Library Evolutionary Algorithms for Clustering (LEAC)

User manual
for LEAC version 1.2
6 January 2022

Hermes Robles-Berumen,
Amelia Zafra,
Sebastian Ventura.

This user guide is for Library LEAC (version 1.2, 6 January 2022), and documents commands for clustering analysis.

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1 Introduction

Library Evolutionary Algorithms for Clustering (LEAC) is a library for the implementation of evolutionary algorithms (EA) to solve the problem of *partitional clustering*, the purpose is to find an optimal partition of a data set X having n $d-$dimensional *objects*[1]. $X = \{x_1, x_2, ..., x_n\}$ in k subsets $C_1, C_2, ..., C_k$ $(k \leq n)$. So that the objects that are in the same group are more similar between them and the objects of the other groups are the most different. Formally under the partitioning approach the problem of clustering is defined by Nanda and Panda [NP14] as

$$\begin{aligned} C_j \neq \emptyset \quad & \forall j = 1, 2....k; \\ C_j \cap C_{j'} = \emptyset \quad & \forall j, j' = 1, ..k \quad \text{and} \quad \cup_{j=1}^{k} C_j = X. \end{aligned} \tag{1.1}$$

Clustering is useful in areas, such as exploratory *pattern-analysis*, *grouping*, *decision-making*, and *machine-learning* and *data mining* [JMF99].

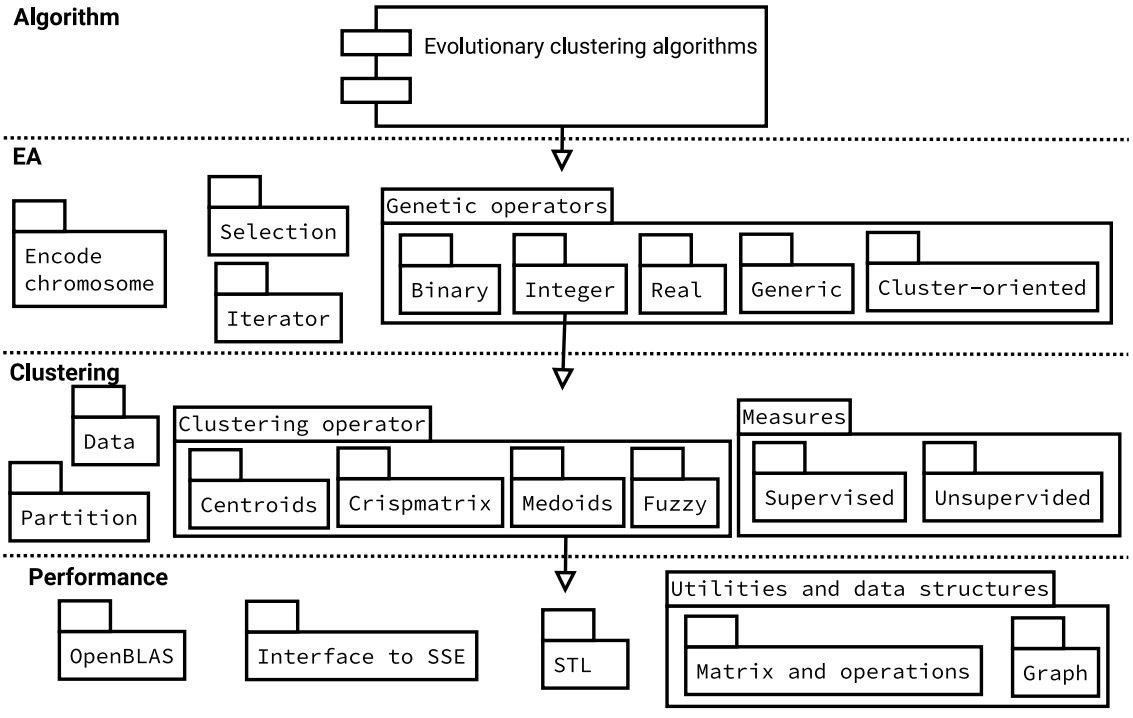

Figure 1.1: *Layered software architecture* of LEAC library

[1] The terms *object*, *instance*, *points* or *prototype* usually have the same meaning in the literature on *clustering analysis* and will be freely interchanged in this document

LEAC library is based on a *layered software architecture* composed of four layers. Each layer consists of a set of related packets as shown in the Figure 1.1. Following, it is described each layer:

`Algorithm`
: It contains final implementations of several evolutionary algorithms for clustering. In the current version of LEAC, there are 25 implemented algorithms (see Table 1.1).

`EA`
: It contains several packets with operators and strategies to configure EAs, such as: encoding criteria, initialization methods, selection methods, crossover and mutation operators and updating and replacement strategies.

`Clustering`
: It contains several packets with specific clustering operators, such as, supervised and unsupervised performance measures and clustering operators based on centroids, crispmatrix or medoids.

`Performance`
: It consists of low-level programmed functions under the current CPU architectures. For example, Data Alignment and Streaming SIMD Extensions (SSE) [Int10]. It allows top layers to work with high performance.

LEAC is a modular library which make easier to develop new evolutionary algorithm proposals for solving the partitional clustering. Moreover, it includes the most representative proposals of Evolutionary Algorithms for partitional clustering. Following the taxonomy given by Hruschka et al. [HCFdC09], a first classification of these algorithms is carried out according to the use of fixed or variable number initial of clusters and the representation of the clusters. Concretely, 25 state-of-the-art proposals were implemented in this library, see Table 1.1. Moreover, LEAC allows you to implement easily new evolutionary algorithm proposals for clustering using the classes developed in the library. Thus, new algorithms can use the diversity of proposed strategies, procedures and genetic operators included in the library to evolve the population according to the flowchart of these algorithms.

LEAC is based on the current standards of the C++ language, the standard template library (STL) and the optimized BLAS library (OpenBLAS) to have a better performance. Moreover, it uses the C++ language characteristics, such as, hybrid language, generic programming, multi-paradigms and lambda function of C++11 and C++14 versions.

Encode	**Fixed-K**	**Variable-K**
Label	1. `gaclustering_fklabel`, Murthy and Chowdhury [MC96] 2. `gka_fklabel`, Krishna and Murty [KM99] 3. `igka_fklabel`, Lu et al. [LLF+04b] 4. `fgka_fklabel`, Lu et al. [LLF+04a]	14. `gga_vklabeldbindex` and 15. `gga_vklabelsilhouette`, Agustín-Blas et al. [ABSSJF+12] 16. `cga_vklabel`, Hruschka and Ebecken [HE03] 17. `eac_vklabel`, Hruschka et al. [HCdC06] 18. `eaci_vklabel`, 19. `eacii_vklabel`, 20. `eaciii_vklabel` and 21. `feac_vklabelssilhouette` and 22. `feac_vklabelrandindex`, Alves et al. [ACH06]
Crisp matrix	5. `gaclustering_fkcrispmatrix`, Bezdek et al. [BBHB94]	
Centroids	6. `gas_fkcentroid`, Maulik and Bandyopadhyay [MB00] 7. `kga_fkcentroid`, Bandyopadhyay and Maulik [BM02a] 8. `gagr_fkcentroid`, Chang et al. [CZZ09] 9. `cbga_fkcentroid_int` and 10. `cbga_fkcentroid`, FrÃ¤nti et al. [FKKN97]	23. `gcuk_vkcentroid`, Bandyopadhyay and Maulik [BM02b] 24. `tgca_vkcentroid`, He and Tan [HT12]
Medoid	11. `gaprototypes_fkmedoid`, Kuncheva and Bezdek [KB97] 12. `hka_fkmedoid`, Sheng and Liu [SL04] 13. `gca_fkmedoid`, Lucasius et al. [LDK93]	
Tree		25. `gaclustering_vktreebinary`, Casillas et al. [CdLM03]
Sub-cluster		26. `clustering_vksubclusterbinary` Tseng and Yang [TY01]

Table 1.1: Evolutionary algorithms implemented in the LEAC library, described by the taxonomy based on Hruschka et al. [HCFdC09]

2 Get and Install LEAC software

For Windows® systems, perform steps 1 through 4. For GNU/Linux systems and Mac OS X®, perform steps 1, 2 and 5 through 7, and optionally 8 and 9 for all.

1. Download LEAC software at the leac project from https://github.com/kdis-lab/leac, select latest releases.
2. Unzip the file `LEAC-1.2.zip` or '`mv ~/Downloads/LEAC-1.2.tar.gz ~/ ; tar zxvf LEAC-1.2.tar.gz`', we recommend you in the directory `c:\LEAC-1.2` for Windows® and `/home/user/LEAC-1.2` for GNU/Linux and Mac OS X®. Verify that the following directories exist within the main directory.

