**grend: An R Package for Model-Based Clustering by Greedy Maximization of the Integrated Classification Likelihood**

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**Abstract**

The *grend* package implements the general and flexible framework of Côme, Jouvin, Latouche, and Bouveyron (2021) for model-based clustering in the R language. Based on the direct maximization of the exact Integrated Classification Likelihood with respect to the partition, it allows jointly performing clustering and selection of the number of groups. This combinatorial problem is handled through an efficient hybrid genetic algorithm, while a final hierarchical step allows accessing coarser partitions and extract an ordering of the clusters. This methodology is applicable in a wide variety of latent variable models and, hence, can handle various data types as well as heterogeneous data. Classical models for continuous, count, categorical and graph data are implemented, and new models may be incorporated thanks to S4 class abstraction. This paper introduces the package, the design choices that guided its development and illustrates its usage on practical use-cases.

**Keywords**: R, model-based, clustering, hierarchical, classification likelihood, genetic algorithms.

**1. Introduction**

Clustering consists in the unsupervised task of grouping a set of objects into distinct groups or clusters. Unveiling relevant structure in datasets, it holds an important part in modern data analysis, with a wide range of applications involving data of different nature. Grounded on a statistical approach, model-based clustering provides a flexible method capable of handling the variety and complexity of modern data such as continuous, count, graphs or mixed data...
in a common framework using finite mixtures or stochastic block models (Bouveyron, Celeux, Murphy, and Raftery 2019). The greed R package, introduced in this paper, builds on this general framework and provides a generic method for clustering various types of data based on the maximization of the Integrated Classification Likelihood (Côme et al. 2021). The method is versatile and thanks to the exploration capabilities of an hybrid genetic algorithm, it does not rely on a carefully chosen - and potentially costly and model dependent - initialization procedures. Throughout the paper, we will discuss specific instances of models and give suitable references for related works and packages for each of the considered data type: count, continuous, mixed-type and graph data.

The clustering problem has been the focus of a lot of attention in the last decades, and the R (R Core Team 2021) community have been a driving force1 with the development of many packages taking advantage of the R programming language capacities in handling and visualizing data. These packages can be divided into three main categories:

1. On the one hand, there are packages implementing distance-based clustering, relying on some ad hoc notion of similarity between observations. Working with vector-valued observations, the well-known k-means (MacQueen 1967) algorithm is implemented in the stats and ClusterR (Mouselimis 2021) packages for Euclidean distances. Refined similarity metrics for k-means such as kernels are available in the kernlab package (Karatzoglou, Smola, Hornik, and Zeileis 2004), together with an implementation of the spectral clustering algorithm (Ng, Jordan, and Weiss 2002). Other partitional methods working with k-medoids and arbitrary distance functions are implemented in the cluster package (Maechler, Rousseeuw, Struyf, Hubert, and Hornik 2021). Finally, the clustMixType (Szepannek 2018) package allows to cluster mixed type data composed of numeric and categorical variables. On the side of graph clustering algorithms, the well-known Louvain algorithm (Blondel, Guillaume, Lambiotte, and Lefebvre 2008) based on modularity maximization is implemented in the igraph (Csardi and Nepusz 2006), and the spectral clustering algorithm is also very popular for clustering binary or weighted adjacency matrices.

2. On the other hand, packages implementing model-based clustering fit a probabilistic model to the data. We distinguish between two main strategies for statistical inference:

(a) Frequentist: The first strategy casts clustering as a parameter estimation problem, traditionally dealt with via maximum likelihood, and most of the time solved with the help of some (possibly variational) EM procedure. The clustering comes as a byproduct since a partition can then be obtained via its posterior distribution given the observation and the point estimates. This approach is implemented in various R packages such as Mclust (Scrucca, Fop, Murphy, and Raftery 2016) for Gaussian mixture models, mixtools (Benaglia, Chauveau, Hunter, and Young 2009) for multinomial mixtures, poLCA (Linzer and Lewis 2011) for mixture of categorical distributions, and blockmodels (Leger, Barbillon, and Chiquet 2020) and sbm (Chiquet, Donnet, and Barbillon 2021) for the simple and bipartite stochastic block models (SBM). The Rmixmod (Langrognet, Lebret, Poli, Iovleff, Auder, and Iovleff 2020) package also provides an R interface with the MIXMOD software

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1 A snapshot highlighting the numerous contributions made is available on a dedicated CRAN “Task Views” page on clustering: https://cran.r-project.org/web/views/Cluster.html
to fit Gaussian or categorical mixtures for continuous or count data clustering. Somewhat closer to our contribution, the flexmix package (Grün and Leisch 2008) also proposes a general framework for fitting mixture models on, possibly heterogeneous, multivariate data using maximum likelihood and an EM procedure. However, it does not cover graph data clustering with SBMs since the latter cannot be cast as simple mixture models and cannot be estimated through regular EM procedures. Their approach is extensible, and new mixture models may be implemented via an S4 class representation of their M-step. While the algorithms strongly differ, our greed package proposes a similar interface, with the possibility to implement new models as S4 classes without impacting the main functions and API.

(b) *Bayesian:* The second strategy relies on Bayesian inference, seeking to accurately estimate the posterior distribution of the model parameters and cluster memberships, usually via Markov chain Monte Carlo methods (MCMC, Robert and Casella 2013). Some of these methods allow inferring the number of clusters through a non-parametric Dirichlet process prior on the group proportions. The main packages implementing Bayesian model-based clustering are rjags (Plummer, Stukalov, and Denwood 2019) and rstan (Stan Development Team 2020), respectively R interface to the JAGS and STAN softwares, each having dedicated modules for finite mixture modelling. Other packages directly focus on mixture modelling such as Bmix (Taddy 2016), bmixture (Mohammadi 2021) or IMIFA (Murphy, Viroli, and Gormley 2021). Note that, in addition to heavy computations, the two principal difficulties of MCMC inference for clustering are label switching and the resulting multimodality of the posterior.

Beyond the R community, most of the aforementioned methods are implemented in popular Python modules. Without being exhaustive, we mention the scikit-learn module (Pedregosa, Varoquaux, Gramfort, Michel, Thirion, Grisel, Blondel, Prettenhofer, Weiss, Dubourg, Vanderplas, Passos, Cournapeau, Brucher, Perrot, and Duchesnay 2011) implementing standard algorithms for multivariate data clustering in its cluster submodule, and the graph-tool module (Peixoto 2014) which implements Bayesian inference for the stochastic block model and its variants.

Our approach lies in between the frequentist and Bayesian approaches, which, while efficient, can be computationally intensive as they require to explore a high-dimensional parameter space, and possibly perform model selection by running the inference procedure on a grid of values for $K$ i.e. the number of clusters. A contrario, we focus on clustering rather than points or posterior estimates of the model parameters, by maximizing an *exact* version of the Integrated Classification Likelihood (ICL, Biernacki, Celeux, and Govaert 2000) directly with respect to the partition. Originally used as a model selection criterion in frequentist settings, the exact ICL is rooted in the Bayesian framework and consists in the joint distribution of the observations and the partition with all other parameters analytically integrated out by a suitable choice of prior distributions. The genetic algorithm of Côme et al. (2021) then solves the highly combinatorial problem of maximizing this objective function with respect to the partition, allowing $K$ to be variable, hence performing clustering and model selection altogether while avoiding grid procedures.

