

ADENINE — A Data Exploration pIpeliNE

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Editor: Editor name

Abstract

Adenine is a machine learning **{Python }** framework for data exploration. Its goal is to help researchers and data scientists achieving a first and quick overview on the main structures underlying their data and to choose the most suitable unsupervised learning pipeline for the problem at hand. This software tool encompasses state-of-the-art techniques for missing values imputing, data preprocessing, dimensionality reduction and clustering tasks. **Adenine** exploits both process- and thread-level parallelism and it is capable of generating nice and clean publication-ready plots along with quantitative descriptions of pipeline results. **Adenine** is available at <http://slipguru.github.io/adenine/> under FreeBSD license.

Keywords: Data exploration, unsupervised learning, RNA-Seq gene expression

1. Introduction

Data exploration is a very insightful starting point for many data analysis projects. Researchers and data scientists are often asked to extract meaningful information from collections of complex and possibly high-dimensional data coming from heterogeneous contexts. For instance, in biomedical scenarios, physicians are likely to be interested in answering some biological questions starting from observations collected from a pool of subjects enrolled in a study. Possible investigations can be: *is there any relevant stratification among subjects?* or *is it possible to discriminate between cases and controls from my observations?*. Starting from a given dataset, the information needed to answer such questions may be non-trivial to extract or even completely absent. In these situations, a preliminary data exploration step is not only a good practice, but also a fundamental starting point for further and deeper investigations. To accomplish this task, several machine learning and data mining techniques were developed over the years. Among those we focus on the four most popular classes of methods: (i) missing values imputing, (ii) data preprocessing, (iii) dimensionality reduction and (iv) unsupervised clustering. **{togliere? viene detto anche dopo}**

In the last few years, a fair number of data exploration software and libraries were released. At a very coarse grain we can group them in two families: GUI-based and command-line applications. Among the first group we recall *Divvy* (Lewis et al., 2013), a software

tool that performs dimensionality reduction and clustering on input datasets. *Divvy* is a light framework; however, its collection of C/C++ algorithm implementations does not cover common strategies such as kernel principal component analysis (KPCA) (Schölkopf et al., 1997) or hierarchical clustering (Friedman et al., 2001) and it does not offer strategies to perform automatic discoveries of the number of clusters. The most notable project that spans between the two families is *Orange* (Demšar et al., 2013), a data mining software suite that offers both visual programming front-end and Python APIs. In the context of data exploration, *Orange* can be successfully employed. However, it does not support automatic pipeline generation and, as of today, *Orange* lacks in several nonlinear methods such as isomap (Tenenbaum et al., 2000), locally linear embedding (Roweis and Saul, 2000) and spectral clustering (Shi and Malik, 2000).

We introduce **Adenine**, a command-line Python tool for data exploration that, starting from a set of unsupervised algorithms, creates textual and graphical reports of an arbitrary number of pipelines. In this context data imputing, preprocessing, dimensionality reduction and clustering strategies are considered as building blocks for data analysis pipelines. The user is only required to specify input data and to select blocks, then **Adenine** takes care of the generation and running of the pipelines composed by all possible combinations of the selected algorithms. Every algorithm implementation of **Adenine** is inherited, or extended, from **scikit-learn** (Pedregosa et al., 2011) which is, to the best of our knowledge, the most complete machine learning open source library freely available online.

{mettere qui?} In order to perform exploratory analysis on large datasets we took advantage of different parallel computing paradigms. Moreover, since **Adenine** makes large use of **numpy** and **scipy**, it automatically benefits from their bindings with optimized linear algebra libraries (such as OpenBLAS¹ or Intel[®] MKL).

2. Tool overview

Adenine is developed around the data analysis concept of *pipeline*. A pipeline is a sequence of the following fundamental steps: (i) missing values imputing, (ii) data preprocessing, (iii) dimensionality reduction and (iv) unsupervised clustering. For each task, different off-the-shelf algorithms are available (see Table 1).

