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AutoClassWeb: a simple web interface for Bayesian clustering

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Abstract

Summary: Data clustering is a common exploration step in the omics era, in particular in genomics and proteomics. Bayesian clustering is a powerful algorithm that can classify several thousands of genes or proteins. AutoClass C, its original implementation handles missing data and determines automatically the best number of clusters but is unfortunately not user-friendly.

Availability and Implementation: We propose AutoClassWeb an easy-to-use web interface for Bayesian clustering with AutoClass. The project is implemented in Python and is published under the 3-Clauses BSD license. This web application is packaged as a Docker image and available in the BioContainer registry for better reproducibility. The code is available at <https://github.com/pierrepo/autoclassweb> along with a detailed documentation.

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1 Motivation

In the omics era, data clustering is a common step in data exploration. Many clustering algorithms are available for this task. Bayesian clustering is such an algorithm and one of its implementation in C (AutoClass C) has been published in 1996 at the Ames Research Center at NASA ([Cheeseman and Stutz, 1996]). The idea behind Bayesian clustering and the AutoClass algorithm is to find a classification that fits the data with the highest probability. The AutoClass algorithm provides some additional and interesting features: it handles missing data and determines automatically the best number of clusters.

AutoClass C has been used in a wide variety of applications (see [Achcar *et al.*, 2009] and [Camadro and Poulain, 2019] for a detailed list). In the context of genomics or proteomics, where several thousands of genes or proteins need to be analyzed at once, this kind of algorithm is pertinent. However, AutoClass C, originally developed by physicists, is not user-friendly: command line interface only, 32-bit binaries, results difficult to parse for subsequent analysis...

More than 10 years ago, Achcar *et al.* published AutoClass@IJM ([Achcar *et al.*, 2009]), a web interface for AutoClass C. This web service drastically simplified the use of AutoClass

C and widen its adoption, notably in biology (according to Google Scholar, this paper has been cited more than 40 times). Unfortunately, this tool is not maintained anymore, and its source code is not publicly available.

To continue to offer this powerful clustering method to the community, we propose AutoClassWeb, a new easy-to-use open-source web-based interface for AutoClass C.

2 Implementation

2.1 AutoClassWrapper

AutoClassWeb utilizes AutoClassWrapper ([Camadro and Poulain, 2019]), a Python wrapper for the AutoClass C algorithm. This wrapper facilitates the preparation and quality control of data, runs the actual classification, and eventually, prepare results in format that allow further analysis.

2.2 Web interface

AutoClassWeb is written in Python and uses the Flask module to build the web interface users interact with.

For better reproducibility and sustainability, AutoClassWeb is packaged in a Docker image stored in the BioContainers ([da Veiga Leprevost *et al.*, 2017]) registry.

The source code of AutoClassWeb is open-source and released under the BSD-3-Clause license, and available on the GitHub development platform <https://github.com/pierrepo/autoclassweb>.

The web service itself has been designed to be easy to use. There is no user authentication and by default, results are kept 30 days before being deleted. A comprehensive *help* page provides all the help and guidance the user might need.

Thanks to Docker technology, AutoClassWeb can be easily deployed on a local machine or on a public web server. For this purpose and to lower the burden of installation, we provide two companion GitHub repositories with detailed instructions, for local installation (<https://github.com/pierrepo/autoclassweb-app>) and server installation (<https://github.com/pierrepo/autoclassweb-server>).

2.3 Code archive

AutoClassWeb source code in its current version 2.2.1 is archived in Software Heritage with the following reference:

swh:1:dir:173e846a5137a4b498ca7da9eca980790631bc1a

3 Usage & performance

3.1 Data submission

Input data must be formatted as tab-separated values (TSV) files. The first line must be a header with column names that are required to be unique. The first column must be gene/protein/object names.

Missing data are allowed and must be encoded with an empty value (*i.e.* nothing).

Three categories of data are supported:

- *real location*: negative and positive values such as position, elevation, microarray log ratio...

- *real scalar*: singly bounded real values, typically bounded below at zero (*i.e.*: length, weight, age).
- *discrete*: qualitative data. For instance, color, phenotype, name...

If the initial input dataset contains several types of data (real scalar, real location, discrete), it is advisable to split this dataset in multiple datasets with homogeneous data type.

