



Big Data to Enable Global Disruption of the Grapevine-powered Industries

D4.3 - Models and Tools for Predictive Analytics over Extremely Large Datasets

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ACRONYMS LIST

BDG	BigDataGrapes
HDFS	Hadoop Distributed File System
RDD	Resilient Distributed Dataset

EXECUTIVE SUMMARY

This accompanying document for deliverable D4.3 (Models and Tools for Predictive Analytics over Extremely Large Datasets) describes the first version of the mechanisms and tools supporting efficient and effective predictive data analytics over the BigDataGrapes (BDG) platform in the context of grapevine-related assets.

The BDG software stack employs efficient and fault-tolerant tools for distributed processing, aimed at providing scalability and reliability for the target applications. On top of this stack, the BDG platform enables distributed predictive big data analytics by effectively exploiting scalable Machine Learning algorithms using efficiently the computational resources of the underlying infrastructure. The software components enabling BDG predictive data analytics have been designed and deployed using Docker containers. They thus include everything needed to run the supported predictive data analytics tools on any system that can run a Docker engine.

The document first introduces the main technologies currently used in the first version of the BDG component for performing efficient and scalable analytics over extremely large dataset. The docker component provided in this deliverable relies on the BDG software stack discussed in Deliverable 2.3 “BigDataGrapes Software Stack Design” and exploits the distributed execution environment provided by the Persistence and Processing Layers of the BDG architecture contributed in Deliverable 4.1 “Methods and Tools for Scalable Distributed Processing”

The document details the steps to be followed to download and deploy the first version of the BDG platform and provides the reader with practical examples of usage of its scalable predictive analytics component. Specifically, we provide three demonstrators released as Jupyter Notebooks implementing three different machine learning tasks by exploiting the BDG infrastructure. The first one shows how to train two kinds of regressors, i.e., linear and random forest regressors, to fit synthetically generated data. We present these results by adding a visualization of the result to allow the reader to understand the limitations of each specific solution. The second demonstrator employs a well-known dataset, i.e., the KDD CUP 1999 dataset, to train a binary logistic regression classifier. We show how to train and evaluate the performance of the classifier by means of a standard metric, i.e., Accuracy. This second demonstrator also shows how the distributed filesystem can be exploited to directly feed with data the machine learning platform. The third demonstrator extends the second one by showing how to train a multi-label classifier on the Red Wine Quality Dataset, a public dataset employed on Kaggle for a machine learning competition. We show how to learn a multi label logistic regression classifier and how to evaluate its performance in terms of Accuracy.

In this first version of D4.3 we assess the effectiveness of different predictive data analytics tools in terms of a standard and popular metrics such as Accuracy. Future versions of the BDG predictive analytics component will provide tools and methods for a deep analysis of the performance of different machine learning libraries by specifically considering the results of WP7 (Cross-sector Rigorous Experimental Testing).

TABLE OF CONTENTS

EXECUTIVE SUMMARY.....	5
1 INTRODUCTION.....	8
2 DISTRIBUTED MACHINE LEARNING OVER BIG DATA	9
2.1 APACHE SPARK.....	9
2.2 APACHE HDFS	9
2.3 MLLIB	9
2.4 H2O SPARKING WATER.....	10
3 BIGDATAGRAPES PREDICTIVE DATA ANALYTICS SETUP.....	11
3.1 REQUIREMENTS	11
3.2 DOCKER COMPONENTS SCHEMA	11
3.3 HOW TO GET THE CODE	11
3.4 DESCRIPTION OF THE DEMONSTRATORS	12
3.4.1 Connection to the BDG Apache Spark enabling distributed computation	13
3.4.2 Reading of the data with Apache Spark (to create a Resilient Distributed Dataset (RDD)	14
3.4.3 Training of three different kinds of machine learning applications with MLLib.....	14
3.4.4 Disconnection from the BDG Apache Spark environment.....	15
3.5 HOW TO RUN THE CODE.....	15
3.6 PERFORMANCE ASSESSMENT.....	15
4 SUMMARY	16

LIST OF FIGURES

Figure 1: BigDataGrapes Components used by the Predictive Data Analytics functionality and their mapping on Docker Containers 11

Figure 2: Snapshot of a Jupyter Notebook taken from the Predictive Data Analytics demonstrator..... 13

Figure 3: Application of three linear regression models (red, green and blue solid lines) trained on synthetic data generated by perturbing linear, square and sine functions with gaussian noise. 14