Step 0: Missing values imputing. In order to cope with real-world datasets where entries are often missing, **Adenine** offers an improved version of the Imputer class provided by **scikit-learn**. Our extension adds a k-nearest neighbor (KNN) imputing method to the pre-existent feature-wise *mean*, *median* and *most frequent* value strategies. (Troyanskaya et al., 2001)

Step 1: Data preprocessing. Collecting data from heterogeneous sources may imply dealing with features lying in very different numerical ranges. This could have a negative influence on the behavior of dimensionality reduction and clustering techniques. To tackle this issue **Adenine** offers different strategies to preprocess data.

Step 2: Dimensionality reduction. Data exploration of high dimensional dataset can be very tricky. However, it is often possible to *decrease* the dimensionality of the problem

1. <http://www.openblas.net/>

Table 1: Pipeline building blocks available in **Adenine**. See **Adenine** documentation for a comprehensive description.

Step	Algorithms	Ref.
Imputing	mean median most frequent KNN	(Troyanskaya et al., 2001)
Preprocessing	recentering standardize normalize min-max	
Dimensionality reduction	PCA incremental PCA randomized PCA kernel PCA isomap locally linear embedding spectral embedding multidimensional scaling t-distributed stochastic neighbor embedding	(Jolliffe, 2002) (Ross et al., 2008) (Halko et al., 2011) (Schölkopf et al., 1997) (Tenenbaum et al., 2000) (Roweis and Saul, 2000) (Ng et al., 2002) (Borg and Groenen, 2005) (Van der Maaten and Hinton, 2008)
Clustering	k-means affinity propagation mean shift spectral hierarchical	(Bishop, 2006) (Frey and Dueck, 2007) (Comaniciu and Meer, 2002) (Shi and Malik, 2000) (Friedman et al., 2001)

estimating by means of different strategies, a low-dimensional embedding in which the data lie. **Adenine** offers a set of linear and nonlinear dimensionality reduction and manifold learning algorithms (see Table 1).

Step 3: Unsupervised clustering. Besides offering a wide range of clustering techniques, **Adenine** implements strategies and heuristics to automatically estimate parameters that yield the most suitable cluster separation. The optimal parameter selection of centroid-based algorithms follows the B -fold cross-validation strategy presented in Algorithm 1, where $\mathcal{S}(X, y)$ is the mean silhouette coefficient (Rousseeuw, 1987) for all input samples. Clustering parameters for affinity propagation, that is the *preference* (Frey and Dueck, 2007) and for k-means techniques, that is the *number of clusters* (Bishop, 2006) can be automatically extracted, while mean shift (Comaniciu and Meer, 2002) has an implicit cluster discovery. For hierarchical (Friedman et al., 2001) and spectral clustering (Shi and Malik, 2000) no automatic discovery of clustering parameters is offered. However, **Adenine** generates graphical aids to evaluate clustering performance with fixed parameters such as, respectively, dendrogram tree and eigenvalues of the Laplacian of the affinity matrix plots.

Algorithm 1 Automatic discovery of the optimal clustering parameter.

```

1: for clustering parameter  $k$  in  $k_1 \dots k_K$  do
2:   for cross-validation split  $b$  in  $1 \dots B$  do
3:      $X_b^{tr}, X_b^{vld} \leftarrow b$ -th training, validation set
4:      $\hat{n} \leftarrow$  fit model on  $X_b^{tr}$ 
5:      $\hat{y} \leftarrow$  predict labels of  $X_b^{vld}$  according to  $\hat{n}$ 
6:      $s_b \leftarrow$  evaluate silhouette score  $\mathcal{S}(X_b^{vld}, \hat{y})$ 
7:   end for
8:    $\bar{S}_k = \frac{1}{B} \sum_{i=1}^B s_i$ 
9: end for
10:  $k_{opt} = \arg \max_k (\bar{S}_k)$ 