In a complementary step, the greed package implements a model-based hierarchical method
Based on the maximization of a modified ICL criterion. Starting from an initial solution provided by the genetic algorithm, it extracts a hierarchy of nested partitions in an ascendant fashion, by finding the best merge according to this new criterion, similarly to the \texttt{hclust()} function of the \texttt{stats} package. This second step unveils hierarchical structures present in the data, which is useful both for interpretation and visualization (Everitt, Landau, and Leese 2011, Section 4), while also giving a dendrogram representation of the hierarchy along with a meaningful pseudo-ordering of the clusters.

The paper is organized in the following way. Section 2 briefly introduces the unified statistical framework considered by Côme \textit{et al.} (2021) and gives specific instances of models, namely finite mixtures and stochastic block models. Then, Section 3 describes the genetic and hierarchical algorithms along with practical package implementation details. Finally, Section 4 presents an overview of the package’s API and practical guidelines, while Section 5 demonstrates its flexibility on practical use-cases, with real-data studies for continuous, categorical, graph and mixed-type data.

2. Model-based clustering

We begin with a brief reminder on model-based approaches to clustering. We will denote as $X$ the set of observations, which can be a collection of $n$ vectors in $\mathbb{R}^p$ in the case of mixture modelling, or an $n \times n$ adjacency matrix in the case of graph clustering. The unobserved partition of $\{1, \ldots, n\}$ will be denoted as $Z = \{z_1, \ldots, z_n\}$ where $z_i$ is a binary vector of size $K$ indicating cluster membership of object $i$.

2.1. Discrete latent variables models

Model-based clustering can be decomposed in a two-stage generative process. First, the partition $Z$ is drawn from a product of multinomial distributions with parameter $\pi$, the latter quantifying the a priori probability to belong to each of the $K$ groups. Second, observations are drawn conditionally on the partition, according to some parametric distribution with parameters $\theta$ depending on the clusters assignments.

Depending on the context, observations may be continuous or discrete vectors in dimension $p$, or edges in a graph. Thus, there are a variety of observational models that can be handled which such an approach. All the models handled by the \texttt{greed} package share the common hypothesis of conditional independence given the full partition $Z$:

$$p(X, Z \mid \pi, \theta) = \prod_{z \in Z} p(z \mid \pi) \prod_{x \in X} p(x \mid Z, \theta),$$

(1)

Such models are called discrete latent variables models (DLVMs, Côme \textit{et al.} 2021) and popular instances for multivariate data and graph clustering are given in Table 1. For the sake of brevity, we do not detail co-clustering with latent block models (LBM) although it fits the definition of DLVMs and is implemented in \texttt{greed}.

As discussed above, standard frequentist approaches casts clustering as a parameter estimation problem, traditionally dealt with a maximum-likelihood approach solved with the help of some (variational) EM procedure in most cases. The clustering comes as a byproduct since a
partition can then be obtained via the posterior distribution of \( Z \mid X, \hat{\pi}, \hat{\theta} \). This approach is implemented in various R packages such as \texttt{Mclust} (Scrucca et al. 2016) for Gaussian mixture models, \texttt{mixtools} (Benaglia et al. 2009) for multinomial mixtures, \texttt{flexmix} (Grün and Leisch 2008) for general finite mixture models or \texttt{blockmodels} (Leger et al. 2020) for the stochastic block model.

| Model name | Observation type | Observational model: \( X \mid Z \) |
|------------|-----------------|-----------------------------------|
| GMM        | Multivariate continuous: \( X \in \mathbb{R}^{n \times p} \) | \( x_i \mid z_{ik} = 1, \theta_k \sim \mathcal{N}_p(x_i \mid m_k, S_k) \) |
| MoM        | Multivariate discrete: \( X \in \mathbb{N}^{n \times p} \) | \( x_i \mid z_{ik} = 1, \theta_k \sim \mathcal{M}_p(x_i \mid \theta_k) \) |
| SBM        | Graphs: \( X \in \mathbb{R}^{n \times n} \) | \( x_{ij} \mid z_{ik} z_{jl} = 1, \theta_{kl} \sim p(x_{ij} \mid \theta_{kl}) \) |

Table 1: Some standard observational models handled by the \texttt{greed} package: Gaussian mixture model (GMM), mixture of multinomial (MoM) and stochastic block models (SBM) for (possibly weighted) graphs. See Table 3 for a complete list of implemented DLVMs.

### 2.2. Exact Integrated Classification Likelihood

Having derived an estimate of the model parameters, the choice of the number of clusters \( K \) is usually delayed post-inference as a model selection problem (Fruhwirth-Schnatter, Celeux, and Robert 2019, Chapter 7). There exists a large variety of model selection criteria, generally involving a penalized likelihood, such as the Akaike Information Criterion (AIC, Akaike 1974) or the Bayesian Information Criterion (BIC, Schwarz 1978) which are commonly implemented in routine packages. Note that, in this framework, performing clustering and model selection requires to estimate the parameters for a grid of models indexed by \( K \), which can be quite cumbersome, even for moderate size problems, as the computational complexity typically grows with \( K \).

Hereafter, we focus on the ICL of Biernacki et al. (2000), a widely used model selection criterion in the clustering context. Adopting a Bayesian point of view on the model parameters \( \theta \) and \( \pi \), it consists in integrating the latter out hence naturally penalizing for complex models. Introducing a factorized prior \( p(\theta, \pi) = p(\theta \mid \beta)p(\pi \mid \alpha) \) with respective hyperparameters \( \beta \) and \( \alpha \), the ICL writes as:

\[
\text{ICL}(Z; \alpha, \beta) = \log \int p(X \mid \theta, Z)p(\theta \mid \beta) \, d\theta + \log \int p(Z \mid \pi)p(\pi \mid \alpha) \, d\pi. \tag{2}
\]

Such integrals are typically non-analytic and usually approximated via Laplace method, leading to a penalized likelihood criterion à la BIC.

However, it is possible to derive exact version of the ICL by choosing conjugate priors for the model parameters \( p(\theta \mid \beta) \) and \( p(\pi \mid \alpha) \):

\[
\text{ICL}_{ex}(Z; \alpha, \beta) = \log p(X \mid Z, \beta) + \log p(Z \mid \alpha). \tag{3}
\]

The first term of the right-hand side is model-dependent, and must be computed on a case-by-case basis² as it depends on the prior on the observational model parameters \( \theta \).