Figure 4: Application of three random forest regressors (red, green and blue solid lines) trained on synthetic data generated by perturbing linear, square and sine functions with gaussian noise. 14

1 INTRODUCTION

The BigDataGrapes platform aims at providing Predictive Data Analytics tools that go beyond the state-of-the-art for what regards their application to large and complex grapevine-related data assets. Having this ambitious goal in mind, even the first version of the predictive analytics component described in this document has been designed by relying on the core technologies and frameworks for efficient processing of large datasets, e.g., Apache Spark, employed on the lower levels of the BDG platform. Machine learning largely benefits from the distributed execution paradigm that serves as the basis for addressing efficiently the analytics and scalability challenges of grapevines-powered industries.

The document first introduces the main technologies currently used in the first version of the *BDG* component for performing efficient and scalable analytics over extremely large dataset. The dockerized component provided in this deliverable relies on the BDG software stack discussed in Deliverable 2.3 “BigDataGrapes Software Stack Design” and exploits the distributed execution environment provided by the Persistence and Processing Layers of the BDG architecture contributed in Deliverable 4.1 “Methods and Tools for Scalable Distributed Processing”.

The BDG platform allows the user to learn and apply predictive data analytics over extremely large dataset. We show these functionalities by discussing three demonstrators implemented as Jupyter Notebooks. The demonstrators deal with three different kinds of machine learning tasks: regression, binary classification and multi-label classification. We present the three applications on three different datasets. The first one is synthetically generated while the other two are the KDD CUP 1999 dataset and the Red Wine Quality, both public. We first present how to train several kinds of models addressing the three tasks, i.e., *linear regressors*, *random forest regressors*, *logistic regression classifiers* by interacting with the BDG distributed infrastructure. We then present how to assess the performance of a learned model in terms of a well-known quality metric, i.e., Accuracy. Moreover, we present some basic visualization of the data to provide the user with a useful visual feedback.

The rest of this document is organized as follows: Section 2 highlights the main technologies used in the BDG software stack to support and implement scalable predictive analytics. Section 3 describes the design and implementation of the first version of the BDG predictive analytics component and details how to set up and run it on the top of the current version of the BDG platform. Moreover, it discusses the three demonstrators that are provided in the deliverable as running examples showing the functionalities of the BDG platform. Finally, Section 4 concludes the document.

2 DISTRIBUTED MACHINE LEARNING OVER BIG DATA

In this Section we introduce the main components allowing BigDataGrapes to perform predictive analytics over extremely large dataset. To provide the reader with a self-contained view of the predictive data analytics functionality supported by the first version of the BDG platform, we first introduce Apache Spark, a scalable big data processing framework that is the de-facto technological state-of-the-art for parallel and distributed batch computations, and Apache HDFS, a distributed file system enabling persistence of information. We finally introduce MLLib, the machine learning library working on Apache Spark that allows distributed and parallel learning from big data of effective models for regression and classification tasks.

2.1 APACHE SPARK

Apache Spark (<https://spark.apache.org/>) is a well-known and open-source framework for big data processing. It has been designed at the University of California, Berkeley's AMPLab in 2009. Later, the Spark project moved to the Apache Software Foundation, which has maintained it since 2010. As previous big data processing frameworks, Spark provides an interface for programming clusters with implicit data parallelism and fault tolerance. The novel key feature that motivates its success and popularity is the introduction of the “Resiliend Distributed Dataset” (RDD), a data structure implementing a read-only multiset of data items distributed over a cluster of machines and guaranteeing fault-tolerance. The introduction of the RDD was needed in response to the limitations of the MapReduce cluster computing paradigm, which forces a particular linear dataflow structure on distributed programs. With MapReduce, programs simply read input data from disk, map a function across the data, reduce the results of the map, and store reduction results on the file system. The functions of the RDD in Spark allows distributed programs to interact with a (deliberately) restricted form of distributed shared memory. This novel approach allows Spark to ease the implementation of both iterative algorithms, that visit the data multiple times in a loop, and interactive/exploratory data analysis, i.e., the repeated database-style querying of data. As a consequence, the latency of this kind of applications is extremely reduced, i.e., by several orders of magnitude compared to a MapReduce implementation (as was common in Apache Hadoop stacks).