   `bin` This is the directory to store all evolutionary algorithms for clustering (EAC) binary or executable programs, which result from the compilation of using LEAC.

   `data` In the data directory, it is stored the data sets to be processed.

   `doc` In the '`docs`' directory you will find all the necessary API documentation for the use of LEAC.

   `eac` It contains the source files of the implementations of the EAC algorithms implemented by the LEAC library.

   `include` It contains LEAC library header files and source code.

   `include_inout`
   It contains the modules for the input of parameters and output of the EAC programs.

   `openblas` It contains only the necessary header files to compile a program with some functionalities of the OpenBlas library.

   `sse_kernel`
   It is a module based on OpenBlas and GotoBLAS2, own of LEAC. The functionality of this module together with that of OpenBlas are the best performance for the processing of high-dimensional data sets. For now, it only works for `x86-64` architecture.

   For GNU/Linux and Mac OS X® go to [Step 5], page 6.
3. Download and install the latest version of the tdm-gcc compiler. In this step, it is chosen the components expand gcc and select openmp and also select the option Add to PATH, as shown in Figure 2.1.
4. With the compiler installed, see [Step 3], page 5, you can compile the EAC applications. Open a `cmd`, you have to change the directory to the LEAC-1.2 directory, For example: '`cd c:\LEAC-1.2\eac`' and execute any of the following three options:

   '`mingw32-make -k -f Makefile DEBUG=yes VERBOSE=yes`'
   To debug and analyze the detailed execution of the programs. These options allow software engineering ilities of correctness and reliability.

   '`mingw32-make -k -f Makefile DEBUG=no VERBOSE=no WITHOUT_PLOT_STAT=no`'
   Optimize and obtain the evolutionary behavior of the population from the fitness function (option `WITHOUT_PLOT_STAT`) in the execution of the programs.

'`mingw32-make -k -f Makefile DEBUG=no VERBOSE=no WITHOUT_PLOT_STAT=yes`'
Versions of optimized programs to have a good performance in the data set processing.

The compilation time of all programs varies according to the capabilities of the computers, but it can be approximately 20 minutes.

To install the applications '`mingw32-make -k -f Makefile install`'

And to eliminate the applications and use another option '`mingw32-make -k -f Makefile clean`'

Go to step [Step 8], page 8.

5. Verify that the compiler is installed, on `terminal` type, if you do not install the missing packages as system administrator (root):

   '`gcc -v`' (>=4.8.5),

   '`g++ -v`' (>=4.8.5),

   '`make -v`' (>=4.0),

   If you can not find the packages, install the missing ones as system administrator (root), with your package manager.

   For GNU/Linux, e.g. run '`apt-get install gcc-4.9 g++-4.9 make`' or '`zypper install gcc gcc-c++ make`'

   For Mac OS X®, if you do not have a version (> = 4.8.5), install through `MacPorts` or `Homebrew`. The procedure using `MacPorts` is described below:

   a. Run in a terminal '`xcode-select --install`' and '`sudo xcodebuild -license`'.
   b. Install XQuartz.
   c. Install MacPorts for your version of the Mac operating system with `pkg` installer High Sierra, Sierra or El Capitan.
   d. Add to the `PATH` variable, where MacPorts is located, e.g, typing the command '`export PATH=/opt/local/bin/port:$PATH`'
   e. Install the gcc compiler by typing the following commands '`sudo port -v selfupdate`',G '`sudo port install gcc5`'.

   For Mac OS X® go to [Step 7], page 7.

6. If you want to compile your applications with high-performance modules `OpenBLAS` and `sse_kernel`, it is necessary to have a `x86-64` architecture with GNU/Linux. If you do not want this option, go to [Step 7], page 7, and compile with the option `WITH_OPEN_BLAS = no`.

   First, you should verify that you have a Fortran compiler installed

   '`gfortran -v`'
   (>=4.8.5),

   '`gfortran -print-file-name=libgfortran.so`'
   To verify that the `libgfortran` library is installed

   If you can not find the packages, you have to install the missing ones as system administrator (root), with your package manager, e.g. run '`apt-get install gfortran-4.9 libgfortran-4.9-dev`' or '`zypper gcc-fortran libgfortran3`'.

Then you need to compile and get three static libraries `OpenBLAS`, `LAPACK` and `sse_kernel`, below are the steps to get each of them.

`OpenBLAS`

a. From the http://www.openblas.net/ page, download the source code of the latest version of `OpenBLAS` (>= 0.2.20).

b. Unzip the file with the command

   '`mv ~/Downloads/OpenBLAS-0.3.17.tar.gz ~/ ; tar zxvf OpenBLAS-0.3.17.tar.gz`'

   and change to the directory '`cd OpenBLAS-0.3.17`'

c. Edit `Makefile.rule` with the next values: '`NO_CBLAS=1, NO_LAPACK=1, NO_LAPACKE=1`' and run '`make FC=gfortran`'

d. Copy `libopenblas.a` static library from the `OpenBLAS-0.3.17` directory to the `openblas` directory of `LEAC-1.2`,

   e.g. '`cp libopenblas.a ~/LEAC-1.2/openblas/`'

`LAPACK`

a. Download lapack-3.10.0.tar.gz (>= 3.8.0). from http://www.netlib.org/lapack/

b. '`mv ~/Downloads/lapack-3.10.0.tar.gz ~/ ; tar zxvf lapack-3.10.0.tar.gz`'

c. '`cd ~/lapack-3.10.0`'

d. '`cp make.inc.example make.inc`'

e. Edit `make.inc` file, and change the variables '`CFLAGS = -O3 -march=native -m64 -fomit-frame-pointer -fPIC -pthread`' and the compilers that you are using '`CC`' and '`FORTRAN`'.

f. Then, you have to execute the

   '`make cblaslib ; make lapacklib ;make lapackelib`'

g. Copy static libraries

   '`cp libcblas.a liblapack.a liblapacke.a ~/LEAC-1.2/openblas/`'

`sse_kernel`

a. Change to `sse_kernel` directory, within `~/LEAC-1.2`, just type

   '`cd ~/LEAC-1.2/sse_kernel/ ; make`'

   to compile the library and get `libssekernel.a`.

7. To compile the EAC applications, you have to change to the `eac` inside the `LEAC-1.2` home directory '`cd ~/LEAC-1.2/eac`'.

   First, edit the Makefile file and change the name of the compiler in the `CXX` variable, (e.g. `g++-mp-5`), by default it is `g++`.

   Select one of the following compilation options:

   '`make -k -f Makefile DEBUG=yes VERBOSE=yes`'
   : To debug and analyze the detailed execution of the programs. These options allow software engineering ilities of correctness and reliability.

   '`make -k -f Makefile DEBUG=no VERBOSE=no WITHOUT_PLOT_STAT=no`'
   : Optimize and obtain the behavior of population from the fitness function (option `WITHOUT_PLOT_STAT`) in the execution of the programs.

'`make -k -f Makefile DEBUG=no VERBOSE=no WITH_OPEN_BLAS=yes WITHOUT_PLOT_STAT=yes`'

For the processing of the high dimensionality data set, this option is recommended to obtain good performance, for this, you have to complete see [Step 6], page 6,

Finally, to copy the binary files to the `bin` directory, type the command:

'`make install`'

8. Optionally, if you do not want to generate the LEAC API documentation with Doxygen, we recommend that you use the integrated API documentation contained in the `docs` directory. If you want to generate it, do the following: download a version Doxygen (>= 1.8.13) or with your package manager, install it.

   For Windows, download doxygen-1.8.14.windows.x64.bin.zip, unzip the file in `c:\`.

   For GNU/Linux, download doxygen-1.8.13, '`tar zxvf doxygen-1.8.13.linux.bin.tar.gz`'. You have also to install the dependency '`apt-get install graphviz`'.

   For Mac OS X®, '`sudo port install graphviz`' and '`sudo port install doxygen`'.

   To obtain the documentation in a terminal, run '`doxygen Doxyfile`' in the `LEAC-1.2` directory, or with the full path where the `doxygen` command is located, e.g. '`C:\doxygen-1.8.14.windows.x64.bin\doxygen Doxyfile`' or '`~/doxygen-1.8.13/bin/doxygen Doxyfile`'.

9. Optional for a visual presentation of the clusters, you can install gnuplot.

   For GNU/Linux, run '`apt-get install gnuplot-x1`' as system administrator (root).

   For Mac OS X®, run '`sudo port install gnuplot`'.