²Detailed computations of ICL_{ex} for the considered models can be found in the Supplementary Materials of Côme et al. (2021)
However, putting a symmetric Dirichlet prior $p(\pi) = \text{Dir}(\pi \mid \alpha = (\alpha, \ldots, \alpha))$ over the group proportions, the second term is universal to any DLVM and is derived thanks to Dirichlet-Multinomial conjugacy:

\[
\text{ICL}_{\text{ex}}(Z; \alpha, \beta) = \log p(X \mid Z, \beta) + \log \left( \frac{\Gamma(K \alpha) \prod_{k=1}^{K} \Gamma(\alpha + n_k)}{\Gamma(\alpha)^K \Gamma(n + \alpha K)} \right),
\]

where $n_k$ is the number of individuals in cluster $k$.

3. Algorithms

3.1. Greedy maximization of the exact ICL

In contrast to inference-based approaches, the *greed* package bypasses the statistical inference step and focuses on the clustering objective of jointly finding some *hard*-partitioning $Z$ as well as its number of clusters $K$. This is done by solving the maximization of $\text{ICL}_{\text{ex}}$ with respect to both $(Z, K)$:

\[
Z^{(K^*)} \in \arg \max_{K, Z} \text{ICL}_{\text{ex}}(Z, K),
\]

the *greed* package implements several algorithms tackling this problem. Naturally, due to the highly multimodal and combinatorial nature of this discrete problem, the proposed algorithms are not guaranteed to converge to a global maximum, but rather to efficiently explore the space of solutions to find relevant local optima at a reasonable computational time and cost. The default algorithm used by the *greed* package is a hybrid genetic algorithm (GA), introduced in detail in (Côme et al. 2021). Standard GAs evolve a population of solutions by selecting some of the most promising ones, crossing them, and possibly mutating them until a specified number of generations or some stopping criterion is reached. Their capacity to efficiently explore huge space of solutions makes them ideal candidate for discrete combinatorial optimization problems such as in Equation (5). Moreover, in order to improve the exploitation capacity of GAs around local optima, one may hybrid them with efficient local search algorithms (see Eiben and Smith 2004, Chap. 10) such as greedy heuristics based on swaps and merge moves. This is the default approach implemented in the *greed* package, and we detail its most central features as a GA: solution representation and the recombination, mutation and selection operators.

**Solutions as partitions.** Since the $\text{ICL}_{\text{ex}}$ function is invariant under permutations of the cluster indexes, the integer encoding representation in $Z$ is redundant for our optimization problem. This fact is also known as the label switching problem and have an important impact on the design of the recombination (crossover) operator for GA. Indeed, simple recombination operators based on crossover points will not consider this particularity and will completely break the structure of the solution (Hruschka, Campello, Freitas, and Ponce Leon F. de Carvalho 2009), leading to slow evolution of the population of solutions. One solution to circumvent this issue is to define the crossover and mutation operators directly over the space of partitions $\{1, \ldots, n\}$ into $K$ clusters with a variable $K$, denoted as $\mathcal{P} = \{C_1, \ldots, C_K\}$. Such
operators will not suffer from the label switching problems and will therefore not break the structures already found. The hybrid GA used in greed is based on such operators.

Combining two partitions: the crossover operator. The crossover operator, recombining two “parents” solutions into a new “child” one, is based on the cross partition operator. The cross partition of two partitions is simply the partition built by considering all the possible intersections between the elements of the two partitions being crossed. More formally:

$$\mathcal{P}^1 \times \mathcal{P}^2 := \{C^1_i \cap C^2_j, \forall i \in \{1, \ldots, |\mathcal{P}^1|\}, j \in \{1, \ldots, |\mathcal{P}^2|\}\} \setminus \emptyset,$$

with $\mathcal{P}^1 = \{C^1_1, \ldots, C^1_{K^1}\}$ and $\mathcal{P}^2 = \{C^2_1, \ldots, C^2_{K^2}\}$ two partitions of $\{1, \ldots, n\}$. This operator produces a new solution which is a refinement of both solutions being crossed, with at most $|\mathcal{P}^1||\mathcal{P}^2|$ clusters. In practice, the two solutions being crossed will agree on some clusters and the number of new clusters after crossover will be smaller. It also defines the coarser clustering which can lead to either $\mathcal{P}^1$ or $\mathcal{P}^2$ using merge operations, i.e. their first common ancestor in the partition lattice. Thus, in case of under-fitting of both parent partitions, crossing alone may already improve the solution. Finally, while this crossing may create superfluous clusters when done near local maxima of ICLex, the greedy local search based on merges used in the hybrid GA efficiently removes these extra clusters.

Mutation & selection. The remaining aspects to set up concern the selection procedures and the mutation operators. For the selection process, the hybrid GA algorithm uses a classical rank-based selection policy (see Eiben and Smith 2004, p. 81-82). In this scheme, at each step, the $V$ solutions selected for building the next generation are selected according to a probability proportional to their rank in terms of ICLex. Eventually, regarding the mutation operator, the hybrid GA algorithm splits a random cluster in two at random. Indeed, while the greedy heuristic, consisting in swaps and merges, can decrease the complexity of the solutions, it is unable to refine a partition. Such a mutation, along with the recombination operator, will help the exploration of candidate solutions with more clusters.

Eventually, note that the first generation of candidates build by the hybrid-GA algorithm are constructed using a simple greedy swap algorithm from totally random starting partitions. Greedy hill-climbing heuristics are therefore used at initialization (swaps) and after each recombination (merges) and mutations (swaps).

Finally, the greed package also comes along with three other optimization algorithms that the user may decide to use for comparison or if suitable:

- A classical genetic algorithm without hybridization with greedy local search.
- A classical greedy hill climbing (swap and merge) algorithm with multiple random starting partitions (see e.g. Côme and Latouche 2015, for the SBM).
- A classical greedy hill climbing algorithm (Côme and Latouche 2015) with one seeded starting point, the seed being produced by a model-dependent heuristic (over-segmented $K$-means for GMM as an example).

3.2. Hierarchical clustering and cluster ordering
Once a solution with a number $K^*$ of clusters have been found by one of the previous algorithms, the *greed* package also provides a hierarchical approach to build a set of ICL dominant solutions for all the value of $K$ between $K^*$ and 1 (see Côme et al. 2021, for details). This is achieved in the same Bayesian paradigm with the ICL$_{ex}$ objective, now considering the Dirichlet prior parameter $\alpha$ as a regularization controlling the granularity of the clustering and unlocking access to simpler, coarser, solutions as it decreases towards 0. The method is based on a log-linear approximation of ICL$_{ex}$ when $\alpha$ is small, which makes it computationally efficient, and produces a hierarchy of nested partitions along with the sequence of the regularization parameters which enabled the fusions $(Z^{(k)}, \alpha^{(k)})_{k=K^*, \ldots, 1}$. Each of these partitions is dominant in terms of ICL when $\alpha$ is in the value range between $\alpha^{(k-1)}$ and $\alpha^{(k)}$. Such a hierarchical processing allows for the exploration of the clustering at coarser scales, together with an optimal ordering of the clusters which is a powerful tool both for visual representation of the results and their analysis. This final ordering is computed in an optimal fashion in order to minimize the sum of merging costs between adjacent clusters while respecting the order constraints imposed by the merge tree (Côme et al. 2021, Section 4). This can be done efficiently thanks to the dynamic programming algorithm of Bar-Joseph, Gifford, and Jaakkola (2001). It is particularly useful for the dendrogram representation of the hierarchy and other visualization tools described in Section 5.

