Analyzing billion-objects catalog interactively: Apache Spark for physicists

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July 10, 2018

ABSTRACT

Apache Spark is a big-data framework for working on large distributed datasets. Although widely used in the industry, it remains confidential in the scientific community or often restricted to software engineers. The goal of this paper is to introduce the framework to newcomers and show that the technology is mature enough to be used without excessive programming skills also by physicists as astronomers or cosmologists to perform analyses over large datasets as those originating from future galactic surveys.

To demonstrate it, we start from a realistic simulation corresponding to 10 years of LSST data-taking (6 billions of galaxies). Then we design, optimize and benchmark a set of Spark python algorithms in order to perform standard operations as adding photometric redshift errors, measuring the selection function or computing power spectra over tomographic bins. Most of the commands executes on the full 110 GB dataset within tens of seconds and can therefore be performed interactively in order to design full-scale cosmological analyses.

Key words. Large-scale structure of Universe- methods: numerical

1. Introduction

In 2002 Google released the mapReduce programming model (see e.g. Dean & Ghemawat 2008) that allows to scale rather simple requests over a large number of computers located in ever-growing data-centers. The open-source implementation of it, and of many other big-data related tools gave rise around 2006 to the Hadoop "ecosystem"\(^1\), its leading product being an efficient distributed filesystem known as HDFS (Shvachko et al. 2010).

In 2009 a research project started at UC. Berkeley (Zaharia et al. 2010, 2012) in order to relieve some of the limitations met by the original algorithms. During the next years, it captured many companies attention due to order of magnitude better performances over huge distributed data sets. It is today an notorious open-source project named Spark owned by the Apache foundation\(^2\) and used by more than 1000 companies.

Spark benefited and contributed to the revival of long-living concepts known as functional programming (FP) that takes roots back to Turing machines and blossom today due to mature computer technologies. FP is not to be opposed to procedural or object-oriented programming. It is a much more theoretical framework, where "functions" can be viewed as "theorems" and their "implementation" as "proofs" (Howard 1980). If you follow a number of rules, you will end up writing expressions that are much more concise and efficient than what you are probably used to do (without knowing it) known as imperative programming and that will be discussed later. In practice, functions are basic types (as Int or Float are) which are composed without ever changing their internal state (immutability). Some FP languages as Haskell or Lisp already existed since a long time, but a major renewal happened in 2004 with the release of the scala language which capitalized on the richness of the java ecosystem, but simplifies its syntax and mixes gracefully well established Object-Oriented concepts with FP programming. Its ambition is to present a language which allows to build in the same way a small or large application and is used today by several major companies (Twitter, Netflix,...).

Spark used and took full advantage of this language to develop its main core. Its API however also exposes efficient bindings to the python or R languages.

While big-data technologies were emerging, ground-based telescopes and their dedicated state-of-the-art cameras were accumulating more and more high-precision data. For cosmology, the BOSs survey\(^3\) spectroscopically imaged \(O(10^6)\) galaxies providing stringent constraints on today’s standard cosmological model (Alam et al. 2017). The next generation spectroscopic survey DESI\(^4\) is planning to survey \(O(10^7)\) ones and the DESI photometric survey\(^5\) already provides such a data volume. The next frontier will be crossed by LSST\(^6\) in the next decade where \(O(10^9)\) galaxies will be collected over 10 years. Keeping in mind that the clustering or weak-lensing analyses also require numerous mock-data simulations, we end up with volumes that are not impressive today for Spark-like technologies.

However current Spark applications in the industry are essentially dedicated to analyzing poorly structured data as computer CSV log-files or learning your preferences over the Internet. Scientific analyzes requires accessing much more structured data. This is why we developed first a low-level interface to FITS-structured data, named spark-fits\(^7\) that was presented in Peloton et al. (2018), hereafter SparkFTS18. It allows as a

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1. https://hadoop.apache.org/
2. http://spark.apache.org/
3. http://www.sdss3.org/index.php
4. http://desi.lbl.gov
5. https://www.darkenergysurvey.org
6. https://www.lsst.org
7. https://astrolabsoftware.github.io/spark-fits
next step, to study here more quantitatively the performances working on realistic data.