   For Windows® the recommendation for the installation is install windows binaries, built by Tatsuro Matsuoka: gp550-20220117-win64-mingw.zip. Unzip in the `c:\gnuplot` directory and add `c:\gnuplot\bin` to the `PATH` environment variable using the following instructions:

   Warning: Adding entries to the `PATH` is normally harmless. However, if you delete any existing entries, you may mess up your `PATH` string, and you could seriously compromise the functioning of your computer. Please be careful. Proceed at your own risk.

   a. Right-click on your `My Computer` icon and select `Properties`.
   b. Click on the `Advanced` tab, then on the `Environment Variables` button (Figure 2.2).

      You should be presented with a dialog box with two text boxes. The top box shows your user settings. The `PATH` entry in this box is the one you have to modify. Note that the bottom text box allows you to change the system `PATH` variable. You should not alter the system path variable in any manner, or you will cause all sorts of problems for you and your computer.
   c. Click on the `PATH` entry in the TOP box, then click on the `Edit` button
   d. Scroll to the end of the string and at the end add '`c:\gnuplot\bin`'
   e. Press `OK -> OK -> OK` and you have finished.

   For Windows®, additionally, you must install epsviewer to view eps files generated by LEAD software applications.

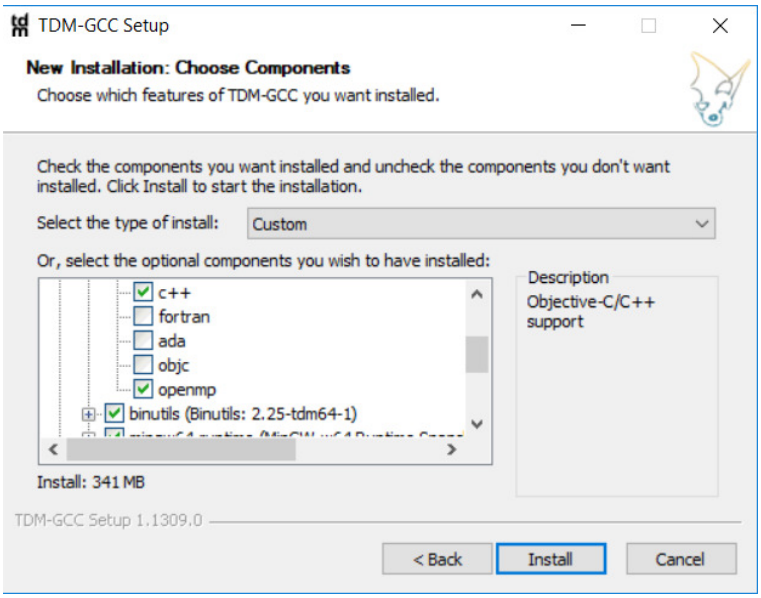

Figure 2.1: Selection of the option openmp in the installation of the tdm-gcc compiler

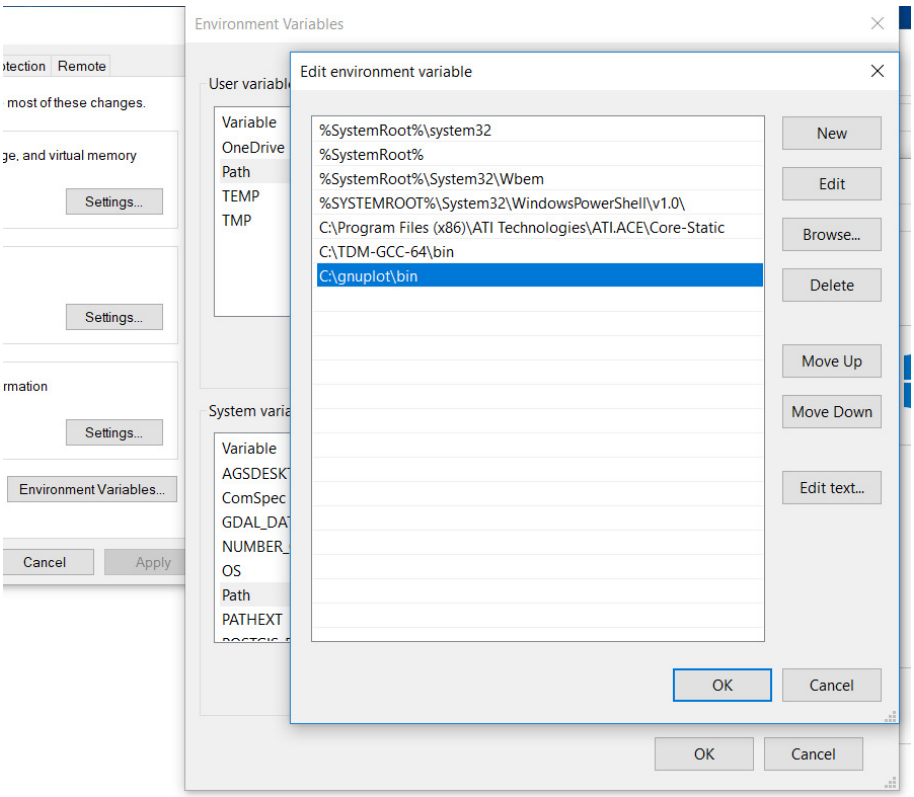

Figure 2.2: Dialog to add the `MinGW` Gnuplot to the `PATH` environment variable

3 LEAC Software

This chapter is composed of three sections. The first section describes the steps to implement an evolutionary algorithm with the components provided by LEAC, documented with two examples included in Appendix A [Example source code], page 89. The complete documentation of the LEAC components can be found in the `docs` folder.

Once that a new algorithm has been built selecting the components and putting them together in a source file, the second section (Section 3.1.10 [Make an executable for a new algorithm], page 41) describes how to create the executable file. Finally, the third section (Section 3.2 [Run an Evolutionary Algorithm included in the library], page 48) describes how to use the algorithms implemented with LEAC. If you want to run any of the algorithms listed in Table 1.1, you can omit the first two sections.

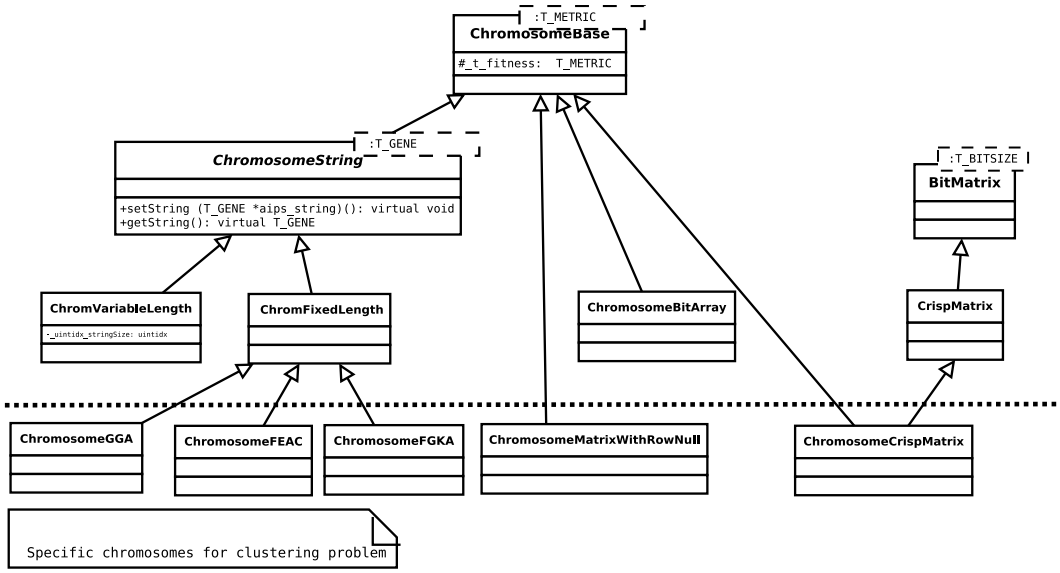

Figure 3.1: Class diagram of the Chromosomes used for encoding

3.1 Develop a new Evolutionary Algorithm in the library

LEAC provides the necessary components to implement an evolutionary algorithm to solve the clustering problem. The following subsections describe the order of the steps to construct an evolutionary algorithm and some of the functions and classes provided by LEAC for each step.

3.1.1 Encoding criterion

Different coding schemes to represent the individual?s genotype have been proposed for solving the traditional clustering problem, such as, binary, integer or real coding. Each type of coding can be associated with a specific phenotype: *centroid*, *medoid*, *label*, *tree*, or *graph-based* representations.

