









Unsupervised random forests of clustering trees

Master 2 Internship

Background

Random Forests¹ (RF) are a powerful machine learning technique. They are most often used for prediction, either in a regression context (with a continuous outcome) or in a classification context (with a categorical outcome). At their core, RF build upon classification and regression trees (CART), overcoming their drawbacks thanks to both i) random sampling (with replacement) of the observations in each tree, and ii) random sampling of variables (without replacement) at each tree node.

RF-related approaches have already been proposed in unsupervised contexts. Notably, some approaches generate synthetic data and apply RF to discriminate between those and real data, finally obtaining a proximity matrix^{2,3}. Besides, Yan et al. propose to apply the k-means on several resampled versions of the data to obtain a set of partitions, that are then all aggregated (through spectral clustering) — an algorithm that takes some inspirations from RF⁴. However, none of these previous works actually propose an extension of RF suitable to clustering problems.

Divisive clustering trees can be constructed for unsupervised classification (or clustering), by minimizing inertia while staying interpretable as decision trees⁵. This approach is implemented in the divclust **@** package. We propose to use those to propose unsupervised random forests of clustering trees.

Subject

This internship aims at leveraging both divisive clustering trees as well as the RF framework to propose a new clustering algorithm. A key contribution of this internship will be the definition of an aggregation strategy of clusterings across trees, which can rely on a consensus similarity matrix and its postprocessing (not unlike solutions adopted in non parametric Bayesian clustering approaches⁶).

Objectives

1. Implement divclust random forests, featuring the ensemble clustering (through partition aggregation across trees).











- 2. Investigate the impact of the RF tuning parameters on the results in numerical studies, in particular the number of trees, the number of randomly selected variables per nodes, and the trees depth.
- 3. Apply this new clustering approach to high-dimensional transcriptomics data in the context of vaccine development against EBOLA⁷, HIV and COVID-19⁸.

Required skills:

- Good knowledge in Biostatistics and/or Statistics
- Programming proficiency with **Q**
- An interest for biomedical research, and in particular in vaccine research
- English proficiency (both written and spoken)
- Scientific curiosity
- Master 1/Bachelor/Engineering school with a major in Biostatistics and/or Statistics

Hosting laboratory:

SISTM team

Inria Bordeaux Sud-Ouest & Inserm U1219 Bordeaux Population Health

Location:

Inserm U1219 Bordeaux Population Health research center – SISTM team Université de Bordeaux – ISPED 146, rue Léo Saignat 33076 Bordeaux Cedex

Duration:

Internship of 4 to 6 month available starting from January 2024.

Compensation:

Intern gratification according to the official recommendations (15% of social security ceiling, i.e. around 685€/month).

Contact:

Send a detailed CV and a motivation letter to both **Boris Hejblum** [boris.hejblum@u-bordeaux.fr] & **Robin Genuer** [robin.genuer@u-bordeaux.fr]

Bibliography

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- 2. Shi, T. & Horvath, S. Unsupervised learning with random forest predictors. *Journal of Computational and Graphical Statistics* **15**, 118–138 (2006).
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- 5. Chavent, M., Lechevallier, Y. & Briant, O. DIVCLUS-t: A monothetic divisive hierarchical clustering method. Computational Statistics & Data Analysis 52, 687–701 (2007).
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- 7. Rechtien, A. et al. Systems Vaccinology Identifies an Early Innate Immune Signature as a Correlate of Antibody Responses to the Ebola Vaccine rVSV-ZEBOV. Cell Reports 20, 2251–2261 (2017).
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