After presenting in a "physicist’s language" what Spark is and what’s its advantages are for data analysis in Sect. 2, we describe how to start using Spark in python in Sect. 3. Then we design and optimize several Spark commands in Sect. 4 with progressive complexity leading to a full tomographic analysis over a simulated set of 10-years of LSST galactic data (Sect. 4.3.7). Several options will be explored and performances discussed.

2. What is Spark and why to use it

While important efforts were put these last decades on optimizing algorithms, data increase now lead to bottlenecks related to data access. This does not only address the question of reading efficiently persistent data (i.e. IO) but also the question of moving data in memory within the registers that perform the computation. The challenge for High Performance Computing (HPC) experts today is to obtain a low arithmetic efficiency (number of data moves over number of operations) on evermore complex computing architectures. This requires a high degree of skills. Instead of moving the data to the algorithm Spark takes the problem the other way by sending the algorithm to the data. This has a number of advantages that are particularly well suited to physics analysis.

Coarse-grain parallelization The use of the mapReduce paradigm allows naturally a high level of parallelization without ever writing complicated code or directives. This is best illustrated by an example. Suppose you are seeking for the maximum value of a huge set of numbers. In Spark, the driver sends instructions (and the code) to each of its executors. This is the map process. Each worker treats its part of the data (here compute the maximum value) and then send it back to the driver that performs the final reduction (here find the maximum of all maxima). The only degree of freedom is the granularity of this decomposition, i.e. the number of partitions which is automatically set by Spark but can be modified.

Automatic pipeline optimization In imperative languages (C, C++, Fortran...) each instruction is performed immediately during execution. Functional Programming introduces lazy evaluation, meaning that in most cases (as for all Spark transformations) nothing is actually performed. Only final actions trigger the full pipeline execution. But before, the direct acyclic graph (DAG) of the pipeline is run through a very efficient optimizer. In practice the code will execute much faster than what a human could ever achieve.

Working in memory Perhaps the most interesting features to data analysts is the ability of caching the data for later reuse. Once the full dataset has been physically read from the filesystem, Spark can put it in cache (partially or totally depending on the cluster memory) within the Least Recently Used cache. Any further computation is then performed much more efficiently. This is for the user as having at disposal a machine with a huge Random Access Memory. Here for instance we will use 110 GB of data in memory but it was shown in SparkFITS18 that 1.2 TB can be available at the NERSC datacenter 8. The key point is that once the data is cached, the user can investigate the data interactively which is impossible with imperative languages where each instruction is run immediately.

Data scaling The success of Spark resides also in the fact that one can design analysis for a partial set of data on a personal laptop and port it to large datacenters without performance loss. The linear scaling for accessing FITS data was demonstrated in SparkFITS18.

3. Working with Spark

Spark basic abstraction is the Resilient Distributed Dataset (RDD) which represents a distributed collection of objects (‘resilient’ meaning that the system is fault-tolerant and guarantees to always returns the data). Many functions and tutorials are related to their usage.

Dataframes were then introduced within the SQL module (Armbrust et al. 2015). They add to the RDD the knowledge of its data structure which allows a higher level of optimization. Although one can retrieve an RDD from a dataframe, you should always try to use the latter in your analyses, especially if you work in python. Indeed the RDD performances are much worse in python than in the native scala language. This is not anymore the case when working with dataframes were similar performances are obtained in most cases as will be verified in Sect. 4.3.8:

Most of astronomers/cosmologists use today the python language for their analyses and we emphasize that pyspark can be run within ipython or a jupyter notebook. We then essentially discuss the python interface although some comparison with scala performances will be presented in 4.3.8. In our opinion, the scala language remains interesting to be looked at and we bring to the attention of the interested reader that:

- there exist some Spark kernels in scala to work in jupyter notebooks;
- the HEALPix package 10 can be build in java (and therefore used in scala) although not including all functionalities,
- the JEP package 11 allows to make calls to external python modules as numpy or matplotlib.