The different encodings are implemented in the LEAC chromosome class hierarchy shown in Figure 3.1. In LEAC, there are three general chromosomes that can be used to implement a large part of the encodings that are:

1. `ChromFixedLength`. Chromosomes with a string of characters, integer or real of fixed length. All instantiated chromosomes will have a fixed length during the evolution. The constructor method is:

   [Constructor on gaencode::ChromFixedLength]
   ChromFixedLength <T_GENE, T_METRIC>()

   Where `T_GENE` it is the type of data of each gene, `T_METRIC` it es the type of data for fitness function

   Before creating the objects, you must specify the length that each chromosome will have with the following method:

   [Method on gaencode::ChromFixedLength]
   static void setStringSize (uintidx *aiuintidx_stringSize*)

   See [Example], page 91,

2. `ChromVariableLength`. It is similar to the previous one, with the difference that the length of each chromosome can vary and can also change during the evolution.

   [Constructor on gaencode::ChromVariableLength]
   ChromVariableLength<T_GENE,T_METRIC>(const uintidx *aiuintidx_stringSize*)

   Where T_GENE it is the type of data of each gene, T_METRIC it es the type of data for fitness function

3. `ChromosomeBitArray`. To model the binary chromosomes. The previous chromosome representation could be used with the `T_GENE` parameter equal to `bool`; however, this representation would have a better efficiency in storage and performance in the application of genetic operators due to bit-level management is performed.

   [Constructor on gaencode::ChromosomeBitArray]
   ChromosomeBitArray<T_BITSIZE,T_METRIC>(const uintidx *aiintidx_numBits*)

   Where `T_BITSIZE` size of the variable to store the bits, `T_METRIC` it es the type of data for fitness function

A classification based on the meaning of the coding (phenotype-genotype), used in different algorithms found in the literature on clustering is described in the following subsections.

3.1.1.1 Cluster labels

a. **String-of-group-numbers encoding**

   It consists of an integer vector of length n, where n is the number of instances. The possible values in the vector are from 1 to k. Thus, the ith element represents that the ith instance belongs to the k cluster.

   To instantiate the *string-of-group-numbers* chromosomes, you can use the class: [gaencode::ChromFixedLength], page 12, where `T_GENE` is the integer type.

b. **Matrix-based binary encoding**

   A $k \times n$ binary matrix can also be used to specify a partition of instances in clusters. It is defined formally by Bezdek et al. [BEF84] and it is called *crisp partition* or *hard partition* (3.1).

$$M_c = \{U_{k\times n} | u_{ji} \in \{0,1\}; \sum_{i=1}^{n} u_{ji} > 0, \text{for all } j,\ \sum_{i=1}^{n} u_{ji} = 1, \text{ for all } i\} \tag{3.1}$$

In this representation, rows represent clusters and columns represent instances. In this case, if the ith object belongs to the jth cluster, then 1 is assigned to element of the jth row and the ith column of the genotype, whereas the other elements of the same column receive 0. You can use the following class:

```
                                    [Constructor on gaencode::ChromosomeCrispMatrix]
ChromosomeCrispMatrix
          <T_BITSIZE,T_CLUSTERIDX, T_METRIC>
          (const uintidx aiuintidx_numRows,
           const uintidx aiuintidx_numColumns)
```

Where T_BITSIZE size of the variable to store the bits, T_CLUSTERIDX is integer index for clusters, T_METRIC is the type of data for fitness function. See [Example ChromosomeCrispMatrix], page 106.

3.1.1.2 Centroid-based

a. **Real encoding**

A chromosome in this encoding is represented as a vector of real numbers that contains the coordinates of each centroid consecutively of the clusters. For an $d$âdimensional space, the length of a genotype is $d \times k$ words, where the first d positions (or genes) represent the d dimensions of the first cluster centroid, the next d positions represent those of the second cluster centroid, and so on until kth cluster:

$$Ch = [g_{11}\ g_{12} \ldots g_{1d}\ g_{21}\ g_{22} \ldots g_{2d} \ldots g_{k1}\ g_{k2} \ldots g_{kd}]$$

To encode a chromosome based on a centroid you can use the same class, see [gaencode::ChromFixedLength], page 12, parameterized for real numbers. See [Example gaencode::ChromFixedLength], page 91.

When a *centroid-based* partition is used, the membership of a objetc to a cluster can be derived by the *nearest object rule* equation (3.2), the rule considers the proximities between the object and the centroids. Thus, the ith object is assigned to the cluster more closer (i.e., the most similar). Formally, given the centroids of the groups μ_j, a object x_i will be assigned to the C_j nearest cluster (equation 3.2).

$$x_i \in C_j \leftrightarrow \|x_i - \mu_j\| \min_k \|x_i - \mu_{j'}\|,\ j' = 1, 2, ..k, \tag{3.2}$$

b. **Binary encoding**

An algorithm based centroids with binary coding is proposed by Tseng and Yang [TY01]. First, a data reduction procedure is used, which consists in calculating an adjacency matrix $A_{n\times n}$ and subsequently the *connected components*. The result is blocks $\{B_1, B_2, ..., B_m\}$, with centroid $\{V_1, V_2, ..., V_m\}$ respectively, so V_i is used as a seed to generate a higher level cluster. Consequently, the chromosomes are of length m. The ith gene with a value of '1' in a chromosome means to use V_i as seeds, which will group the V_i by proximity represented by a gene with value '0'.

3.1.1.3 Medoid-based

Another way to partition a data set is by selecting the most *representative object* of each cluster. In the literature, there are two proposals for integer and binary encoding which are described in the following subsections:

a. **Integer encoding**

   Integer encoding scheme involves using an array of k elements to provide a medoid-based partition of a data set in kth cluster. In this case, each array element represents the index of the object x_i, for $i = 1, 2, ..., n$, where n is the number of objects in the data set.

   For implementation, you can use `gaencode::ChromFixedLength` with *T_GENE* parameterized by an unsigned type as data type. See [gaencode::ChromFixedLength], page 12.

b. **Binary encoding**

   Kuncheva and Bezdek [KB97] use binary encoding to define a medoid-based partition. Each chromosome has a length equal to the number of objects. % n. A bit with index i indicates that the object x_i is a prototype of a cluster C_j. The elements of C_j will be determined by rule (equation 3.2), changing the centroid μ_j by the medoid m_j.

   For implementation, you can use `gaencode::ChromosomeBitArray`, see [gaencode::ChromosomeBitArray], page 12.

3.1.1.4 Graph-based

a. **Binary encoding**

   Casillas et al. [CdLM03] use graph-based coding for objects they get *minimum spanning tree* (MST). The genes represent the edges of the graph and the vertices the n objects in the data set. The MST has $n - 1$ edges. This is the length of the chromosome. In the binary chromosome a value of '`0`' means that this edge remains while a gene with value '`1`' means that this edge is eliminated. The number of elements with value '`1`' represents the value of $k - 1$, where k is the number of clusters.

3.1.2 Initialization methods

Before initializing the population, you must create a container from the `STL` library, such as `std::vector` or `std::list`, to store the individuals of the population and pool mating, see [Example a vector of chromosomes], page 91.

Several approaches are proposed for the initialization of the population. The simplest procedure to initialize the population is random, objects are randomly assigned to a cluster. Such an initialization strategy usually results in unfavorable initial partitions, since the initial clusters are likely to be mixed up to a high degree. However, it constitutes an effective approach to test the algorithms against hard evaluation scenarios [HCFdC09].

LEAC implements different forms of initialization, for the case of `ChromosomeString` objects, the following general function can be used:

[Function]

```
void gagenericop::initializeGenes
          initializeGenes
          (ITERATOR       iterator_first,
           const ITERATOR iterator_last,
```

```
const FUNCTION function)
```

Iterate over the genes of the `ChromosomaString` with the `begin` and `end` method of `ITERATOR`. The function is a lambda function that can generate random values of a distribution and the values are assigned to each gene.

He and Tan [HT12] proposes a more sophisticated initialization, see file tgca_vkcentroid.hpp.

In the study cases of this document, see Section A.2 [GA algorithm], page 104, and Section A.1 [KGA algorithm], page 89. They use an initialization of centroids selected randomly from the instances:

[Function]

```
void clusteringop::randomInitialize
        (mat::MatrixBase<T_FEATURE> &aomatrixt_centroids,
         const INPUT_ITERATOR aiiterator_instfirst,
         const INPUT_ITERATOR aiiterator_instlast)
```

See [Example clusteringop::randomInitialize], page 109,

where all instances are distributed in groups around these centroids by *nearest object rule* (equation 3.2).

