex
- RAPIDS (cuDF)

https://koalas.readthedocs.io/en/latest/
https://modin.readthedocs.io/en/latest/
https://vaex.readthedocs.io/en/latest/

Multi-dimensional arrays

- PySpark: not supported
- Dask: dask.array, xarray
- Ray: possible with task interface
- cuPy (GPU/CUDA)



Machine learning

- PySpark: ML (linear, tree, etc)
- Ray: distributed DL training, reinforcement learning, hyperparameter tuning
- Dask: extend scikit-learn, hyperparameter tuning, XGBoost
- RAPIDS (cuML): scikit-learn parity, XGBoost

Unofficial guide to accelerating Python

- Use “traditional” PyData tools on your laptop until you can’t

Unofficial guide to accelerating Python

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- **Then, use parallel computing / out of core tools *on your laptop***
  - Dask, Ray, Modin, Vaex
  - RAPIDS if you have a GPU

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- **Then, use a cluster in the cloud**
  - Dask, Spark, Ray

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- Then, use a cluster in the cloud
  - Dask, Spark, Ray
- ***Use the best tool for each workload!***

Resources

- Videos
  - Is Spark still relevant? Multi-node CPU and single-node GPU workloads
  - High-Performance Data Science at Scale with RAPIDS, Dask, and GPUs
  - Ray: A System for Scalable Python and ML
  - Scaling Interactive Pandas Workflows with Modin
  - Dask: A Pythonic Distributed Data Science Framework
- Articles
  - Ray comparison to Dask
  - Scaling Pandas: Comparing Dask, Ray, Modin, Vaex, and RAPIDS

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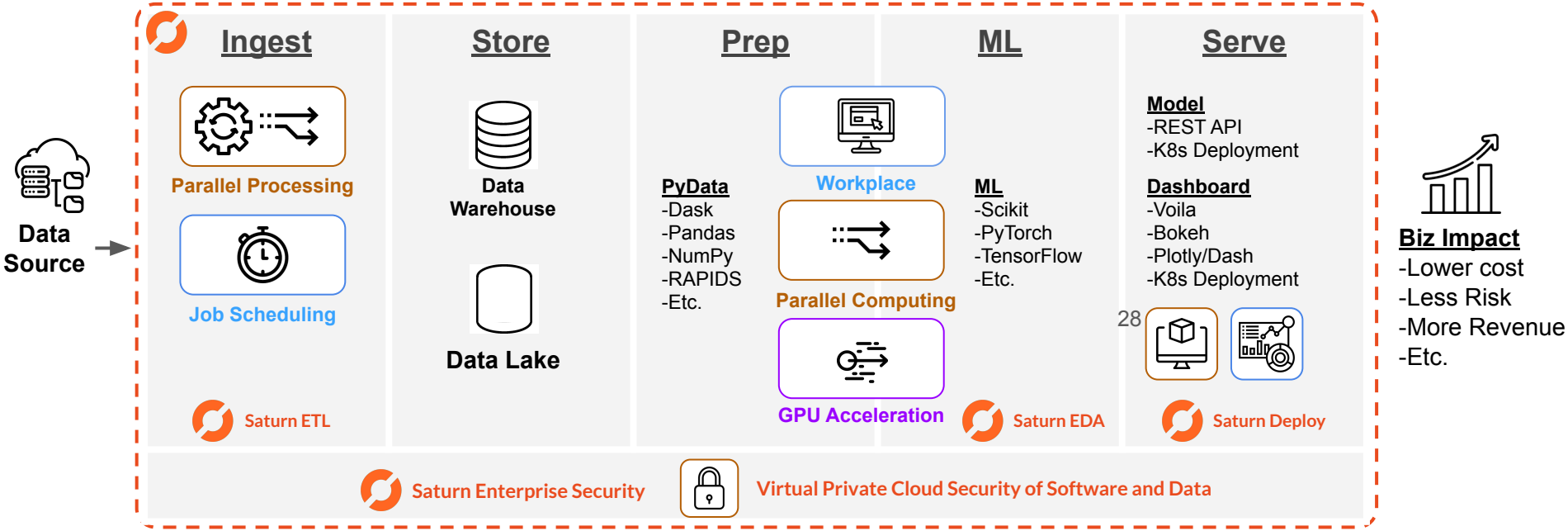
Saturn enables end-to-end DS and ML in Python



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[7 day free trial!]

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