Concerning data formats, spark-fits allows the reading of FITS distributed binary tables and also in recent versions of images. Some connectors also exist to read the HDF5 format (references in SparkFITS18).

4. A full interactive analysis

We present a suite of rather standard operations a scientist can perform using the output of a 10 years LSST simulation presented in Sect. 4.1. Commands were run interactively in the pyspark shell on a cluster described in Sect. 4.2. They will be explicitly shown (as boxed) and their output follows next. We benchmark different options in some cases and focus more on performances in Sect. 4.3.8.

8https://www.nersc.gov
9e.g. http://toree.incubator.apache.org
10http://healpix.sourceforge.net
11https://pypi.org/project/jep
4.1. Simulation

In order to work with physics-oriented data, we built a galactic catalog using the CoLoRe fast simulation\(^\text{12}\) corresponding to 10 years of LSST data-taking. Point-like galaxies are generated in the \(z \in [0, 2.5]\) redshift range assuming a standard \(\Lambda\)CDM cosmology, with a selection function coming from the LSST/DESC 2pt validation working group\(^\text{13}\) and shown on Fig.1.

We generated a catalog of 6 billions of galaxies which contains their type, RA/DEC positions, cosmological redshift and redshift-space distortion (RSD) contribution. The CoLoRe simulation was run at NERSC and produced 32 FITS files of 112GB in total, that were imported to our HDFS cluster. By importing we mean simply recopied to the HDFS cluster. Then spark-fits gives transparent access to all Spark advantages.

4.2. Infrastructure

The cluster we used for this work, located at Université Paris-Sud in France\(^\text{14}\) is rather modest in order to illustrate the fact that you do not need huge resources to achieve spectacular results. It consists of nine 36 GB machines, each with 18 cores, running over HDFS. Since the total memory fraction dedicated to the cache is set to 0.6, the usable memory amount (\(\sim 170\) GB) is largely sufficient to hold our full dataset. We then used the following setup

- 1 driver (4 GB RAM)
- 8 executors (ie. workers) each using 17 cores and 30 GB of RAM.

The python interactive shell is then run with

```
pyspark --driver-memory 4g \
    --total-executor-cores 136 \
    --executor-cores 17 \
    --executor-memory 30g
```

4.3. Spark analysis

4.3.1. Using dataframes

Dataframes in Spark come from the Spark.SQL module. Similar to the pandas one\(^\text{15}\), they can be viewed as a set of named columns over which you can perform operations but in a distributed environment. Some native Spark functions acts on them and should be used as much as possible, since they have been very optimized. They are available with:

```
from pyspark.sql import functions as F
```

Once substantial data reduction has been achieved, we can recover a standard pandas dataframe with the `toPandas()` method which opens the door to further standard python analysis.

4.3.2. Reading the data

We begin by loading the (set of) FITS files using spark-fits. CoLoRe FITS format stores separately the cosmological ("Z\_COSMO") and RSD ("DZ\_RSD") redshifts, but since we only want to work on their sum, we construct the \(z\) column on the fly:

```
sparkfits="com.astrolabsoftware.sparkfits"

gal=spark.read.format("sparkfits")\  
   .option("hdu",1)\  
   .load("hdfs:path/to/fits/directory")\  
   .select("RA", "Dec", \  
      (F.col("Z\_COSMO")+F.col("DZ\_RSD")))\  
   .alias("z")
```

This represents a (Spark) dataframe object. We show two ways of accessing columns in the select function, either simply through their names (strings) or, when some operations are to be performed, through `F.col(..)` that returns Columns objects. Other dataframe standard ways to access columns are through `gal.RA` or `gal['RA']`. Note the use of the "\(z\)" alias to rename the new column.