And finally, with the centroids obtained, it is possible to obtain a partition of the objects in the data set:

[Function]

```
void clusteringop::getPartition
        (mat::CrispMatrix<T_BITSIZE,T_CLUSTERIDX> &aobcrispmatrix_partition,
         mat::MatrixRow<T_FEATURE> &aimatrixt_instances,
         mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
         dist::Dist<T_DIST,T_FEATURE> &aifunc2p_dist)
```

See [Example clusteringop::getPartition], page 109,

For the initialization of the other partition representations, LEAC provides equivalent functions found in the header files:

- `clustering_operator_centroids.hpp`
- `clustering_operator_crispmatrix.hpp`
- `clustering_operator_fuzzy.hpp`
- `clustering_operator_medoids.hpp`

3.1.3 Fitness function

The evolutionary algorithms are based on the optimization of an objective function that guides the evolutionary search, it is known as *fitness function*. In the clustering problem, different measures are used for *fitness function*, these are classified as *unsupervised measures* (Section 3.1.3.2 [Unsupervised measures], page 18) and *supervised measures* (Section 3.1.3.3 [Supervised measures], page 28). Unsupervised measures usually use a distance to describe relationships *inter* and *intra cluster*.

3.1.3.1 Distances

Distance measures are a key point in clustering to find the similarity between two objects x_i and x'_i. The most common is the *Euclidean distance* $\|x_i - x'_i\|$. LEAC offers a module in the `dist_euclidean.hpp` file to calculate the distances and the class diagram is shown in Figure 3.2.

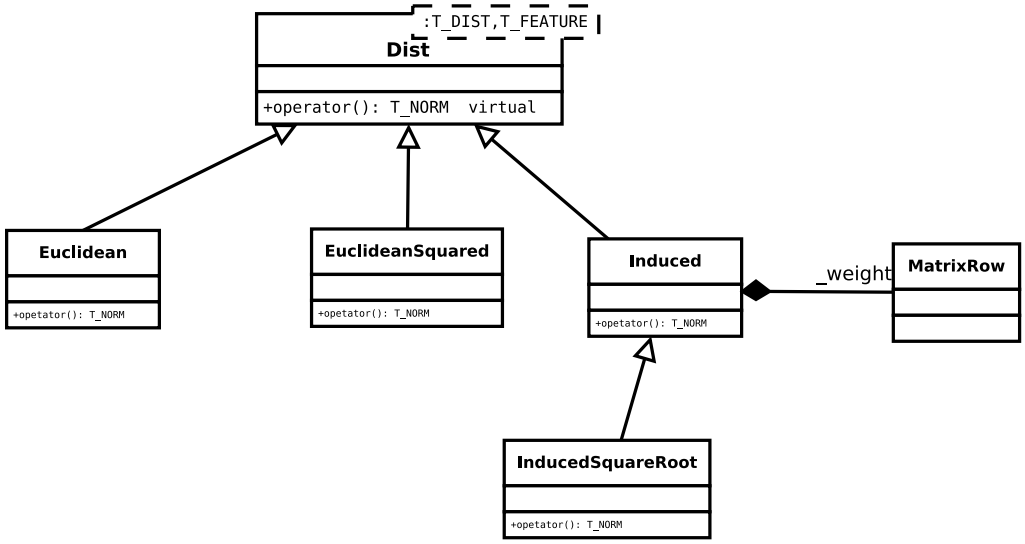

Figure 3.2: Class diagrams of the Distances

All classes derived from `Dist` define the *function call operator* that allows you to find the distance between two x_i and $x_{i'}$ objects:

[Method on dist::Dist]

```
T_DIST operator()(const T_FEATURE*, const T_FEATURE*, const uintidx)
```

To instantiate a `dist::Dist` object the following constructors are used:

1. Euclidean distance

   [Constructor on dist::Euclidean]

   ```
   Euclidean<T_DIST,T_FEATURE>()
   ```

2. Euclidean square distance

   [Constructor on dist::Induced]

   ```
   Induced<T_DIST,T_FEATURE>(const mat::MatrixRow<T_DIST>& aimatrix_weight)
   ```

   See [Example dist::Induced], page 17,

3. Induced distance

   The *induced distance* is a generic measure obtained by multiplying the transposed vector of point x_i to $x_{i'}$ by the *matrix of weight* A and with the vector not transposed (equation 3.3).

   $$D_{Ind}(x_i, x_{i'}) = (x_i - x_{i'})^T A (x_i - x_{i'}) \tag{3.3}$$

   To calculate the *matrix of weights,* A, we have the following functions:

   a. Identity matrix

      [Function]

      ```
      mat::MatrixRow<T_FEATURE> mat::getIdentity (const uintidx aiui_dimension)
      ```

      If the *identity matrix* is used, the induced distance is equivalent to the *Square Euclidean distance* ($A = I$). See [Example mat::getIdentity], page 17,

b. Mahalanobis matrix

[Function]

```
mat::MatrixRow<T_FEATURE> dist::getMatrixMahalonobis
          (INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast)
```

It is the inverse of the *covariance matrix* C_x of the data set X. When it is used an matrix of weights, the *induced distance* is equivalent to *Mahalanobis distance* ($A = C_x^{-1}$). See [Example dist::getMatrixMahalonobis], page 18,

c. Diagonal matrix

[Function]

```
mat::MatrixRow<T_FEATURE> dist::getMatrixDiagonal
          (T_FEATURE* aiarrayt_varianceFeactures)
```

It is the inverse matrix of the variance of the attributes in the main diagonal ($A = D_x^{-1}$). See [Example dist::getMatrixDiagonal], page 17,

The following is an example taken from the main_gas_clustering.cpp file which shows how you can create an instance of a distance metric and select one of them at run time depending on the parameters provided by the user:

```
/*Declaration of a reference to a generic object
    of type of dist::Dist.
    DATATYPE_REAL is the type of data obtained when
       calculating the distance.
    DATATYPE_FEATURE is the data type of the dimensions
       of the instances or objects
*/
dist::Dist<DATATYPE_REAL,DATATYPE_FEATURE>
  *pfunct2p_distAlg = NULL;

/*Create a dist::Dist object based on the parameter provided
     by the user, which will have a polymorphic behavior
*/
switch ( linparam_ClusteringGA.getOpDistance() ) {
case INPARAMCLUSTERING_DISTANCE_EUCLIDEAN:
  pfunct2p_distAlg =
    new dist::Euclidean<DATATYPE_REAL,DATATYPE_FEATURE>();
  break;
case INPARAMCLUSTERING_DISTANCE_EUCLIDEAN_SQ:
  pfunct2p_distAlg =
    new dist::EuclideanSquared<DATATYPE_REAL,DATATYPE_FEATURE>();
  break;
case INPARAMCLUSTERING_DISTANCE_EUCLIDEAN_INDUCED:


  pfunct2p_distAlg =
    new dist::Induced<DATATYPE_REAL,DATATYPE_FEATURE>
    (mat::getIdentity
     <DATATYPE_REAL>
     (data::Instance<DATATYPE_FEATURE>::getNumDimensions()));
  break;
case INPARAMCLUSTERING_DISTANCE_DIAGONAL_INDUCED:

  pfunct2p_distAlg =
    new dist::Induced<DATATYPE_REAL,DATATYPE_FEATURE>
    (stats::getMatrixDiagonal<DATATYPE_FEATURE>
```

```
      (larray_desvstdFeactures)
    );
  break;
case INPARAMCLUSTERING_DISTANCE_MAHALONOBIS_INDUCED:

  pfunct2p_distAlg =
    new dist::Induced<DATATYPE_REAL,DATATYPE_FEATURE>
    (stats::getMatrixMahalonobis
      (lvectorptinst_instances.begin(),
       lvectorptinst_instances.end()
      )
    );
  break;
default:
  throw std::invalid_argument("main_gas_clustering: undefined norm");
  break;
}
```

3.1.3.2 Unsupervised measures

This type of evaluation tries to determine the quality of a given obtained partition of the data without any external information available. For this reason, unsupervised measures are also called as internal measures [ABSSJF+12]. All *unsupervised measures* function of the library are defined in the header file unsupervised_measures.hpp In order to use these metrics, you have to include files or simply the leac.hpp library which contains all the header files.