### 3.3. Implementation details

One of the main features of the *greed* package is its flexibility, as it can handle any observational model, *i.e.* any DLVM, for which a tractable exact ICL expression can be derived. The implementation reflects this fact and, while most of the standard DLVMs are implemented, new observational models can seamlessly be integrated without impacting the main functions and API. Each observational model must obey an interface and implements methods that compute the difference of ICL$_{ex}$ induced by an elementary change of a solution (*i.e.* a swap or a merge) and to compute the observational part of the ICL$_{ex}$ criterion in Equation (3), denoted as $\log p(\mathbf{X} | \mathbf{Z}, \mathbf{\beta})$. For the available models, the swap and merge moves are efficiently implemented, only updating the necessary terms rather than computing the whole ICL$_{ex}$ twice and taking the differences. Moreover, whenever possible we took advantage of possible computational speedups, *e.g.* for Mixture of regressions models we used Woodbury identity to efficiently perform rank-one updates of the inverse of the covariance matrices induced by the swaps.

The remaining part of the code base is generic for all models. On the computational side, the main demanding methods were developed in C++ thanks to the Rcpp package (Eddelbuettel and Balamuta 2017) taking advantages of sparse matrix computational efficiency provided by the RcppArmadillo and Matrix packages (Eddelbuettel and Sanderson 2014; Bates and Maechler 2019). The greedy swap and merge methods are implemented in C++ and the high-level optimization algorithms GA, hybrid GA, multiple restarts and seeded greedy algorithms in R. Eventually, the future package (Bengtsson 2019) was used to enable easy parallelization of the computations in the hybrid GA and multistarts algorithms. Finally, the observational model and the optimization algorithm are defined with S4 classes which we detail in the next section on some concrete use cases.
Figure 1: Timings of one swap pass for the SBM (left) and Diagonal-GMM (right) models. For the SBM, the data were simulated using a planted partition model with 4 equiprobable clusters, 4000 nodes, an off-diagonal connection probability of $10^{-3}$ and a diagonal connection probability drawn at random between 0.01 and 0.3. This scheme leads to graphs with 250K to 1.25M edges. For the GMM, the datasets were simulated with a 3-component GMM in dimensions 10. The number of data points was drawn at random between 300 and 3000. In both cases, the swap algorithm was initiated with $K = 10$ clusters and 80 datasets were simulated. The timings were done on a Xeon(R) CPU, at 3.50GHz, and without parallelization.

A note on numerical performances and algorithms complexities. All the optimization algorithms proposed by the greed package rely on combinations of locally optimal swap and merge moves. The time complexity of the latter are model dependent: a whole epoch of swap moves for an SBM (or it’s degree corrected version) is in $\mathcal{O}(M \cdot K^2)$, with $M$ the number of edges in the graph and $K$ the current number of clusters, whereas it reaches a complexity in $\mathcal{O}(N \cdot K \cdot D)$ for a Diagonal-GMM model. Figure 1 clearly illustrates this relationship on simulated data for both models. The timings are shown for one epoch of a swap, and the linear relationships with the number of edges for SBM and with the number of data-points for GMM clearly appears. The timings are reasonable with respect to the problems sizes.

Regarding the merge moves, the complexities are also model dependent. However, as in standard agglomerative procedures, the necessary statistics only have to be computed once at the beginning. For example, the cost of this operation is in $\mathcal{O}(M)$ for the graphs models and in $\mathcal{O}(N \cdot P)$ for classical mixture, where $P$ is a model dependent constant. Then, the cost of computing the ICL variation for one merge is in $\mathcal{O}(P)$, with $P = K$ for SBM like models and $P = d$ for Diagonal-GMM models, for example. Note that it does not depend on $N$ or $M$ anymore. Merge moves are used twice in the algorithm: first in the GA in order to merge redundant clusters after the cross-partition operator in Equation (6), and second in the hierarchical clustering algorithm used to complete the hierarchy after the genetic algorithm has converged. These two use cases do not exhibit the same overall complexity. Indeed, the GA takes advantage of the specific structure yielded by the cross-partition operator to avoid exploring irrelevant pairs of clusters. To do so, merge moves are only considered between pairs of clusters that share a common parent in one of the two parent partitions, see Côme et al.

\[^3\text{greed}\] uses a sparse representation of the adjacency matrix to reach this complexity.
(2021, end of p.6) for details. Moreover, the hierarchy is not built entirely during the GA greedy merge steps, hence further reducing the computational costs. Thus, in practice, the greedy merge heuristic does not reach its worst-case complexity - which is in $O(K^2 \cdot (K + P))$ - during the GA, and it is quite economical compared to the swaps operations costs thanks to the low values of $K$. Concerning the final hierarchical step algorithm, after the GA convergence, the complete hierarchy is built and all possible merges are considered at each step. Therefore, its complexity reaches the bound $O(K^2 \cdot (K + P))$, which is still reasonable for low values $K = K^*$ found by the GA.

Naturally, discussing each global algorithm complexity is quite difficult, since they are influenced by many factors such as population size, number of generations before convergence, mutations probabilities, etc. Nevertheless, one may put in perspectives the different use cases of the algorithms: the hybrid-GA and multistarts algorithms are quite comparable in terms of computational time, provided that the population size of the hybrid-GA is equal to the number of starting points of the multistarts algorithm. The former being more efficient than the latter on all the implemented models, it is the default of the package. The seeded algorithm may be advantageous to users that want to quickly explore large datasets, provided that the seeding algorithm is efficient. Indeed, it is less computationally intensive since only one swap epoch is performed, compared to several dozen for multistarts and hybrid-GA.

A notable aspect of the package is its ability to handle graphs with thousands of nodes in a very reasonable amount of time (less than 1 minute) making it competitive with respect to existing frequentist or Bayesian approaches. As an illustration, in the simulation settings of Figure 1, the whole procedure runs in 30.2 seconds on average for a SBM graph with 4000 nodes and more than 400K edges.

Finally, greed is seamlessly adaptable to parallel computing as described in Section 4.5. This can be easily used to obtain a sensible speedup in performance when datasets become large\(^4\).

### 4. Guidelines for Users

This section provides an overview of a basic usage of the package. We also describe the S4 classes and methods facilitating the manipulation and exploration of the results. As a complement to this section and to the usual R package documentation, a complete documentation including model-specific vignettes is available as a pkgdown website at [https://comeetie.github.io/greed/](https://comeetie.github.io/greed/).