You can now print the dataframe schema:

```
gal.printSchema()
```

```
root
    |-- RA: float (nullable = true)
    |-- Dec: float (nullable = true)
    |-- z: float (nullable = true)
```

It is important to understand that, at this level (almost) nothing is performed, only the FITS header is read to get the data structure. It is the principle of lazy evaluation. Only when it will be clearer to Spark about what we want to do with those data, will the system trigger real loading.

4.3.3. Adding photometric smearing

We would like to add now the effect of the photo-z (PZ) resolution of the instrument. For LSST this will be close to a Gaussian smearing with a standard deviation somewhere in the range \(\sigma_z/(1 + z) \in [0.03 - 0.05]\) (LSST Science Collaboration et al. 2009).

In the optimistic case, we add a column to the `gal` dataframe with

```
from pyspark.sql import functions as F

gal=gal.select(F.col("z")\  
    .cast("float")\  
    .subtract(\  
      (0.03 + (0.05 - 0.03)/(1 + F.col("z").cast("float")))\  
      .cast("float")\  
      .cast("float"))\  
    .alias("z\_PZ")
```

```
root
    |-- RA: float (nullable = true)
    |-- Dec: float (nullable = true)
    |-- z: float (nullable = true)
    |-- z\_PZ: float (nullable = true)
```

This time Spark will perform the addition before returning the dataframe. This is typically what you want to do with photometric redshifts.

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\(^\text{12}\)https://github.com/damonge/CoLoRe
\(^\text{13}\)https://github.com/LSSTDESC/2pt_validation
\(^\text{14}\)https://www.informatique-scientifique.u-psud.fr/services/spark.html
\(^\text{15}\)https://pandas.pydata.org/
from pyspark.sql.functions import randn
gal = gal.withColumn("zrec", gal.z + 0.03 * (1 + gal.z) * randn()).astype('float')

Again, when executed nothing happens, the pipeline just grows.
We can investigate a few samples, which now triggers a real action:

gal.show(5)

This is the very idea of lazy evaluation: if you only want to look at a few samples does it worth loading all (110 GB) of the data? Here Spark analyzes the full pipeline, optimizes it and works only on the first block, which is why this happens within seconds (see Table 1).

4.3.4. Caching

Now we have defined which data we want to use in our analysis we put them in cache. This is achieved with the cache() function. Some finer level of details can be obtained with the persist(level) function that allows to specify the storage level. cache() corresponds to persist(MEMORY_ONLY). You may use persist(MEMORY_AND_DISK) if your cluster does not have enough total memory. It was shown in SparkFITS18 that good performances can still be obtained in this case. Note that serializing the objects might also improve performances (e.g. level=MEMORY_ONLY_SER) but it was not observed in our case.

In order to trigger caching one must call an action as counting the total number of galaxies which requires access to the full data:

```
print(gal.cache.count())
```

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In our case, putting all the data in cache by counting them takes about 90 s, with about 20 s coming from the PZ computation.

4.3.5. Getting some basic statistical information

Some basic statistical informations may be obtained on some (or all) variables with:

```
gal.describe(['z', 'zrec']).show()
```

Table 1 gives the measured user-time in each case: once the data are in cache, all those commands run in seconds.

### 4.3.6. Histograms

We now wish to go further and study the redshift distribution of galaxies. Although RDDs provides some command to build histograms, we will show that it is much more efficient to design a function using dataframes capabilities. We use a standard mapReduce method:

1. add a new column to the dataframe containing the bin number,
2. group the data by this number,
3. count the number of values in each group,
4. sort the bin index by ascending order.