2.2 APACHE HDFS

The Apache Hadoop software library (<http://hadoop.apache.org/>) is a framework supporting the distributed processing of large data sets across clusters of computers using simple programming models. It is designed to scale out from single servers to thousands of machines, each offering local computation and storage. Among the Apache Hadoop's core components, there is the Hadoop File System (HDFS). HDFS or Hadoop File System is the file system in which the data is stored. The stored data may be structured, semi-structured or unstructured thus containing for example either the tables of a relational database, or a set of json or log files. HDFS is designed for massive scalability, it stores unlimited amounts of data in a single platform. As the data grow, it is possible to simply add more servers to scale linearly. Furthermore, a key feature of HDFS is reliability. It automatically performs multiple copies of the data stored, letting it always available for access and protection from data loss. Built-in fault tolerance means servers can fail but a system will remain available for all workloads.

2.3 MLLIB

MLlib (<https://spark.apache.org/mllib/>) is the machine learning library for Apache Spark. It is a fully-fledged tool containing many algorithms and utilities for several tasks ranging from classification (logistic regression, naive Bayes, etc.) to regression (generalized linear regression, survival regression, isolation regression, etc.) and gradient-boosted algorithms based on trees, e.g., random forests, multiple additive regression trees. It also provides distributed methods for clustering (K-means, Gaussian mixtures (GMMs), etc.) and for mining frequent itemsets, association rules, and sequential patterns. MLLib also provides utilities for data pre-processing exploiting the underlying distributed Spark environment. Pre-processing of data includes feature

transformations (standardization, normalization, hashing) and easy statistics on data (summaries, hypothesis testing, etc). All this processing blocks can be also combined together toward the definition of a “Pipeline” of machine learning techniques that enable model evaluation and efficient hyper-parameter tuning. The persistence of the results is also implemented by the definition of methods for saving and loading models and pipelines to/from the file system.

2.4 H2O SPARKING WATER

Sparkling Water (<https://www.h2o.ai/products/h2o-sparkling-water/>) allows users to combine the fast, scalable machine learning algorithms of H2O with the capabilities of Apache Spark. Sparkling Water stems from H2O, an in-memory platform for machine learning, the potential of performing effective and efficient machine learning on big data. Sparkling Water and Apache Spark allows for a seamless experience for users who want to interact with distributed databases/filesystems, build a model and make predictions, and then use the results again in Apache Spark. It is used for exploring and analysing datasets held in cloud computing systems and in the Apache HDFS as well as in the conventional operating-systems Linux, macOS, and Microsoft Windows. The H2O software is written in Java, Python, and R. Its graphical-user interface is compatible with four browsers: Chrome, Safari, Firefox, and Internet Explorer.

3 BIGDATAGRAPES PREDICTIVE DATA ANALYTICS SETUP

The BDG platform relies on MLLib, the Apache HDFS file system and Apache Spark to allow the BDG users to develop methods for predictive data analytics, i.e., classification, regression, and clustering algorithms, and to interact and use them on the BDG distributed infrastructure. In the following sections we detail how to setup and install the BDG Predictive Data Analytics component and how to run the toy demonstrators provided in the first version of the deliverable. Demonstrators are implemented in Python as Jupyter Notebooks (<http://jupyter.org/>).

3.1 REQUIREMENTS

The Predictive Big Data Analytics functionality of the BDG platform is available after setting up the BDG architecture as detailed in D4.1. Interested users should refer to D4.1 and follow all the steps reported in Section 3 to setup a working BDG architecture.

3.2 DOCKER COMPONENTS SCHEMA

Figure 1 shows the components used by the Predictive Data Analytics functionality of BDG and their implementation as Docker components. In the Figure we made transparent all the components of the BDG architecture not explicitly needed by this functionality. As detailed above, the Predictive Data Analytics functionality relies on MLLib, Spark and HDFS to perform machine learning tasks over extremely large datasets. We also report the addresses and ports used by these containers. Particularly, the Spark component is composed of one master node/container and many workers nodes/containers linked to the master. Similarly, the HDFS component has one *namenode* container and many *datanodes* containers.