#### 4.1. The greed function

The package's main entry point is the `greed()` function, which performs the clustering and presents a flexible API as illustrated in the block of code below.

```r
> library("greed")
> sol = greed(
+   X , # dataset to cluster
+   K = 20 , # number of initial clusters (optional)
+   model = Gmm() , # model to use and its prior parameters (optional)
)```

\(^4\)For small datasets, the communication costs may exceed the gains from parallelism.
The `greed()` function only has one mandatory argument, `X`, which contains a dataset to cluster. All remaining arguments are optional:

- **K** represents the initial number of clusters and is set to 20 by default. Note that this value is an initial guess, and the available optimization algorithms may return a partition with more or less clusters.

- **model** is an S4 object inheriting from the abstract class `DlvmPrior` and containing the observational model used to compute $ICL_{ex}$ along with its (model-specific) hyperparameters. If not provided, `greed` will try to infer a compatible model with the provided dataset. For example, if `X` is a symmetric binary sparse `dgCmatrix` the model will be set to an `Sbm()` model. Or else, if the provided dataset is a `data.frame` with only columns of `factor` type, an `Lca()` model will then be used. The list of available observational models, their prior parameters and allowed inputs is summarized in Table 3.

- **alg** determines the clustering algorithm used by the `greed()` function. The algorithm is an S4 object inheriting from the abstract `Alg` class and containing the relevant hyperparameters (e.g. probability of mutation, etc.). By default, the hybrid GA described in Section 3 is used, but other maximization heuristics may be used such as standard greedy hill-climbing with multiple random starts, or a standard GA without greedy local search.

### 4.2. Analysing the clustering result

The `greed()` function return an S4 object that inherits from the `IclPath` S4 class, e.g. a `SbmPath` object when the model used is an `Sbm` or a `GmmPath` object when the model used is a `Gmm`. Thus, any clustering result shares the same structure and can be analyzed with the same set of S4 methods, independently from the specified model, illustrating the generic aspect of the methodology. These methods are listed in Table 2 along with their description, and Section 5 presents several uses in concrete examples.

As a quick illustration, we present the results and usage of these methods in the case of graph clustering with SBM (this model will be presented in more details in Section 5.3) using a nested hierarchical community structure in the simulation. The simulations deals with 12 clusters arranged in three levels: 2 big clusters, each composed of three medium clusters, themselves decomposed in two smaller groups. We choose a community structure where nodes inside the same blocks tend to connect more. The connectivity matrix $\theta$ of the simulation is displayed in Figure 2 and the model in Equation (9).

```r
R> N <- 800  # Number of node
R> K <- 12    # Number of cluster
R> pi <- rep(1/K, K)  # Clusters proportions
R> sbmsim <- rsbm(N, pi, theta)  # Simulation
R> sol <- greed(sbmsim$x, model = Sbm())  # Clustering
```
Table 2: S4 methods associated to the IclPath class allowing analysing the results sol of the \texttt{greed()} function.

The algorithm found the true clustering structure. In addition, the dendrogram and the block adjacency matrix of Figure 3 highlight the hierarchical structure of the dataset.

\begin{verbatim}
R> tree <- plot(sol, type="tree")
R> blocks <- plot(sol, type='blocks')
R> ggarrange(blocks,tree)
\end{verbatim}

The \texttt{cut()} function may then be used to inspect the clustering at the “medium” ($K = 6$) and “top” ($K = 2$) levels of the hierarchy. In the following code block, we illustrate the usage of the \texttt{K()}, \texttt{ICL()} and \texttt{clustering()} functions on these coarser solutions.

\begin{verbatim}
R> sol_medium = cut(sol, 6)
\end{verbatim}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2}
\caption{Connectivity matrix of the SBM hierarchical simulation.}
\end{figure}
Figure 3: Blocks representation (left) and dendrogram (right) of the hierarchical SBM clustering found by greed.

\begin{verbatim}
R> K(sol_medium)
[1] 6
R> ICL(sol_medium)
[1] -61080.25
R> sol_top = cut(sol, 2)
R> table(clustering(sol_top), sbmsim$cl)

     1 2 3 4 5 6 7 8 9 10 11 12
1  54 52 73 78 71 63 0 0 0 0 0 0
2   0 0 0 0 0 0 63 65 78 70 57 76
\end{verbatim}

To finish, the `coef()` method may be used on `sol`, returning an estimate $\hat{\theta}$ of the connectivity matrix. Note how, in this specific example, the cluster permutation given by the dendrogram allows to directly compare $\hat{\theta}$ to the true $\theta$, which is typically not the case in regular inference procedure.

\begin{verbatim}
R> hat_theta= coef(sol)$theta
R> mean(abs(hat_theta-theta)) # l1 relative error, no permutation needed.
[1] 0.001154612
\end{verbatim}

4.3. Available models and prior specification

The list of currently implemented DLVM is available in Table 3, describing the name of the hyperparameters as well as the allowed inputs $X$ for each model. A summary of implemented models is also available through the helper function `available_models()`. 
Table 3: S4 classes of the observational models handled by the greed package along with their prior hyperparameters name and the classes of the input datasets that these models can process. Informative hyperparameters fixed in a data-driven way are highlighted with a (*) symbol.

Any observational model may be created with prior hyperparameters \( \beta \) values automatically chosen, \textit{e.g.} by just calling \texttt{Gmm()} or \texttt{Sbm()}. In this case, the chosen value for the prior hyperparameters corresponds to non-informative uniform prior whenever possible, as in the MoM, LCA an SBM models. Whenever non-informative priors are unavailable, they are chosen in a data-driven way. For example, the \( p \) hyperparameter for \texttt{DcSbm()} and \texttt{DcLbm()} is set to the average connection probability between two nodes. The help and documentation of each model precisely describes its hyperparameters and their default values. Moreover, if any prior information is available, their value may be specified by the user, one may for example use \texttt{Gmm(tau=0.3)} to create a \texttt{Gmm()} model prior with hyperparameter \( \tau \) (controlling the variance of the Gaussian prior on the means) equal to 0.3. However, two models have one mandatory argument the Mixture of Regression model must be provided with a formula describing the linear model to use \texttt{MoR(y~x)} and eventually, the \texttt{CombinedModels} class that enable the stacking of several observational models on the same individuals, must be provided with a list of models to use for each view, its usage will be covered in Section 5.4.

### 4.4. Controlling optimization algorithms and their hyperparameters

As explained above, optimization algorithms used by \texttt{greed()} are represented as S4 object inheriting from the class \texttt{Alg}. In this representation, an algorithm has all its hyperparameters stored as attributes of the object, allowing fine-grained control when instantiating the object. For example, in the case of the hybrid GA briefly introduced in Section 3 - and used as a default by \texttt{greed()} - one may customize the behaviour via its \texttt{Hybrid()} constructor and
specify some of the following parameters:

- **pop_size**: size of the populations (default to 20)
- **nb_max_gen**: maximal number of generations (default to 10)
- **prob_mutation**: mutation probability (default to 0.25)
- **Kmax**: maximum number of clusters (default to 100)

A user desiring to increase the exploration capacities of the algorithm may increase the population size, at the expanse of an increased computational time, by using something like `Hybrid(pop_size=50)`. Increasing the two other parameters `nb_max_gen` and `prob_mutation` will also help with the exploration capacities of the algorithm but to a lesser extent. Eventually, the **Kmax** parameter allows the user to set an upper bound for the desired number of cluster. Indeed, this specific algorithm may in fact find a larger number of clusters than the initial value provided to `greed()`. Thus, this upper bound avoids the computations of solutions with too many clusters.

The list of implemented algorithm is available via the helper function `available_algorithms()`. `Seed()` do not have any hyperparameters while `Multistarts()` only one - **nb_start** - corresponding to the number of different random initialization used. Eventually, `Genetic()` share the same parameters as `Hybrid()`.

### 4.5. Parallel computing.

Parallel processing is implemented in `greed` through the `future` package, providing a unified and straightforward framework for sequential and parallel processing. A `future::plan` must simply be set by the user (default is sequential with no parallelism). For instance, in order to run `greed()` on 10 cores in multiple sessions, the following commands should be used before any call to `greed()`.