Adding the \(z\) bin number column (labeled “bin”) is done most efficiently using standard column operations:

```
Nbins=100
dz=(zmax-zmin)/Nbins
zbin=gal.select(gal.z,
((gal.z-zmin-dz/2)/dz).astype('int').alias('bin'))
```

Then, grouping by the bin column, counting its members and sorting in ascending order is performed by:

```
h=zbin.groupBy("bin")
 .count()
 .orderBy(F.asc("bin"))
```

where the groupBy operation is the most expensive, since it triggers data exchange between executors (called shuffle), the ordering acting only on the bin values, i.e. after the data reduction.

Finally we may want to add the bin locations, drop the bin number and go back to the python world by recovering a standard pandas object:

```
pd=h.select("bin",
 (zmin+dz/2+h.bin*dz).alias('zbin'),
 "count")
 .drop("bin")
 .toPandas()
```

The histogram is obtained in about 10 s (Table 1) which is impressive for running on 6 \(10^9\) data. We can now study for instance how the selection function varies depending on the PZ smearing parameters which is shown on Fig.2.
In order to prepare for the next part, let us see how to build the histogram by calling an external function. Operations may be applied onto dataframes with a User Defined Function (UDF) as:

```
binNum=F.udf(lambda z: int((z-zmin-dz/2)/dz))

zbin=gal.select(gal.z,)
    .alias('bin'))

binNum(gal.z)
```

But there are performances issues since from the previous 10 s we get to 2 mins.

To alleviate this issue, Spark introduced recently (v2.3.0) pandas_udf’s which allow some level of vectorization using pandas.Series. The UDF is re-written as:

```
import pandas as pd
from pyspark.sql.functions \n    import pandas_udf, PandasUDFType

@pandas_udf("float", PandasUDFType.SCALAR)
def binNumber(z):
    return pd.Series((z-zmin)/dz)

zbin=gal.select(gal.z,)
    .alias('bin'))

binNumber("z").astype('int')
```

The user-time becomes 40 s which is better although not optimal and will be discussed more in Sect. 4.3.8. The main lesson from this part for python users is to always work with dataframes and whenever possible with the native Spark SQL functions.

### 4.3.7. Tomography

Measuring galactic density power-spectra over some redshift bins (called tomographic “shells”) is a nearly optimal method in cosmology to study galaxy clustering, especially for photometric surveys (Crocce et al. 2011; Asorey et al. 2012). Measuring the cross-correlation between nearby shells gives also access to Redshift-Space-Distorsions even in photometric surveys where the radial information is strongly suppressed (Ross et al. 2011). Cross-correlation between far-away bins is also of interest: since, neglecting magnification lensing, no cosmological signal is expected there, any observed correlation singles-out some remaining systematics (as PZ distribution outliers).

Such studies can be efficiently performed with Spark. We have chosen 10 tomographic bins marked out as vertical lines on

![Fig. 2. Difference of galactic density with/without photometric smearing for two configurations given in the legend.](image)

We end up with a standard HEALPix map on which can perform further analysis. An example is shown on Fig. 4. We note that the python packages must be available on each executor.

Concerning performances (Table 1), each shell projection is obtained in about 30s, quite independently of the galaxy population. All the 10 shells are obtained in about 5 mins.
From the maps, one can then compute auto and cross spectra using standard healpy functions. We illustrate some of the results we obtain for a few of them on Fig. 5.

4.3.8. Performances

We already discussed the user-time measured for each step. They are summarized in Table 1. But are we far from the best possible ones in Spark? The native Spark language is scala which generally leads to the best performances. So we have recoded and run all the previous commands in scala and compare performances in Table 1.