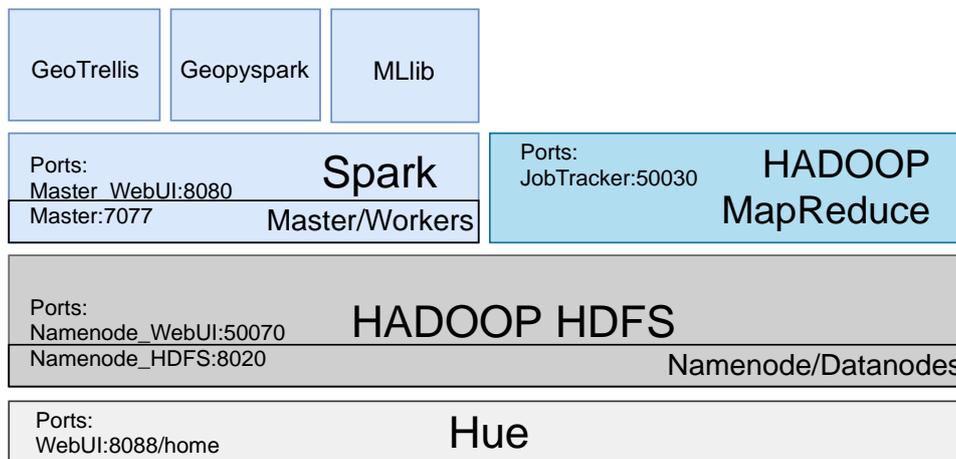


Figure 1: BigDataGrapes Components used by the Predictive Data Analytics functionality and their mapping on Docker Containers

3.3 HOW TO GET THE CODE

To get the code demonstrating the Predictive Data Analytics functionality of BDG, clone the following GitHub repository

```
$ git clone https://github.com/BigDataGrapes-EU/deliverable-D4.3.git
```

The repository contains three Jupyter Notebooks and a Bash shell script that should be used to initialize the Big Data Grapes Platform. The script should be executed after cloning the repository by running the Bash command below:

```
$ ./run-components.sh
```

The Bash script above downloads the Docker images and builds the environment according to the predefined configuration settings. The Bash script also starts the Docker containers of the BigDataGrapes software stack components.

Finally, to execute the demonstrators, run the following Bash command:

```
$ ./run-jupyter_notebooks.sh
```

The Bash script above starts the Jupyter notebooks for predictive data analytics using the BigDataGrapes platform.

3.4 DESCRIPTION OF THE DEMONSTRATORS

The Predictive Data Analytics demonstrator consists of Python code made available in three Jupyter Notebook files. The first one shows how to train linear and random forest regressors with MLLib on synthetic data. The second one details how to perform a classification task with MLLib on a real-world public dataset, the KDD Cup 1999 challenge. The third one shows how to train multi-label classifiers with MLLib on the Red Wine Quality Dataset.

Jupyter Notebook (<http://jupyter.org/>) is an open-source Web application that allows the user to create and share documents that contain live code, equations, visualizations and narrative text. They are extremely useful for data cleaning and transformation, numerical simulation, statistical modeling, data visualization, machine learning, and much more. The Notebook supports over 40 programming languages. Code inside a notebook can produce rich, interactive output. More importantly, Jupyter Notebook can exploit big data tools, such as Apache Spark, from Python, R and Scala.



Figure 2 shows a snapshot of one of the Jupyter Notebooks of the demo. A Jupyter Notebook is a sequence of cells containing code, text, images, etc. The execution of each cell allows to run the code inside it. The output of each cell is then shown in the notebook so to allow easy interaction with the user.

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This deliverable (D4.3) presents how to train machine learning models with the BigDataGrapes distributed processing architecture. In particular, we present how to train classifiers with MLLib (<https://spark.apache.org/mllib/>).



```
In [1]: from pyspark import SparkContext
```

```
In [2]: import math
import urllib
import random
import numpy as np
import pydoop.hdfs as hdfs

from numpy import array
from pyspark.mllib.regression import LabeledPoint
```

```
In [3]: %matplotlib inline
import matplotlib.pyplot as plt
```

Connection to the BDG Apache Spark

```
In [4]: # standalone mode below
#sc = SparkContext(appName="Classification-WineDataset", master="master[*]")

# distributed mode below
sc = SparkContext(appName="Classification-WineDataset", master="spark://spark-master:7077")

# setting logger level
sc.setLogLevel("ERROR")
```

Figure 2: Snapshot of a Jupyter Notebook taken from the Predictive Data Analytics demonstrator.

The three demonstrators of the Predictive Data Analytics functionality of BDG are both structured around four different steps that are detailed in the following.