3.2 Clustering

Upon submission, input data are quality checked and formatted to be usable by AutoClass C. The web interface provides a quick summary (*Hide/show logs*) of input data, a unique job identifier for the run and a link to the status page.

The status page lists running, failed and completed runs with their respective identifier (*Job name*), creation date, status and running time (in hours, minutes and seconds).

This page auto-refreshes itself every 5 minutes (by default).

3.3 Results

Once a job is completed, a green button lets the user download results. Results are bundled in a zip archive with the following files:

- `xxx_autoclass_out.cdt` and `xxx_autoclass_out_withproba.cdt` can be open with Java TreeView ([Saldanha, 2004]), where `xxx` stands for the unique identifier of the job. The file `xxx_autoclass_out_withproba.cdt` exhibits the probability for each gene/protein/object to belong to each class.
- `xxx_autoclass_out_stats.tsv` contains means and standard deviations of numeric columns (real scalar and real location) for each class.
- `xxx_autoclass_out_dendrogram.png` is a dendrogram plot that visualizes the distance between all classes.
- `xxx_autoclass_out.tsv` contains all the data with the class assignment and membership probabilities for all classes. This file is in the Tab-separated values format and can then easily be parsed with Excel, R, Python...

3.4 Performance

The AutoClass C algorithm has been designed to run on a single CPU (core) only.

The running time depends exponentially on the size of the input dataset. Figure 1 illustrates the running time as a function of the number of lines in the input dataset (all with 64 columns).

Note that a parallel version of AutoClass C has been published ([Pizzuti and Talia, 2003]). Unfortunately, the source code is not available, and the project does not appear to have been continued.

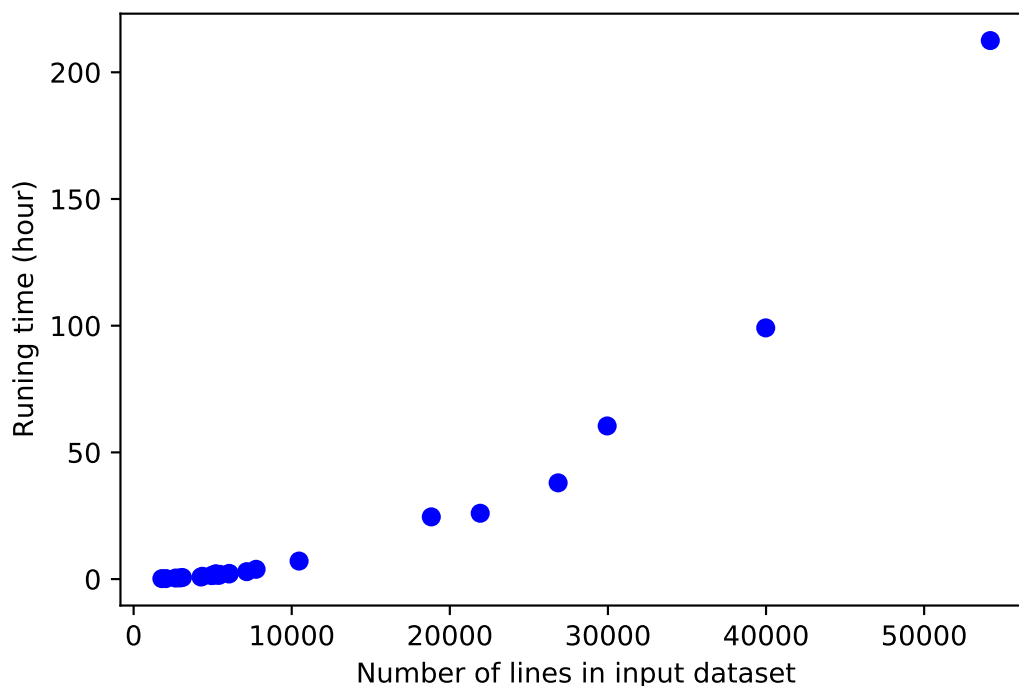


Figure 1: Running time (in hour) vs dataset size.

4 Discussion & conclusion

Data clustering is an essential step of most modern omics analysis. The AutoClass algorithm albeit very powerful is not very used, mostly because its original implementation AutoClass C is not user-friendly. AutoClassWeb provides an easy-to-use web-based user interface for Autoclass. The project is open-source, packaged in a Docker image available in BioContainers for better reproducibility and sustainability.

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