```r
R> future::plan(multisession, workers=10)
```

Finally, note that `future` supports many parallel processing paradigms and options. Details are provided in `plan()` documentation as well as in the package’s vignettes. In `greed`, the parallelism will be used with the `Multistarts()` (one process per starting points), `Genetic()` and `Hybrid()` algorithms (one process per elements of the population). The interest of enabling parallel processing can be limited and even counterproductive for small datasets so it is best to reserve its use for massive datasets.

### 5. Applications

In this section, we demonstrate the use of the `greed` package on continuous, categorical, graph and heterogeneous data clustering problems through the lens of illustrative real datasets. Each of these applications uses some underlying standard observational model, *i.e.* a DLVM, which we will briefly introduce, along with the model-specific hyperparameters \( \beta \).

#### 5.1. Continuous data clustering with Gaussian mixtures
We are interested in clustering a set of \( n \) multivariate observations in dimension \( p \), \( X = \{ x_i \}_{i=1,\ldots,n} \). As explained in Section 2, Gaussian mixture models (GMMs) are a widely used DLVM in this context. Without any constraints, the Bayesian formulation of GMMs leading to a tractable exact ICL expression uses a Normal and inverse-Wishart conjugate prior on the mean and covariances \( \theta = (\mu_k, \Sigma_k)_k \) (Bertoletti, Friel, and Rastelli 2015). This prior is defined with hyperparameters \( \beta = (\mu, \tau, n_0, \varepsilon) \) and the hierarchical formulation is as follows:

\[
\begin{align}
\pi & \sim \text{Dirichlet}_K(\alpha) \\
Z_i & \sim \mathcal{M}(1, \pi) \\
\Sigma_k^{-1} & \sim \text{Wishart}(\varepsilon^{-1}, n_0) \\
\mu_k & \sim \mathcal{N}(\mu, \frac{1}{\tau} \Sigma_k) \\
X_i|Z_{ik} = 1 & \sim \mathcal{N}(\mu_k, \Sigma_k)
\end{align}
\]

These priors are informative and may therefore have a sensible impact on the obtained results. By default, the priors parameters are set in a data driven fashion as follows: \( \mu = \bar{X}, \tau = 0.01, n_0 = d, \varepsilon = 0.1\text{diag}({\hat{\Sigma}_X}) \), where \( \Sigma_X \) denotes the empirical covariance matrix. These values were chosen to accommodate a variety of situation but they can still be specified by the user and their impact investigated through a sensitivity analysis.

When the number of variables \( p \) becomes large, it can be of interest to reduce the flexibility of a GMM by adding a specific set of constraints. The diagonal covariance model, with constraint \( \Sigma_k = \text{diag}(\sigma_{k1}, \ldots, \sigma_{kp}) \), is implemented in \texttt{greed} through its \texttt{DiagGmm} S4 class. Its hierarchical formulation is similar to that of Equation (7), except the Wishart prior on \( \Sigma_k \) is now replaced by a Gamma prior on each \( \sigma_{kj} \) with shape \( \kappa \) and rate \( \beta \) hyperparameters. The latter have default values set to 1 and to the mean of the empirical columns variances respectively.

The diabetes data

Let us describe a first use case on the \texttt{diabetes} dataset from the \texttt{mclust} package a small dataset suitable for illustration purposes. The data describes \( p = 3 \) biological variables for \( n = 145 \) patients with \( K = 3 \) different types of diabetes: normal, overt and chemical. We are interested in the clustering of this dataset to see if the three biological variables can discriminate between the three diabetes type. We begin by applying the \texttt{greed} function with a \texttt{Gmm} object with default hyperparameters, and compare the obtained clusters with the known diabetes types of the patients.

R> data("diabetes")
R> X=diabetes[, -1]
R> sol = greed(X, model=Gmm())

R> table(diabetes$class, clustering(sol))
The `gmpairs` function allows to get an overview of the clustering results by plotting every biplot combinations of the original variables with the estimated clusters membership and Gaussian ellipses highlighted in each cluster.

```r
R> gmpairs(sol, X)
```

If a user wants to experiment with other values of the prior hyperparameters, the most important is $\varepsilon$, which control the clusters' covariance matrices Wishart prior. This amounts to specify the prior on the dispersion inside each class. For instance, one may specify a priori belief that the variance is small inside clusters, which amounts to diminish the $0.1$ coefficient in front of $\hat{\Sigma}_X$. In this case, it makes sense to decrease $\tau$ in the same proportions to keep a flat priors on the clusters means. For the diabetes data such a choice leads to an interesting solution, where the strong prior constraint leads to one cluster being created to fit one outlier in the “chemical” diabetes.

```r
R> sol_dense = greed(X, model=Gmm(epsilon=0.01*diag(diag(cov(X))), tau =0.001))
R> gmpairs(sol_dense,X)
```

5.2. Categorical data clustering with Latent class analysis

*The model*
Figure 4: Matrix pairs plots of the clustering with user specified hyperparameters on the diabetes data.

We are interested in the clustering of categorical datasets, which are typically found in survey data or item response theory. In this context, we observe \( n \) individuals described by \( p \) variables, taking one among \( d_j \) modalities for each variable \( j \). Latent class analysis (LCA) is a generative model for categorical data clustering which posits conditional independence of the factor variables conditionally on the (unknown) partition, hence fitting the definition of a DLVM. Below is a description of its Bayesian formulation with the use of proper conjugate priors

\[
\begin{align*}
\pi &\sim \text{Dirichlet}_K(\alpha), \\
\forall k, \forall j, \quad \theta_{kj} &\sim \text{Dirichlet}_{d_j}(\beta), \\
Z_i &\sim \mathcal{M}_K(1, \pi), \\
\forall j = 1, \ldots, p, \quad X_{ij} | Z_{ik} = 1 &\sim \mathcal{M}_{d_j}(1, \theta_{kj}),
\end{align*}
\]

For each cluster \( k \) and variable \( j \), the vector \( \theta_{kj} \) represents the probability of each of the \( d_j \) modalities. With the choice of priors above, the LCA model admits an exact ICL expression similar to the mixture of multinomials model\(^5\). Specifying priors hyper-parameters for such a model is less sensible than in the GMM case since uninformative priors are available when there is a lack of prior information.

**Illustration: the mushroom dataset**

\(^5\)The derivation may be found in Section 3 of the supplementary materials of Côme et al. (2021)
This dataset originally comes from UCI Machine Learning Repository and describes 8124 mushrooms with 22 phenotype categorical variables. Each mushroom is classified as “edible” or “poisonous” and the goal is to recover the mushroom class from its phenotype. The mushroom dataset is attached to the greed package and can be loaded as follow:

```r
R> data("mushroom")
```

We illustrate the method on a subsample of size $n = 1000$ mushrooms.