3.4.1 Connection to the BDG Apache Spark enabling distributed computation

This is a preliminary operations allowing Jupyter Notebook to connect to the Spark context used for the computation, i.e., the master node that manage the distributed computation on the cluster. Data generation/download for the regression/classification demonstrators works as follows:

- In the regression demonstrator we generate synthetic data and we preliminary plot them to allow the user to understand their shape and complexity.
- The binary classification demonstrator exploits real data from a well-known data challenge: KDD Cup 1999. The dataset is used for the Third International Knowledge Discovery and Data Mining Tools Competition, which was held in conjunction with KDD-99 The Fifth International Conference on Knowledge Discovery and Data Mining. The competition task was to build a network intrusion detector, a predictive model capable of distinguishing between “bad” connections, called intrusions or attacks, and “good” normal connections. This database contains a standard set of data to be audited, which includes a wide variety of intrusions simulated in a military network environment. The demonstrator shows how to build a Logistic Regression Classifier with MLLib. We also show how to interact with the BDG HDFS distributed file system by downloading and storing the dataset on HDFS.
- The multi-label classification demonstrator is built around the Red Wine Quality Dataset made available on Kaggle (<https://www.kaggle.com/piyushgoyal443/red-wine-dataset/discussion>). The dataset is related to red variants of the Portuguese "Vinho Verde" wine. Due to privacy and logistic issues, only physicochemical (inputs) and sensory (the output) variables are available (e.g. there is no data about grape types, wine brand, wine selling price, etc.). The dataset is made up of 1599 instances. Each instance has 11 attributes and one label, i.e., the quality of the wine produced expressed on a ten-grade scale, i.e., $\{1, 2, \dots, 10\}$. The classes are ordered and not balanced.

3.4.2 Reading of the data with Apache Spark (to create a Resilient Distributed Dataset (RDD))

The three demonstrators read the datasets used in two different ways. While the regression demonstrator shows how to build Spark RDDs from NumPy arrays the second and the third one, i.e., the ones dealing with classification read data from HDFS showing an example of interaction with the BDG distributed file system.

3.4.3 Training of three different kinds of machine learning applications with MLlib

- Regression (Linear and Random Forest Regressors): We intentionally generate data by perturbing results from linear, square, and sine functions with gaussian noise. The visualization of the results of the regression clearly show that the three lines fitted follow the shape of the data used to fit them. Indeed, this kind of regressors are very simple yet not totally able to deal with the complexity of square and sine data (Figure 3).

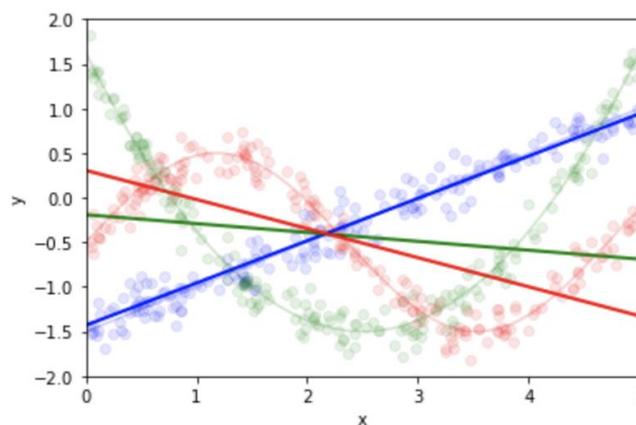


Figure 3: Application of three linear regression models (red, green and blue solid lines) trained on synthetic data generated by perturbing linear, square and sine functions with gaussian noise.

- We then add a more complex (non-linear) regressor, i.e., random forest, to deal with the complexity of the data. The prediction produced is now more accurate as Figure 4 shows.

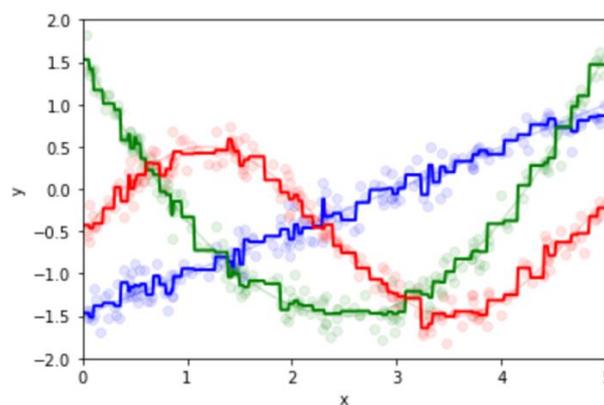


Figure 4: Application of three random forest regressors (red, green and blue solid lines) trained on synthetic data generated by perturbing linear, square and sine functions with gaussian noise.

