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ADENINE: A Data ExplorationN pIpeliNE

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Abstract

ADENINE is a machine learning 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 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 available at `http://slipguru.github.io/adenine/` under FreeBSD license.

Keywords: data exploration, unsupervised learning, dimensionality reduction, clustering

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. 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.

In the last few years, a fair number of data exploration software and libraries were released. Roughly, 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 data sets. *Divvy* is a light framework; however, its collection of C/C++ algorithm implementations does not cover common strategies such as kernel principal component analysis (Schölkopf et al., 1997) or hierarchical clustering (Friedman et al., 2001) and it does not offer strategies to perform automatic

Step	Algorithm	Reference
Imputing	mean	
	median	
	most frequent	
	k-nearest neighbors	(Troyanskaya et al., 2001)
Preprocessing	recentering	
	standardize	
	normalize	
	min-max	
Dimensionality reduction	principal component analysis (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)

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

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).

In this paper, 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. Data imputing, preprocessing, dimensionality reduction and clustering strategies are considered as building blocks for constructing data analysis pipelines. The user is simply required to specify input data and to select blocks. ADENINE, then, takes care of generating and running the pipelines obtained by all possible combinations of the selected blocks. 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 Python library freely available online.

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 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).

ADENINE offers an improved version of the `Imputer` class provided by SCIKIT-LEARN to cope with real-world data sets, where entries are often missing. Our extension adds a k-nearest neighbors imputing method (Troyanskaya et al., 2001) to the pre-existent feature-wise *mean*, *median* and *most frequent* strategies.

ADENINE presents different data preprocessing strategies to tackle undesired effects that may arise from heterogeneous measures possibly lying in very different numerical range.

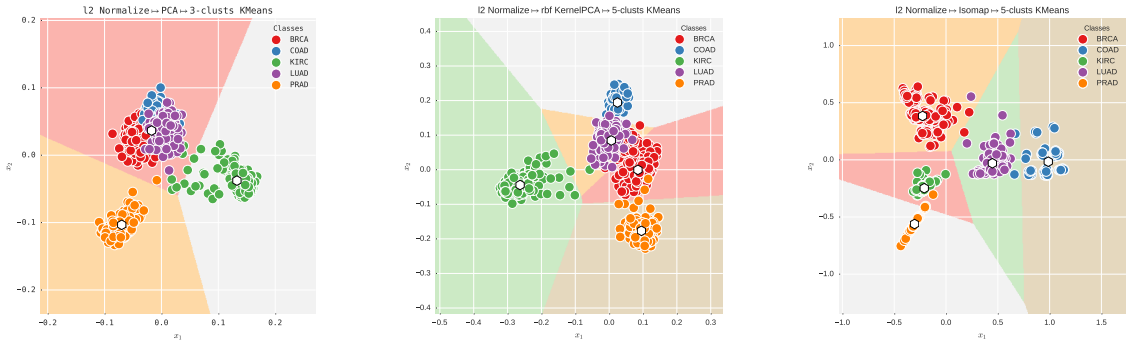
ADENINE includes a set of linear and nonlinear dimensionality reduction and manifold learning algorithms particularly suited for the exploration of high dimensional data set that otherwise can be very tricky. In fact, it is often possible to *decrease* the dimensionality of the problem estimating a low-dimensional embedding in which the data lie.

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.

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
$k_{opt} = \arg\max_k (\bar{S}_k)$

For affinity propagation (Frey and Dueck, 2007) and k-means (Bishop, 2006) clustering parameters can be automatically defined (*preference* and *number of clusters*, respectively). 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, graphical aids are generated to evaluate clustering performance such as dendrogram tree and eigenvalues of the Laplacian of the affinity matrix plots, respectively.



(a) (b) (c)

Figure 1: k-means on three different 2D projections of an RNA-Seq data set.

3. Usage Example

Figure 1 shows one of several possible comparisons between three pipelines on an RNA-Seq gene expression data set available both on UCI Machine Learning Repository and ADENINE documentation webpage. Exploratory data analysis is performed by executing 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,feat_names,class_names = data_source.load("custom","data.csv","labels.csv")
step1 = {"Normalize":[True,{"norm":"l2"}]} #Preprocessing
step2 = {"PCA":[True,{"n_components":2}],"KernelPCA":[True,{"kernel": ["rbf"], \
"n_components":2,"gamma":2}],"Isomap":[True,{"n_components":2}]} #Dim. Reduction
step3 = {"KMeans":[True,{"n_clusters":["auto"]}]} #Clustering
```

Each `step` variable refers to a dictionary having the name of the building block as key and a list as value. Each list has a *on**off* trigger in first position followed by a dictionary of keyword arguments for the class implementing the corresponding method. When more than one method is specified in a single step, or more than a single parameter is passed as list, ADENINE generates the pipelines composed of all possible combinations. For a comprehensive description of options available in the configuration file we refer to ADENINE documentation and tutorials: `http://slipguru.unige.it/Software/adenine`.

The configuration snippet above generates three pipelines with similar structure. All three of them have ℓ^2-normalized samples, projected on a 2D space by PCA (pipeline a), Gaussian kernel PCA with $\gamma = 2$ (pipeline b) and isomap (pipeline c); on the dimensionality-reduced data set a k-means clustering with automatic cluster discovery is eventually performed as in Algorithm 1. Results of such pipelines are all stored in a single output folder. Once the process is completed, plots and reports can be automatically generated running `ade_analysis.py` with the output folder previously created as the only input argument.

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