# ADENINE — A Data Exploration plpeline

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#### Abstract

Abstract here.

**Keywords:** Exploratory data analysis, unsupervised learning, dimensionality reduction, clustering

#### 1. Introduction

# 2. Implementation

From an implementative standpoint, adenine is built upon the concept of *pipeline*, that is a sequence of four fundamental steps: (i) missing values imputing, (ii) data preprocessing, (iii) dimensionality reduction and (iv) clustering (see Figure 1).

Figure 1: adenine workflow

For each step, a fair number of off-the-shelf algorithm implementations are available (see Table 2). The vast majority of such implementations is inherited, or extended from scikit-learn (Pedregosa et al., 2011), a collection of machine learning tools implemented in Python. For the first step, adenine offers an extended version of the sklearn.preprocessing.Imputer class that adds the KNN imputing method to the pre-existent features-wise mean, median and most frequent choices.

In order to obtain exploratory analysis of fairly big datasets, adenine exploits the use of parallel computing in several ways. Each pipeline is designed to be completely independent from each other

## 3. Experiments and results

To assess the quality of the obtained results, we tested adenine on a set of synthetic and real dataset.

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## 4. Conclusions

Table 1: Pipelines building blocks and relative references (which are not reported when the definition is given in Section 2).

| Step                     | Algorithms   | Ref.   |
|--------------------------|--|--|
| Imputing                 | Mean<br>Median<br>KNN  | (Troyanskaya et al., 2001)   |
| Preprocessing            | Recentering Standardize Normalize MinMax   |  |
| Dimensionality reduction | Principal component Analysis (PCA) Incremental PCA Randomized PCA Kernel PCA Isomap Locally linear embedding Spectral embedding Multidimensional scaling t-Distributed Stochastic Neighbor Embedding (t-SNE) | (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)<br>(Frey and Dueck, 2007)<br>(Comaniciu and Meer, 2002)<br>(Shi and Malik, 2000)<br>(Friedman et al., 2001)   |

## References

Christopher M Bishop. Pattern recognition. Machine Learning, 2006.

Ingwer Borg and Patrick JF Groenen. Modern multidimensional scaling: Theory and applications. Springer Science & Business Media, 2005.

Dorin Comaniciu and Peter Meer. Mean shift: A robust approach toward feature space analysis. Pattern Analysis and Machine Intelligence, IEEE Transactions on, 24(5):603–619, 2002.

Brendan J Frey and Delbert Dueck. Clustering by passing messages between data points. science, 315(5814):972–976, 2007.

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- Jerome Friedman, Trevor Hastie, and Robert Tibshirani. The elements of statistical learning, volume 1. Springer series in statistics Springer, Berlin, 2001.
- Nathan Halko, Per-Gunnar Martinsson, and Joel A Tropp. Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions. *SIAM review*, 53(2):217–288, 2011.
- Ian Jolliffe. Principal component analysis. Wiley Online Library, 2002.
- Andrew Y Ng, Michael I Jordan, Yair Weiss, et al. On spectral clustering: Analysis and an algorithm. Advances in neural information processing systems, 2:849–856, 2002.
- F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.
- David A Ross, Jongwoo Lim, Ruei-Sung Lin, and Ming-Hsuan Yang. Incremental learning for robust visual tracking. *International Journal of Computer Vision*, 77(1-3):125–141, 2008.
- Sam T Roweis and Lawrence K Saul. Nonlinear dimensionality reduction by locally linear embedding. *Science*, 290(5500):2323–2326, 2000.
- Bernhard Schölkopf, Alexander Smola, and Klaus-Robert Müller. Kernel principal component analysis. In *Artificial Neural NetworksICANN'97*, pages 583–588. Springer, 1997.
- Jianbo Shi and Jitendra Malik. Normalized cuts and image segmentation. *Pattern Analysis and Machine Intelligence*, *IEEE Transactions on*, 22(8):888–905, 2000.
- Joshua B Tenenbaum, Vin De Silva, and John C Langford. A global geometric framework for nonlinear dimensionality reduction. *science*, 290(5500):2319–2323, 2000.
- Olga Troyanskaya, Michael Cantor, Gavin Sherlock, Pat Brown, Trevor Hastie, Robert Tibshirani, David Botstein, and Russ B Altman. Missing value estimation methods for dna microarrays. *Bioinformatics*, 17(6):520–525, 2001.
- Laurens Van der Maaten and Geoffrey Hinton. Visualizing data using t-sne. *Journal of Machine Learning Research*, 9(2579-2605):85, 2008.