- Binary Classification (Logistic Regression Classifier): In the binary classification demonstrator we train a binary classifier by employing logistic regression. The demonstrator is built around the KDD 1999 dataset that comes split in train/test. Train and test data are read from HDFS to allow Apache Spark to build two RDDs that are then used to build the classifier. We first build the classifier on training data.

We then perform an evaluation step by computing the accuracy metric, i.e., the proportion of true results (both true positives and true negatives) among the total number of cases examined, on the test set of the dataset. This information is then returned to the used to allow an easy comparison of the performance with other classifiers.

- **Multi-label Classification (Logistic Regression Classifier):** In the multi-label classification demonstrator we train a multi label classifier by employing logistic regression. The demonstrator is built around the Red Wine Quality Dataset that we split in train/test. The dataset is made up of examples labeled with a “quality” label expressed on a ten-grade scale. We thus learn a classifier to guess the correct class, i.e., quality of each wine. We learn the classifier after loading data from HDFS. We then perform an evaluation step by computing the accuracy metric, i.e., the proportion of true results (both true positives and true negatives) among the total number of cases examined, on the test set of the dataset. This information is then returned to the used to allow an easy comparison of the performance with other classifiers.

3.4.4 Disconnection from the BDG Apache Spark environment

This is the last, yet very important, phase needed to disconnect the Jupyter Notebook from the BDG big data platform. The operation allows for freeing the resources allocated and used by the computation. Each step above is documented inside the Jupyter Notebooks. We clearly identify each part by adding a textual cell describing when a specific step starts. We also add several cells allowing for visualizing the dataset and the intermediate results.

3.5 HOW TO RUN THE CODE

To run the demonstrators, after following the instructions detailed in Section 3.3, the user should point her browser to the following Jupyter Notebook URL: http://<server_address>:9999

The password used to protect the Jupyter Notebook instance is “bigdatagrapes”.

After a successful login the user can open the files below:

- D4.3-PredictiveDataAnalyticsWithMLLib-Regression-Py2.ipynb
- D4.3-PredictiveDataAnalyticsWithMLLib-Classification-Py2-KDDCUP1999.ipynb
- D4.3-PredictiveDataAnalyticsWithMLLib-MultiLabelClassification-Py2-WineDataset.ipynb

The execution of the code can be done by running each cell from the beginning to the end of each notebook and wait for the result.

3.6 PERFORMANCE ASSESSMENT

In this first version of D4.3 we simply assess the effectiveness of different predictive data analytics tools in terms of a standard and popular metrics such as Accuracy. Future versions of the BDG predictive analytics component will provide tools and methods for a deep analysis of the performance of different machine learning libraries by specifically considering the results of WP7 (Cross-sector Rigorous Experimental Testing). In particular WP7 will provide guidelines and methodologies for the rigorous testing of the BDG technical solutions under realistic conditions and assumptions. We recall that a preliminary, first version of the BDG testing methodology that will allow the project to reliably measure and compare the efficiency of the developed components is presented in D7.1 (Scalability and Robustness Experimental Methodology).

4 SUMMARY

This accompanying document for deliverable D4.3 (Models and Tools for Predictive Analytics over Extremely Large Datasets) describes the first version of the mechanisms and tools supporting efficient and effective predictive data analytics over the BigDataGrapes (BDG) platform in the context of grapevine-related assets.

The BDG software stack employs efficient and fault-tolerant tools for distributed processing, aimed at providing scalability and reliability for the target applications. On top of this stack, the BDG platform enables distributed predictive big data analytics by effectively exploiting scalable Machine Learning algorithms using efficiently the computational resources of the underlying infrastructure. The software components enabling BDG predictive data analytics have been designed and deployed using Docker containers. They thus include everything needed to run the supported predictive data analytics tools on any system that can run a Docker engine.

In this first version of D4.3 we assess the effectiveness of different predictive data analytics tools in terms of a standard and popular metrics such as Accuracy. Future versions of the BDG predictive analytics component will provide tools and methods for a deep analysis of the performance of different machine learning libraries by specifically considering the results of WP7 (Cross-sector Rigorous Experimental Testing).