```r
R> X <- mushroom[, -1]
R> subset <- sample(1:nrow(X), size = 1000)
R> labels <- mushroom$edibility[subset]
R> sol_mush <- greed(X[subset,], model=Lca())
```

The hybrid genetic algorithm found a solution with $K = 13$ clusters which is quite over-segmented. However, the hierarchical structure of the clustering depicted in Figure 5 (and generated with the code block below) displays a good separation between two main types of clusters.

```r
R> plot(sol_mush, type=’tree’)
```

A clear hierarchical structure appears, with $K = 2$ or $K = 4$ main clusters. Thus, we can cut the tree at this height and look at the solution.

```r
R> sol4 = cut(sol_mush, 4)
R> table(labels, clustering(sol4))
```
Here, we clearly see that the order of merges is consistent with the edibility labels. While some poisonous mushrooms have been categorized as edible, this might be the consequence of the way the labels have been set, since mushrooms for which the edibility status was unknown were classified as poisonous by default. While this choice is reasonable from a strict health perspective, it might be too conservative. Furthermore, as the data documentation specifies, "there is no simple rule for determining the edibility of a mushroom". Thus, the unsupervised problem is hard and the obtained clustering is already satisfactory.

5.3. Graph clustering with the stochastic block model

The model

Graph data arise in various scientific fields from biology to sociology, and accounts for relationship between objects. These objects are expressed as nodes, while a relationship between two objects is expressed as an edge. Hence, graph data may be expressed and stored in an adjacency matrix $X = \{x_{ij}\}$ where $x_{ij} = 1$ means that objects $i$ and $j$ are connected.

Stochastic block model (SBMs) form a family of random graph models for the adjacency matrix $X$, widely used for graph clustering. In these models, the probability of an edge $(i,j)$ is driven by the cluster membership of node $i$ and $j$, hence the block terminology.

They can be expressed in the DLVM framework and the greed package handles two of these models: the classical binary SBM and its degree-corrected variant with Poisson emissions. The Bayesian formulation of a binary SBM is as follows

$$
\begin{align*}
\pi &\sim \text{Dirichlet}_K(\alpha), \\
\theta_{k,l} &\sim \text{Beta}(a_0, b_0), \\
Z_i &\sim \mathcal{M}(1, \pi), \\
\forall(i,j), \quad x_{ij} | Z_{ik}Z_{jl} = 1 &\sim \mathcal{B}(\theta_{k,l}).
\end{align*}
$$

This model class is implemented in the Sbm class. Here, the model hyperparameters are:

- $\alpha$ which is set to 1 by default.
- The beta distribution parameters $a_0$ and $b_0$ on the connectivity matrix $\theta$. A non-informative prior can be chose with $a_0 = b_0 = 1$, which is the default value in Sbm.

Note that the greed package also handles the degree-corrected variant of SBM in the DcSbm class, allowing for integer valued edges. The underlying model and its DLVM formulation are described in depth in the Supplementary Materials of Côme et al. (2021).

A real-data example: the Book dataset

The Books dataset was gathered by Valdis Krebs and is attached to the greed package. It consist of an undirected co-purchasing network of $N = 105$ books on US politics. Two books...
Figure 6: Block matrix representation of the DcSbm and Sbm solution found with greed on the Book network.

have an edge between them if they have been frequently co-purchased together. We have access to the labels of each book according to its political inclination: conservative ("n"), liberal ("l") or neutral ("n"). We will compare the fit obtained with `greed()` and the two network models namely `Sbm()` and `DcSbm()`.

```r
R> data("Books")
R> sol_dcsbm <- greed(Books$X,model = DcSbm(type="undirected"))
R> ICL(sol_dcsbm)
[1] -1344.987
R> sol_sbm <- greed(Books$X,model = Sbm(type="undirected"))
R> ICL(sol_sbm)
[1] -1252.718
```

For this dataset, the regular SBM model seems to reach a better ICL solution than its degree-corrected variant. Still, Figure 6 allows visualizing both aggregated adjacency matrices and comparing them.

```r
R> bl_sbm = plot(sol_sbm,type='blocks')
R> bl_dcsbm = plot(sol_dcsbm,type='blocks')
R> ggarrange(bl_sbm,bl_dcsbm)
```

In addition, external R packages may be used to display a graph layout with node color as clusters and node size as book popularity (computed using centrality degree). In Figure 7, we represent the result for the SBM solution with 5 clusters. One can see a hierarchical clustering structure appearing, with a central cluster of neutral books in between two densely connected set. In each of these two dense set, there is a clear distinction between popular books (heavily purchased) and more peripheral ones, indicated by node size.

---

We emphasize that the `greed()` function is able to automatically detect if the network model type should be "directed" or "undirected". We specified it in the code chunk for the sake of clarity.
Finally, we can look at both models solutions and their confusion matrix. We see that both partitions make sense according to the available political labels.

```R
R> # Regular SBM
R> table(clustering(sol_sbm), Books$label)

          c l n
1     8 0 0
2    34 0 3
3    6 5 8
```
One of the distinctive features of the DLVM framework is that several observational models may be combined together. This is particularly useful when dealing with heterogeneous or mixed-type data, frequently arising in modern applications.

**Statistical justification**

In this context, we have different representations – or *views* – related to the same *n* objects, \( X = \{X_v\}_{v=1,...,V} \) where \( X_v \) is the *v*-th view of the data. From the statistical point of view, we are simply stacking observational models \( \mathcal{M}_v \) on each view, with a conditional independence assumption with respect the common (and unknown) partition:

\[
p(X_1, \ldots, X_V \mid Z) = p(X_1 \mid \mathcal{M}_1, Z) \times \ldots \times p(X_V \mid \mathcal{M}_V, Z).
\]

Then, the ICL\(_{ex}\) of the whole dataset is simply the sum of the individual ICL\(_{ex}\) of the *V* models, and the algorithms implemented in *greed* still apply.

**The CombinedModels class**

From an implementation point of view, all the combined models may have their own hyper-parameters \( \beta_v \), with the only constraint that they must share the same partition \( Z \) and thus the same (symmetric) Dirichlet prior with hyperparameter \( \alpha \) on the cluster proportions \( \pi \).

The `CombinedModels` S4 class implement this approach, and its constructor takes two arguments

- **models** a named list of size *V* containing S4 objects of class `DlvmPrior-class` instantiating each observational model and their hyperparameters \( \beta_v \).

- **alpha** the cluster proportions the Dirichlet hyperparameter, same as before (default to 1)

Here, the `DlvmPrior-class` is used instead of the `Dlvm-class`. It ensures that only the observational models hyperparameters \( \beta_v \) can be specified, and not one \( \alpha_v \) per model.
The data are provided with a named list, and the model is created with the `CombinedModels` constructor, which must also be provided with a list of `models` priors, with the same `names` as in the data list. The next cell gives the possible skeleton of a call to `greed()` in this context, where may be replaced by any of the implemented models described in Table 3.