The measures used in the evolutionary algorithms are described below:

1. **Sum of quadratic errors (SSE)**

   A common clustering criterion or quality indicator is the *sum of squared error* (SSE), defined by Chang et al. [CZZ09] (equation 3.4).

$$\text{SSE} = \sum_{C_j} \sum_{x_i \in C_j} (x_i - \mu_j)^T (x_i - \mu_j) = \sum_{C_j} \sum_{x_i \in C_j} \|x_i - \mu_j\|^2 \tag{3.4}$$

   Where x_i represents the ith instance of the data set. We use the following convention for subscripts i; $i \in \{1, 2, ..., n\}$, for the instances. The subscript for the groups is j; $j \in \{1, 2, ..., k\}$ and the centroid of cluster C_j is denoted as μ_j.

   SSE is also defined by Krishna and Murty [KM99], using [Crisp Partition], page 12, and calling it *total within-cluster variation* (TWCV), equation 3.5.

$$\text{TWCV} = \sum_{j=1}^{k} \text{WCV}^{(j)} = \sum_{j=1}^{k} \sum_{i=1}^{n} u_{ij} \sum_{l=1}^{d} (x_{il} - \mu_{jl})^2 \tag{3.5}$$

   To refer to the dimensions of the objects, it is used l: $l \in \{1, 2, ..., d\}$, so lth object denotes the dimension of x_{il}.

   Or with some slight variation *Sum of Euclidean Distance* SED equation 3.6.

$$\text{SED} = \sum_{C_j} \sum_{x_i \in C_j} \|x_i - \mu_j\| \tag{3.6}$$

This is the most straightforward and popular evaluation distance in the literature. It only considers cohesion of clusters in order to evaluate the quality of a given partition data [ABSSJF+12].

This metric generally is used by different algorithms when the number of clusters k is known and is used by [BM02a] [CZZ09].

For the calculation of SSE, you have three functions. Different distances can be passed as parameter *aifunc2p_dist* (see Section 3.1.3.1 [Distances], page 15) to obtain the variations of the metric:

[Function]

```
std::pair<T_METRIC,bool> um::SSE
          (const mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

The partition is derived by *aimatrixt_centroids*. See [Equation (3.2)], page 13. See [Example um::SSE], page 95,

Other functions for the calculation of *SSE* that depend on the way to specify the membership of an object to a cluster, are the following:

[Function]

```
T_METRIC um::SSE
          (const mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           T_CLUSTERIDX *aiarraymmidx_memberShip,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

[Function]

```
std::pair<T_METRIC,bool> um::SSE
          (const mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const partition::Partition<T_CLUSTERIDX>
           &aipartition_clusters,
           dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

Depending on the encoding used, there is a set of partition clusters classes (`partition::Partition`) for calculating metrics generically. See Figure 3.3. For example, a partition based on equation 3.2 can use the following constructor:

[Constructor on partition::PartitionCentroids]

```
PartitionCentroids<T_FEATURE,T_CLUSTERIDX,T_DIST,INPUT_ITERATOR>
          (mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
           const INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const dist::Dist<T_DIST,T_FEATURE>& aifunc2p_dist)
```

And a partition based on a crisp matrix (equation 4.1) can use the following constructor:

[Constructor on partition::PartitionCrispMatrix]

```
PartitionCrispMatrix<T_BITSIZE,T_CLUSTERIDX>
          (const mat::CrispMatrix<T_BITSIZE,T_CLUSTERIDX> &aibitcrisp_matrix)
```

See [Example partition::PartitionCrispMatrix], page 112,

To avoid defining the template parameters for the case of a partition, you can use the function `makePartition`:

[Function]

```
T_METRIC partition::makePartition
          (mat::MatrixRow<T_FEATURE>  &aimatrixt_centroids,
           const INPUT_ITERATOR  aiiterator_instfirst,
           const INPUT_ITERATOR  aiiterator_instlast,
           const T_CLUSTERIDX  aimcidx_numClusters,
           const dist::Dist<T_DIST,T_FEATURE>  &aifunc2p_dist)
```

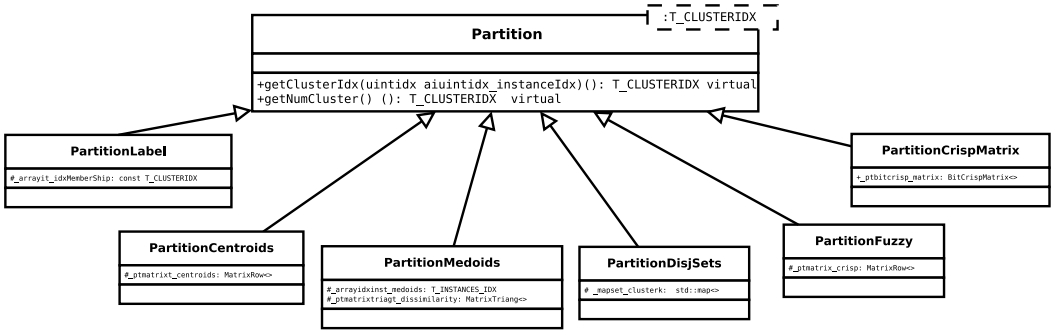

Figure 3.3: Class diagram of the partitions used to calculate the metrics

2. **Distortion**

   The distortion of a cluster is a measure defined by FrÃ□nti et al. [FKKN97]. Similar to SSE, but it considers the number of instances and attributes (equation 3.7).

$$\text{distortion}(C) = \frac{1}{n \cdot d} \sum_{i=j}^{n} D(x_i, f_C(x_i))^2 \tag{3.7}$$

   Where D is the Euclidean distance, $f_C(x_i)$ is a mapping which gives the closest centroid in solution C for a instance x_i, n is the number of instances, and d is the number of attributes of the instances.

   The function that allows to calculate the measure of the distortion is:

   [Function]

```
std::pair<T_METRIC,bool> um::distortion
          (const mat::MatrixBase<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           T_CLUSTERIDX *aiarraycidx_memberShip,
           const dist::Dist<T_METRIC,T_FEATURE>  &aifunc2p_dist,
           const FUNCINSTFREQUENCY func_instfrequency)
```

3. **Sum of Euclidean Distance for Medoid**

   For *k-medoid*, replacing the centroids by the most representative instance in equation 3.6, it is obtained the cost function sum of Euclidean distance to the most representative instance defined by equation 3.8.

$$\text{SEDmedoid} = \sum_{C_j} \sum_{x_i \in C_j} \|x_i - m_j\| \tag{3.8}$$

   Where m_j represents the *medoid* or *prototype* of cluster C_j.

   [Function]

```
T_METRIC um::SSEMedoid
          (const uintidx *aiarrayidxinst_medoids,
           const T_CLUSTERIDX aimcidx_numClustersK,
           const mat::MatrixTriang<T_METRIC> &aimatrixtriagt_dissimilarity)
```

The `medoids::getMatrixDissimilarity` function calculates and returns the triangular distance matrix using a specified distance measure. Used to get other measures for example `um::SSEMedoid`. This is in `medoids_clustering.hpp` file.

[Function]

```
mat::MatrixTriang<T_DIST> medoids::getMatrixDissimilarity
          (INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const dist::Dist<T_DIST,T_FEATURE> &aifunc2p_dista)
```

4. **Least-squared errors functional**

   A *fuzzy c-partitions* is represented by a matrix (equation 3.9) defined by Bezdek et al. [BEF84].

$$M_{fc} = \{U_{k\times n} | u_{ji} \in [0,1]; \sum_{i=1}^{n} u_{ji} > 0, \text{for all } j,\ \sum_{i=1}^{n} u_{ji} = 1, \text{ for all } i\}, \tag{3.9}$$

   Several clustering criteria have been proposed for identifying optimal fuzzy c-partitions in X, the most popular and well-studied criterion is associated with matrices M_{fc} (equation 3.9) is called *least-squared errors functional* (equation 3.10) described in [BEF84].

$$J_m(U,\mu) = \sum_{i=1}^{n}\sum_{j=1}^{k} u_{ji}^{m} D_{Ind}(x_i - \mu_j), \tag{3.10}$$

   Where

   $U \in M_{fc}$ (equation 3.9), fuzzy c-partition of X,

   $\mu = [\mu_1, \mu_2, ..., \mu_k]$ centroids,

   m weighting exponent; $1 \leq m < \infty$,

   $D_{Ind}(x_k, \mu_i)$ is one of the *induced distances* from x_i to μ_j. See [Induced distance], page 16,

[Function]

```
T_METRIC um::jm
          (mat::MatrixRow<T_METRIC> &aimatrixt_u,
           mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           T_METRIC aif_m,
           dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

   For hard clustering, the equation 3.10 is rewritten as equation 3.11.

$$J_1(U,\mu) = \sum_{i=1}^{n}\sum_{j=1}^{k} u_{ji} D_{Ind}(x_i - \mu_i) \tag{3.11}$$

