Structural Bioinformatics Training Workshop & Hackathon 2018

mmtfPyspark Advanced

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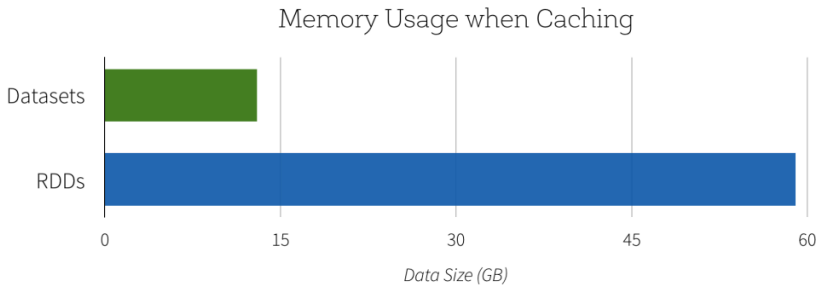
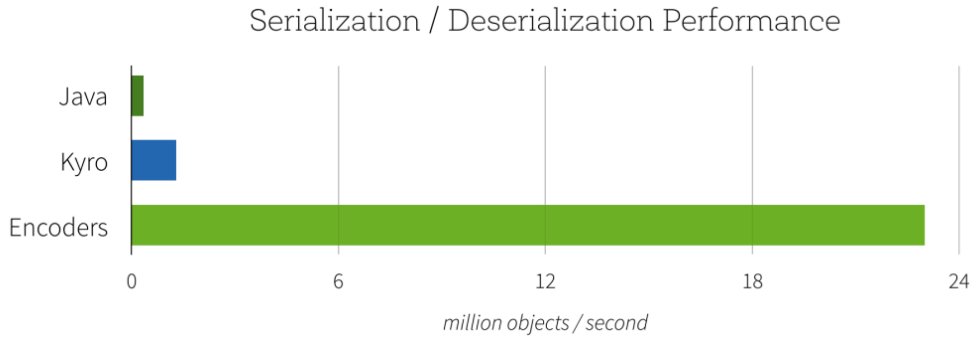
Introduction

- **Spark SQL and Dataset API**
  - Augmenting MMTF data with metadata from PDB and other 3rd party resources
  - Creating datasets of molecular interactions
  - Querying and analyzing datasets

Spark Dataset

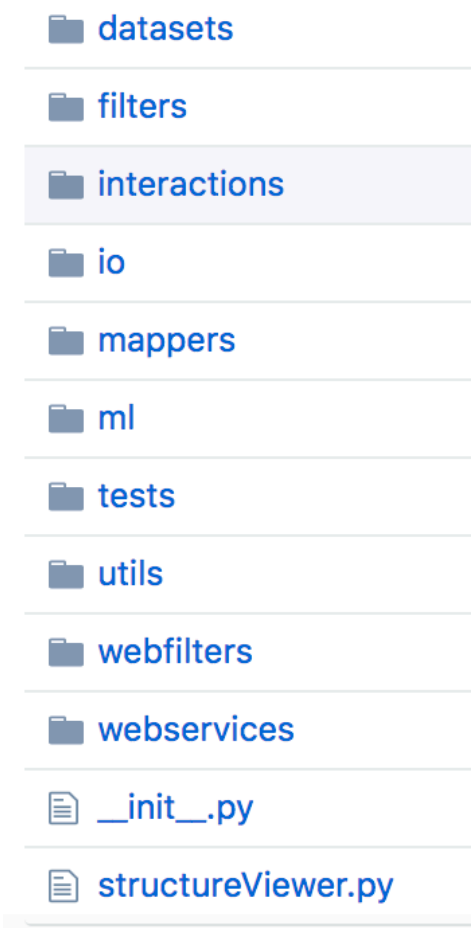
- Table of typed objects with a relational schema
- Similar to Python Pandas and R Dataframes
- Distributed data structure optimized for performance
- Distributed SQL queries on Dataset (Spark SQL)





Source: https://databricks.com/blog/2016/01/04/introducing-apache-spark-datasets.html

mmtfPyspark Modules Covered



- **datasets**
  - Datasets calculated from structure
  - Metadata retrieved from external resources
- **interactions**
  - Ligand-polymer interactions
  - Polymer-polymer interactions

Jupyter Notebook Tutorials

https://github.com/sbl-sdsc/mmtf-workshop-2018/tree/master/4-mmtf-pyspark-advanced

- 1-Metadata
- 2-JoiningDatasets
- 3-MutationsToStructure
- Problem-1 (Solution-1)
- 4-CreateDatasets
- Problem-2 (Solution-2)

Summary

- **Spark Dataset API provides an efficient distributed tabular data structure**
- **Can be queried using Spark SQL**
- **We used datasets to**
  - get additional metadata not available in MMTF
  - store and query the results of structural calculations

Resources

- **Spark SQL, DataFrames and Datasets Guide**
  - https://spark.apache.org/docs/latest/sql-programming-guide.html
- **MMTF Website**
  - https://mmtf.rcsb.org
- **GitHub Repository**
  - https://github.com/sbl-sdsc/mmtf-pyspark
  - https://github.com/sbl-sdsc/mmtf-spark

- **RCSB PDB Web Services and Query System**
  - Rose, PW, et al. (2013) The RCSB Protein Data Bank: new resources for research and education, Nucleic Acids Res 41: D475-D482. https://doi.org/10.1093/nar/gks1200
  - Rose, PW, et al. (2011) The RCSB Protein Data Bank: redesigned web site and web services, Nucleic Acids Res 39: D392-D401. https://doi.org/10.1093/nar/gkq1021

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