```r
my_combined_mod <- CombinedModels(models = list("mod1"=<Mod1>Prior(beta1),
                                             ..., 
                                             "modV"=<ModV>Prior(beta_V)),
                                         alpha=1)
X = list("mod1"=X_1, ..., "modV"=X_V)
sol = greed(X, model = my_combined_mod)
```

Eventually, one can retrieve a fitted submodel on a specific view via the `extractSubModel()` method and use all the classical methods of individuals model on the result, as illustrated in the next code chunk.

```
submod_1 = extractSubModel(sol, "mod1")
```

We now illustrate the method on a concrete heterogeneous dataset mixing continuous and categorical variables, with `GmmPrior()` and `LcaPrior()` respectively stacked on each view. However, we emphasize that a `CombinedModels` may be built with any combination of models (including graph models), and that each model may appear multiple times. For example, it can be used to create models for multilayered networks and/or networks with nodes attributes.

### Illustration on the Fifa data-set

The `Fifa` dataset is attached to `greed` and contains several features of soccer players in the Fifa 2020 videogame (see `?Fifa`). After loading the dataset, we begin by a small pre-processing only keeping players being worth more than 1 000 000 euros, while removing columns corresponding to the players’ names, nationalities, values, a boolean indicating if the player is a goal keeper, and the player `x` and `y` coordinate on a 2-D view of the field. These coordinates will be useful later when analysing the clustering result.

```r
R> data("Fifa")
R> X <- Fifa[,,-c(1,2)] %>%
           filter(value_eur>1000000) %>%
           select(-value_eur,-GK,-pos_x,-pos_y)
```

This leaves us with a dataset of `n = 2266` rows and `p = 24` columns. The features correspond to players’ characteristics (such as age, height or weight), skills statistics (pace, shooting, ...) and a set of binary factors that indicates the possible field positions of each player (e.g. attack right or middle centre) as well as their preferred foot.

The next code block demonstrates the `CombinedModels` approach and its instantiation for this dataset. The data are split into categorical and continuous views with `LcaPrior()` and `GmmPrior()` models respectively.

---

For example of such complex models we refers the reader to the packages vignettes and in particular the [Graph Clustering](https://comeetie.github.io/greed/) and [Combined Models](https://comeetie.github.io/greed/) vignettes available online at https://comeetie.github.io/greed/.
R> data <- list(categorical = X %>% select_if(is.factor),
+    cont = X %>% select_if(function(v){!is.factor(v)}))
R> cbmods <- CombinedModels(models=list(categorical=LcaPrior(),cont=GmmPrior()))
R> sol = greed(data,model = cbmods)

**Note:** Be careful, names in the models list and in the data list must match.

The resulting model being fitted, the `extractSubModel()` method allows retrieving each sub-model, via its name in the `models` list, and thus to use the plotting capabilities of `greed` on all views. For example, Figure 8 investigates the categorical part of the model and plot the marginal distribution of the factor variables in each cluster thanks to the `marginals` plot type implemented specifically for LCA. We see that the estimated clusters agree quite strongly with the field positions features. The preferred foot feature also have a clear impact on two clusters.

R> plot(extractSubModel(sol,"categorical"),type="marginals")

For the continuous features, Figure 9 shows the `violins` plot type specifically implemented for GMMs. Again, the clusters seem well organized and the hierarchical ordering has produced a meaningful ordering as can be seen with the shooting feature. We will go back to this point later.

R> plot(extractSubModel(sol,"cont"),type="violins")

Figure 10 shows the plot of `marginals` density plots in each clusters. The bimodal aspect of the defending features clearly appears in this visualization, while the mixture of the remaining features is clearly poorly separated.

R> plot(extractSubModel(sol,"cont"),type="marginals")

Finally, in order to clearly show the alignment of the cluster with field position, Figure 11 displays the average position on the field for each cluster.

R> clust_positions = Fifa[,c(-1,2)] %>%
+    filter(value_eur>1000000) %>%
+    select(pos_x,pos_y) %>%
+    mutate(cluster=clustering(sol)) %>%
+    group_by(cluster) %>%
+    summarize(pos_x=mean(pos_x),pos_y=mean(pos_y))
R> ggplot(clust_positions)+
+    annotate_pitch()+
+    geom_text(aes(x=pos_x,y=pos_y,label=cluster),size=5,col="red")+
+    theme_pitch()
Figure 8: Marginal plots of the Lca part of the model over categorical features.
Figure 9: Violins plots of the Gmm part of the model over continuous features.
Figure 10: Marginal plots of the Gmm part of the model over continuous features.
The organization of the clusters clearly appears, cluster 7 correspond to central defensive players, cluster 5 and 6 to lateral defensive players (recall that the preferred foot of this player were quite different between these two clusters with almost only right footed players in cluster 6 and left footed players in cluster 5).

6. Conclusion

This paper introduced greed, a new R package for model-based clustering with a flexible interface and a wide range of applications from multivariate data to graphs and heterogeneous data. In particular, the package implements two new algorithms. First, a hybrid GA algorithm that performs both clustering and model-selection altogether. Second, a hierarchical post-processing which allows cluster ordering and extraction of coarser solutions, hence enabling multiscale analysis of the clustering results. Combined, these two algorithms offer a competitive approach in terms of computational time, ease of use and results interpretability. The generic aspect of the approach is reflected in the package implementation, with S4 class representation of observational models and the possibility to implement new ones. Moreover, the implementation of popular observational models allows to handle a wide variety of datasets, of possibly heterogenous nature, as illustrated on real datasets. We emphasize that the key advantage of the hybrid-GA - enabling its genericity - is its random initialization, making it independent from carefully chosen seeding procedures. Indeed, the latter is both heavily model-dependent and may also have a strong influence of the convergence of classical EM-like algorithms extensively used in model-based clustering. To finish, while already versatile, we lay several possible extensions to the package in order to widen its scope. First, a desirable feature would be to allow for multiple measurement data, without changing the generic interface. Second, handling missing data is also a desirable feature in modern appli-
applications. The DLVM framework allows for a generic approach in two contexts: either with a missing at random hypothesis, or when the missing pattern is supposed to only depend on $Z$. Finally, handling models for which there exists no explicit formula of the $ICL_{ex}$ criterion is a natural direction. However, it would required the adaptation of the two main algorithms to handle the approximation steps and is therefore postpone to future works.

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