```

3. Usage Example

In this section we show how to use **Adenine** to perform an exploratory analysis on a relatively small dataset. Once **Adenine** is installed, all we need to do is to execute the **Python** script `ade_run.py` specifying as single input argument a configuration file (with `.py` extension) which should look like the snippet below.

```

1 from adenine.utils import data_source
2 X, y, feats, classes = data_source.load('custom', 'data.csv', 'labels.csv')
3 step1 = {'Normalize': [True, {'norm': 'l2'}]} # Preprocessing
4 step2 = {'KernelPCA': [True, {'kernel': ['rbf'], 'n_components': 3, 'gamma':
5 2}], 'Isomap': [True, {'n_components': 3}]} # Dimensionality reduction
6 step3 = {'KMeans': [True, {'n_clusters': ['auto']}]} # Clustering

```

Each `step` variable refers to a `dict` having the name of the building block as key and a `list` as value. Each list has a boolean *on/off* trigger in first position followed by a `dict` of keyword arguments for the class implementing the correspondent method. When more than one method is specified in a single step (or a single parameter is passed as `list`) **Adenine** generates the pipelines made by all possible combinations. For a comprehensive description of options specifiable in the configuration file we refer to **Adenine** documentation and tutorials². The configuration file above generates two pipelines with similar structure. They both have ℓ^2 -normalized samples, projected on a three-dimensional space by Gaussian KPCA with $\gamma = 2$ (pipeline 1) and isomap (pipeline 2); on the dimensionality-reduced dataset a k-means clustering with automatic cluster discovery (as in Algorithm 1) is eventually performed. Results of this first step are all stored in a single output folder. Once the analysis are completed, plots and reports can be automatically generated running the **Python** script `ade_analysis.py` specifying the output folder previously created as single input argument. Figure 1 shows one of several possible comparisons between the two pipelines.

2. www.slipguru.unige.it/Software/Adenine

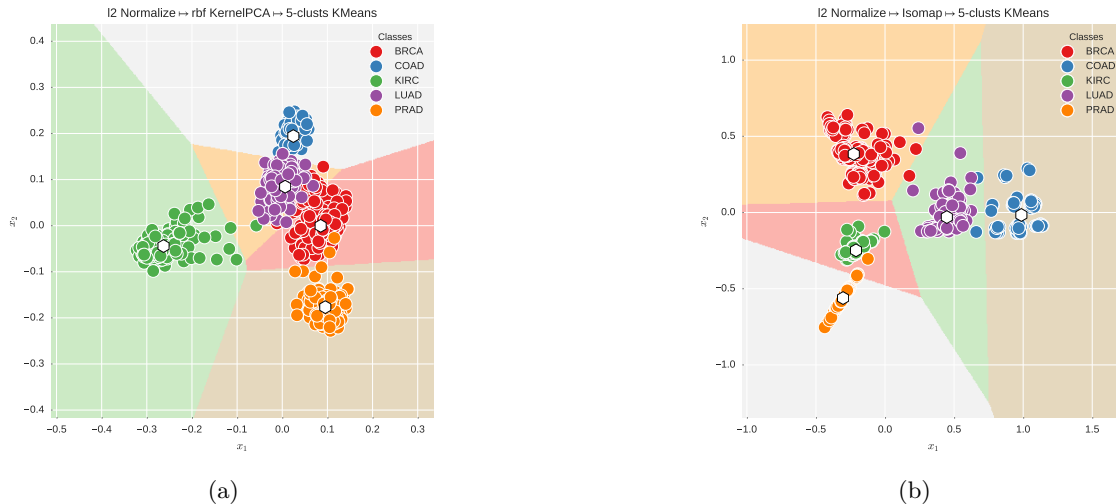


Figure 1: K-means performance after two different nonlinear projections. Data-points colors refer to real classes, while backgrounds are colored according to clustering predictions. The dataset is composed by a random extraction of 801 samples (with dimension 20531) measuring RNA-Seq gene expression of patients affected by 5 different types of tumor: breast invasive carcinoma (BRCA), kidney renal clear cell carcinoma (KIRC), colon (COAD), lung (LUAD) and prostate adenocarcinoma (PRAD). This reduced dataset is available from **Adenine** documentation website and it comes from the cancer genome atlas pan-cancer analysis project (Weinstein et al., 2013). In both cases our algorithm automatically discovers the correct number of clusters, even if the isomap projection improves the clustering performance.

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