[Function]

```
T_METRIC um::j1
```

```
(mat::BitMatrix<T_BITSIZE> &aimatrix_crisp,
 mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
 INPUT_ITERATOR aiiterator_instfirst,
 const INPUT_ITERATOR aiiterator_instlast,
 dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

See [Example um::j1], page 109,

5. **Davis-Bouldin Index**

   Davis Bouldin index (DB), defined by Davies and Bouldin [DB79], is a function of the ratio of the sum of *within-cluster scatter* to *between-cluster separation*, DB index for the partitioning of k clusters is defined by equation 3.12.

$$DB = \frac{1}{k}\sum_{j} R_{C_j, C_{1\leq j'\leq k}}, \quad j' = 1, 2, ..., k \quad \text{and} \quad j \neq j' \tag{3.12}$$

   in which the index for the jth cluster against all clusters least the same $R_{C_j, C_{1\leq j'\leq k}}$ is given by

$$R_{C_j, C_{1\leq j'\leq k}} = \max_{j',\, j' \neq j} R_{C_j, C_{j'}}$$

   where $R_{C_j, C_{j'}}$ is a measure between a pair of clusters defined by

$$R_{C_j, C_{j'}} = \frac{S_{q,C_j} + S_{q,C_{j'}}}{d_{jj',t}}$$

   and the scatter S_{q,C_j} within for jth cluster, is computed as

$$S_{q,C_j} = \left(\frac{1}{|C_j|}\sum_{x_i \in C_j} \{|x_i - \mu_j|_2^q\}\right)^{1/q}$$

   S_q is the q^{th} root of the q^{th} moment of the points in the jth cluster with respect to their mean, and it is a measure of the dispersion of the points in the jth cluster. $d_{jj',t}$ is the Minkowski distance of order t between the centroids that characterize clusters j and j'.

   DB measure is used in [BM02b].

[Function]

```
T_METRIC um::DBindex
          (const mat::MatrixBase<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const partition::Partition<T_CLUSTERIDX> &aipartition_clusters,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

6. **Silhouette**

   This metric known as silhouette was proposed by Kaufman and Rousseeuw [KR90]. It considers an object x_i which belongs to cluster C_j. The average dissimilarity of x_i to all other objects of C_j is denoted by $a(x_i)$. Now, let us take into account cluster $C_{j'}$. The average dissimilarity of x_i to all objects of $C_{j'}$, will be called $D(x_i, C_{j'})$. After computing $D(x_i, C_{j'})$ for all clusters $C_j \neq Cj'$ the smallest one is selected, i.e.

$b(x_i) = \min D(x_i, C_{j'})$. This value represents the dissimilarity of x_i to its neighbor cluster, and the silhouette $s(x_i)$ is defined by equation 3.13.

$$s(x_i) = \frac{b(x_i) - a(x_i)}{\max\{a(x_i), b(x_i)\}}, \tag{3.13}$$

The higher $s(x_i)$ has a better assignment of the object x_i to a given cluster and

$$-1 \leq s(x_i) \leq 1$$

It is used in [HE03] and [ABSSJF+12].

[Function]

```
T_METRIC um::silhouette
          (mat::MatrixTriang<T_METRIC> &aimatrixtriagrt_dissimilarity,
           ds::PartitionLinkedNumInst<T_CLUSTERIDX,
           T_INSTANCES_CLUSTER_K> &aipartlinknuminst_memberShip)
```

7. **Simplified silhouette**

Alves et al. [ACH06] propose a metric based on [KR90], computation time of Silhouette measure (equation 3.13). The computational cost of Silhouette is $O(n^2)$, which is often not sufficiently efficient for real-world clustering applications (e.g. data mining, text mining, gene-expression data analysis). To avoid this limitation, they propose a simplified silhouette based on the computation of distances between objects and cluster centroids which are the mean vectors of the clusters. More specifically, the term $a(i)$ of equation 3.13 represents the dissimilarity of object x_i to the centroid of its cluster (C_j). Similarly, instead of computing $D(x_i, C'_j)$ as the average dissimilarity of x_i to all objects of C'_j, $C_j \neq Cj'$, only the distance between x_i and the centroid of C'_j must be computed. With these modifications, the computational cost of $O(n^2)$ is reduce to $O(n)$.

[Function]

```
std::vector<T_METRIC> um::simplifiedSilhouette
          (const mat::MatrixBase<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const partition::Partition<T_CLUSTERIDX> &aipartition_clusters,
           const std::vector<T_INSTANCES_CLUSTER_K> &aivectorit_numInstClusterK,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

8. **CS measure**

The CS measure defined by Chou et al. [CSL04] and later by Das et al. [DAK08] is given by the equation 3.14.

$$CS(C) = \frac{\frac{1}{k}\sum_{j=1}^{k}\left\{\frac{1}{|C_j|}\sum_{x_i \in C_j}\max_{x_{i'} \in C_j}\{D(x_i, x_{i'})\}\right\}}{\frac{1}{k}\sum_{j=1}^{k}\left\{\min_{j \in k, j \neq j'}\{D(\mu_j, \mu_{j'})\}\right\}} \tag{3.14}$$

Where

D is a distance function,

x_i and $x_{i'}$ are instances in the same cluster,

μ_j and $\mu_{j'}$ are the centroids of two different cluster.

Chou et al. [CSL04], within-cluster scatter to between-cluster separation. The smallest $CS(C)$ indicates a valid optimal partition. The CS measure is similar to the DI (see [Dunn's index], page 24) and the DB (see [Davis-Bouldin Index], page 22).

[Function]

```
T_METRIC um::CSmeasure
          (INPUT_ITERATOR aiiterator_instfirst,
           const mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
           const ds::PartitionLinkedNumInst<T_CLUSTERIDX,T_INSTANCES_CLUSTER_K>
               &aipartlinknuminst_memberShip,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

9. **Dunn's index**

   Dunn's index (DI) gives good results when the groups are well separated [CSL04] (equation 3.15).

$$DI(C) = \min_{j \in C} \left\{ \min_{j' \in C, j' \neq j} \left\{ \frac{\delta(C_j, C_{j'})}{\max_{j'' \in C} \{\Delta(C_{j''})\}} \right\} \right\} \tag{3.15}$$

   Where

$$\delta(C_j, C_{j'}) = \min \{D(x_i, x_{i'}) | x_i \in C_j, x_{i'} \in C_{j'}\},$$

$$\Delta(C_j) = \max \{D(x_i, x_{i'}) | x_i, x_{i'} \in C_j\},$$

   and x_i and $x_{i'}$ are instances.

   The main drawback with the direct implementation of Dunn's index is its computational load because calculating $DI(C)$ becomes computationally very expensive, when the number of clusters k and the size of the data set n increases. The largest $DI(C)$ indicates a valid optimal partition [CSL04].

   [Function]

```
T_METRIC um::DunnIndex
          (INPUT_ITERATOR aiiterator_instfirst,
           const ds::PartitionLinked<T_CLUSTERIDX> &aipartlink_memberShip,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

   To improve performance in the DI evaluation, it is used the following function. It uses a function `mat::MatrixTriang` to precalculate the distance between objects, and reduce the time of calculation of the distance from one object to another, especially for objects with a large dimension d:

   [Function]

```
T_METRIC um::DunnIndex
          (mat::MatrixTriang<T_METRIC> &aimatrixtriagrt_dissimilarity,
           ds::PartitionLinked<T_CLUSTERIDX> &aipartlinknuminst_memberShip)
```

10. **Simplified Dunn's index**

    Simplified Dunn's index tries to reduce the complexity of the calculation of [Dunn's measure], page 24, from $O(n^2)$ to $O(n)$. This measure is defined in equation 3.16.

$$SDI(C) = \min_{j \in C} \left\{ \min_{j' \in C, j' \neq j} \left\{ \frac{\delta(C_j, C_{j'})}{\max_{j'' \in C} \{\Delta(C_{j''})\}} \right\} \right\} \tag{3.16}$$

Where

$$\delta(C_j, C_{j'}) = \min\{D(\mu_j, \mu_{j''})|j \neq j''\}$$

$$\Delta(C_j) = \max\{D(x_i, \mu_j)|x_i \in C_j\}$$

For implementation, the function to calculate *Simplified Dunn's index*

[Function]

```
T_METRIC um::simplifiedDunnIndex
          (const mat::MatrixBase<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const ds::PartitionLinked<T_CLUSTERIDX> &aipartlink_memberShip,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

11. **Variance ratio criterion**

The *variance ratio criterion* (VRC), also called *Calinski-Harabasz index*, was proposed in [CH74]. It is based on the internal cluster cohesion and the external cluster isolation. The corresponding internal cohesion is calculated by the within-group sum of square distances [HT12].