The initialization phase ("load(HDU)") is slightly longer in scala than in python. Caching the $10^9$ data which is the most demanding part but only needs to be performed once, is obtained in our case in about 1.5 mins in each case. Then, the "statistics" part is slightly more efficient in python. As far as.

| Section     | Analysis                                      | Python (min, max) | Scala (min, max) |
|-------------|-----------------------------------------------|-------------------|------------------|
| 4.3.2       | load(HDU)                                     | $2.8 \pm 0.1$     | $8.8 \pm 0.2$    |
|             | PZ + show(5)                                  | $12.4 \pm 0.6$    | $13.7 \pm 1.2$   |
| 4.3.4       | cache (count)                                 | $97.7 \pm 4.0$    | $95.4 \pm 5.0$   |
| 4.3.5       | stat(z)                                       | $3.9 \pm 1.5$     | $4.9 \pm 2.5$    |
|             | stat(all)                                     | $9.8 \pm 1.0$     | $11.0 \pm 0.9$   |
|             | minmax(z)                                     | $1.8 \pm 0.3$     | $3.2 \pm 0.7$    |
| 4.3.6       | histo (dataframe)                             | $11.5 \pm 1.5$    | $13.0 \pm 0.8$   |
|             | histo (UDF)                                   | $114.9 \pm 5.6$   | $13.9 \pm 1.2$   |
|             | histo (pandas UDF)                            | $43.3 \pm 4.5$    | -                |
| 4.3.7       | 1 shell                                       | $30 \pm 3$        | $13 \pm 2$       |
|             | all shells (10)                               | $307 \pm 34$      | $130 \pm 18$     |

Table 1. User-time (in seconds) for the various analysis steps described in the text using the python commands (first column) and the scala ones (second column). Results were obtained by running sequentially the commands from the top to the bottom of the table, 10 times and then were averaged.

We have shown why Spark is a valuable tool today for scientists to investigate large datasets as simulated or real galactic.
catalogs used in cosmology. More astronomy-related operations, as neighbor finding or cross-matching two catalogs, will be discussed in a forthcoming paper. Using Spark does not require learning a new language since it can be used within a python shell where we have shown that, using Spark SQL dataframes, most operations behave perfectly. One just needs to assemble efficiently some quite simple functions. The key-point is to think in a “distributed way” (ie. map-reduce) and we give some concrete examples about how to start doing it. Note that the Spark framework can be downloaded and experimented on a personal computer. Its strong point is that any local development generally scale when ported to a larger infrastructure.

In the current days of ever-growing massive data, it worths investing in a technology which gives access to physicists to interactive analysis of billions of objects. We have shown how a 6 billion-objects realistic galactic catalog could be analyzed interactively, histograms build in about 10 s, and tomographic bins in 50 s.

We worked on purpose on a rather modest cluster consisting of 8 workers and that much higher performances can be obtained on larger datacenters. Our cluster is however sufficient to hold all the data (110 GB) in cache which is essential for interactive analysis. If the dataset cannot hold in memory one can still:

- in the phase of designing the analysis, put in cache only the fraction of data that fits into memory using the sample function which takes a random fraction of the data,
- then, in a final run still use the cache with a MEMORY_AND_DISK storage level (see Sect. 4.3.4) and run the full analysis.

We emphasize that Spark addresses the question of accessing the data not algorithmic performances. It is in no way opposite to HPC developments and nothing prevents us from combining both. We only began to scratch the surface of connecting some external (optimized) code and have shown that, for a user working in python, pandas_udf’s provide a simple and reasonably efficient way to do it. But there also exist many efficient codes written in C/C++ or Fortran. Should we throw them? We began investigating the java-native-access library (JNA) that allows to link these codes to scala and then be used within a Spark pipeline. The first results, that are outside the scope of this paper, are promising. The balance between accessing the data and algorithmic performances remains to be found and is probably problem-specific. This is an exciting perspective, that would allow to re-appropriate a technology born once in a public lab. It is the goal of the Astrolab organization that everyone interested in such a project is invited to join.

Acknowledgements

We acknowledge the use of the HEALPix package and the CoLoRe fast simulation with support from David Alonso, Anze Slosar and Javier Sanchez that we kindly thank. The Spark work was performed at the VirtualData center at Université Paris Sud and we thank Adrien Ramparison for the upgrades and maintenance of the cluster. The CoLoRe simulation was run at the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

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