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ADENINE — A Data ExploratioN pIpeliNE

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Abstract

In this paper we introduce `Adenine`, a machine learning `Python` framework for data exploration. The main goal of `Adenine` is twofold: helping researchers and data scientists achieving a first and quick overview on the main structures underlying their data and choosing 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 released under FreeBSD license and it can be downloaded from http://slipguru.github.io/adenine/.

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 immediate, non-trivial to extract or even completely absent. In these situations, a preliminary data exploration step is not only 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.

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. Although its interface is designed to be Mac OS X specific, 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, hence it requires the user to manually create each pipeline. On the other hand, 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 an 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.

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 2).

Step 0: Missing values imputing. In real-world datasets groups of entries are often missing. In order to cope with this issue we developed in `Adenine` an improved version of the `Imputer` class offered by `scikit-learn`. Our extension adds a k-nearest neighbor (KNN) imputing method to the pre-existent features-wise *mean*, *median* and *most frequent* value strategies. We chose to add the KNN imputing method to the *naïve* strategies offered by `scikit-learn` because of the robustness demonstrated in the microarray reconstruction experiments described in (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 can sometimes have a negative influence on the behavior of dimensionality reduction and clustering techniques. To tackle this issue `Adenine` offers four different strategies: (i) *Recenter*: transforming samples in order to have zero-mean; (ii) *Standardize*: transforming recentered samples in order to have unit-variance; (iii) *Normalize*: scaling samples in order to have ℓ^p unitary norm (with $p = 1$ or 2); (iv) *MinMax*: scaling features to a given range.

Step 2: Dimensionality reduction. Data exploration of high dimensional dataset can be very tricky. Visualizing samples in high dimension is much less intuitive than

Table 1: Pipeline building blocks available in `Adenine`. Correspondent references are not specified for methods defined Section 2.

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

representing them in two or three-dimensional plots. However, it is often possible to *decrease* the dimensionality of the problem estimating, by means of different strategies, a low-dimensional embedding in which the data lie. To accomplish this task `Adenine` offers a set of linear and nonlinear dimensionality reduction and manifold learning algorithms (see Table 1).

Step 3: Unsupervised clustering. Cluster analysis is the last step of our pipelines. `Adenine` offers strategies ad heuristics to automatically estimate the parameter that yields 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. The tuning parameter for the affinity propagation technique (Frey and Dueck, 2007) is the so-called *preference* and it affects the number of discovered clusters. For k-means (Bishop, 2006) the tuning parameter is directly the *number of clusters*, 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 number of clusters discovery is offered. However, graphical aids to evaluate the performance with

fixed parameters are generated as, respectively, dendrogram tree and eigenvalues of the Laplacian of the affinity matrix plot.

Algorithm 1 Automatic discovery of the optimal clustering parameter.

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

In order to perform exploratory analysis on large datasets, we took advantage of different parallel computing paradigms. `Adenine` pipelines are designed to be independent from each other, therefore they all run in parallel as separate `Python` processes on different cores. Moreover, since `Adenine` makes large use of `numpy` and `scipy`, it automatically benefits from their bindings with optimized linear algebra libraries (such as OpenBLAS[1] or Intel® MKL).

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.

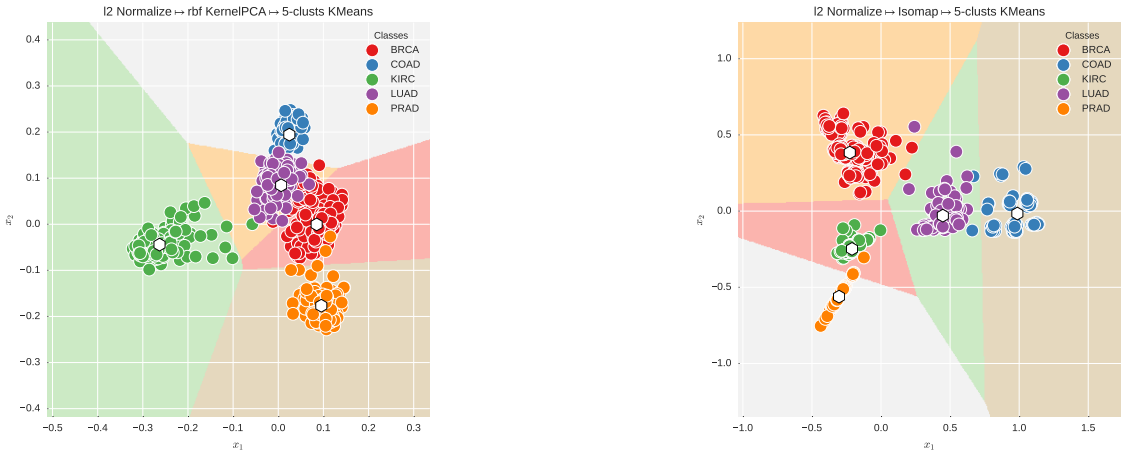
```
from adenine.utils import data_source
X, y, feats, classes = data_source.load('custom', 'data.csv', 'labels.csv')
step1 = {'Normalize': [True, {'norm': 'l2'}]} # Preprocessing
step2 = {'KernelPCA': [True, {'kernel': ['rbf'], 'n_components': 3, 'gamma':
2}], 'Isomap': [True, {'n_components': 3}]} # Dimensionality reduction
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, `Adenine` takes automatically care of implementing the pipelines made by all possible combinations. Several other options can be specified in the configuration file, we refer to `Adenine` documentation and tutorials[2] for a comprehensive description. So, using the configuration file above, `Adenine` will generate two pipelines

1. http://www.openblas.net/
2. www.slipguru.unige.it/Software/Adenine

with similar structure. They will 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.

The 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. In Figure 1, one of several possible comparisons between the two pipelines is presented.



(a) (b)

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 analyzed in this experiment is 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). We can notice that in both cases our algorithm automatically discovers the correct number of clusters, although the isomap projection improves the clustering performance.

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