The index is defined in equation 3.17.

$$VRC_k = \frac{SS_B}{SS_W} \cdot \frac{(n-k)}{(k-1)} \tag{3.17}$$

Where SS_B is the overall between-cluster variance, SS_W is the overall within-cluster variance, k is the number of cluster, and n is the number of instances.

The overall between-cluster variance SS_B is defined as

$$SS_B = \sum_{j=i}^{k} |C_j| \|\mu_j - M\|^2$$

Where μ_j is the centroid of cluster j, M is the overall mean of the instances. The overall within-cluster variance SS_W is defined as

$$SS_W = \sum_{j=1}^{k} \sum_{x_i \in C_j} \|x_i - \mu_j\|^2$$

The VRC should be maximized. Use in [CdLM03] and [HT12].

[Function]

```
T_METRIC um::VRC
          (const mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const partition::Partition<T_CLUSTERIDX> &aipartition_clusters,
           const dist::Dist<T_METRIC,T_FEATURE>  &aifunc2p_dist)
```

12. **Intra-cluster and inter-cluster distance**

The definition of *intra-cluster and inter-cluster distance* (DIIC) by Tseng and Yang in [TY01] is given by the equation 3.18.

$$DIIC = \sum_{i=1}^{k} D_{inter}(C_j)w - D_{intra}(C_j) \tag{3.18}$$

Where $D_{intra}(C_j)$ is the intra-cluster distance

$$D_{intra}(C_j) = \sum_{B_l \subset C_j} \|v_l - \mu_j\| \cdot |B_l|$$

and $D_{inter}(C_j)$ is the inter-cluster distance

$$D_{inter}(C_j) = \sum_{B_l \subset C_j} \left(\begin{matrix} min \\ j \neq k \end{matrix} \|v_l - \mu_j\| \right) \cdot |B_l|$$

And w is a weight. If the value of w is small, it is emphasized the importance of $D_{intra}(C_j)$. This tends to produce more clusters and each cluster tends to be compact. If the value of w is chosen to be large, it is emphasized the importance of $D_{inter}(C_j)$. This tends to produce fewer clusters and each cluster tends to be loose [TY01].

[Function]

```
T_METRIC um::Dintra
          (const mat::MatrixRow<T_FEATURE> &aimatrixrowt_S,
           const mat::MatrixRow<T_FEATURE> &aimatrixrowt_Vi,
           const std::vector<T_INSTANCES_CLUSTER_K> &aivectort_numInstBi,
           const partition::Partition<T_CLUSTERIDX> &aipartition_clustersBkinCi,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

[Function]

```
T_METRIC um::Dinter
          (const mat::MatrixRow<T_FEATURE> &aimatrixrowt_S,
           const mat::MatrixRow<T_FEATURE> &aimatrixrowt_Vi,
           const std::vector<T_INSTANCES_CLUSTER_K> &aivectort_numInstBi,
           const partition::Partition<T_CLUSTERIDX> &aipartition_clustersBkinCi,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

This metric can only be calculated when having subgroups. Given k clusters $C_1, C_2, ..., C_k$ each C_j with S_j centroid, is constructed from the subgroups B_i with V_i centroid. This way of clustering is a characteristic particular feature of the algorithm described in [TY01].

13. **Validity index I**

The *validity index I* or simply *Index I* is described by Maulik and Bandyopadhyay in [MB02] and [BM07]. It is used as a metric to measure clustering performance. It was proposed as a measure to indicate the (goodness) validity of the solution in the cluster. It is defined in equation 3.19.

$$I(k) = \left(\frac{1}{k} \cdot \frac{E_1}{E_k} \cdot D_k \right)^p, \tag{3.19}$$

Where k is the number of clusters

$$E_k = \sum_{j=1}^{k} \sum_{i=1}^{n} u_{ji} \|x_i - \mu_j\|,$$

and

$$D_k = \max_{j,j'=1}^{k} \|\mu_{j'} - \mu_j\|$$

$U(X) = [u_{ji}]_{k\times n}$ is a fuzzy c-partitions matrix of the objects, n is the total number of objects x_i, and μ_j is the jth centroid. The value of k that maximizes $I(k)$ is considered the correct number of clusters.

[Function]

```
T_METRIC um::indexI
          (mat::MatrixRow<T_METRIC> &aimatrixt_u,
           mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist,
           const T_METRIC airt_p = 2.0)
```

If partition of the objects is a crisp partitioning, the following condition holds: $u_{ji} = 1$, if $x_i \in C_j$; otherwise, $u_{ji} = 0$, and you can use:

[Function]

```
T_METRIC um::indexI
          (const mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const partition::Partition<T_CLUSTERIDX> &aipartition_clusters,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist,
           const T_METRIC airt_p = 2.0)
```

14. **Xie-Beni index**

The index of Xie-Beni (XB) was defined by Xie and Beni [XB91] and it is used for *fuzzy c-partitions*, see [Definition fuzzy c-partitions], page 21. This index can be extended to a crisp partition, see [crisp partition], page 12. Note that M_c is imbedded in M_{fc}.

The Xie-Beni index is defined as the quotient of the total variance σ, and minimal separation of groups d_{min} equation 3.20.

$$XB = \frac{\sigma}{n \cdot (d_{min})^2} \tag{3.20}$$

In detail,

$$\sigma = \sum_{j=1}^{k} \sum_{x_i}^{n} u_{ji}^2 \|x_i - \mu_j\|^2,$$

$$d_{min} = \min_{j,j'=1,j\neq j'}^{k} \|\mu_j - \mu_{j'}\|$$

$$XB = \frac{\sum_{j=1}^{k} \sum_{x_i}^{n} u_{ji}^2 \|x_i - \mu_j\|^2}{n \cdot (d_{min})^2}$$

[Function]

```
T_METRIC um::xb
          (mat::MatrixRow<T_METRIC> &aimatrixt_u,
           mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
```

```
                INPUT_ITERATOR aiiterator_instfirst,
                const INPUT_ITERATOR aiiterator_instlast,
                dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

And the function to calculate the XB to a hard partition (see [partition::Partition], page 19).

[Function]

```
T_METRIC um::xb
          (const mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const partition::Partition<T_CLUSTERIDX> aipartition_clusters,
           const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

3.1.3.3 Supervised measures

1. **Rand Index**

   The *Rand Index* was defined by Rand [Ran71]. It is used for two partitions of the same data set X, C in k cluster and R in k' known clases. Alves et al. [ACH06] indicate that these measures can be seen as an absolute criterion or referential standard that allows the use of classification data sets for performance assessment, not only of *classifiers* with the same number of clusters and class ($k = k'$), if not also different ($k \neq k'$). In the same article, they write *Rand Index* as $\Omega(R, C)$ given by equation 3.21.

$$\Omega(R, C) = \frac{a + d}{a + b + c + d} \tag{3.21}$$

   Where:

   - a is the number of pairs of data objects belonging to the same class in R and to the same cluster in C.
   - b is the number of pairs of data objects belonging to the same class in R yet to different clusters in C.
   - c is the number of pairs of data objects belonging to different classes in R yet to the same cluster in C.
   - d is the number of pairs of data objects belonging to different classes in R and to different clusters in C.

   The function that obtains the *Rand Index* is

[Function]

```
T_METRIC sm::randIndex
          (const sm::ConfusionMatchingMatrix<T_INSTANCES_CLUSTER_K>
               &aimatchmatrix_confusion)
```

   To obtain the Rand Index, you must first obtain the confusion matrix:

[Function]

```
sm::ConfusionMatchingMatrix<T_INSTANCES_CLUSTER_K> sm::getConfusionMatrix
          (INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const partition::Partition<T_CLUSTERIDX> &aipartition_clusters,
           const FUNCINSTFREQUENCY func_instfrequency,
           const FUNCINSTCLASS func_instclass)
```

   See [Example sm::getConfusionMatrix], page 112,

2. **Purity**

   Purity is a simple and transparent evaluation measure. Each cluster is assigned to the class which is most frequent in the cluster, and then the accuracy of this assignment is measured by counting the number of correctly assigned objects and dividing by n. For more information on Purity see [MRS08]. It is given in equation 3.22.

$$\text{purity}(C, R) = \frac{1}{n} \sum_{j} \max_{j'} |C_j \cap R_{j'}| \tag{3.22}$$

   Where C and R are two partitions of the same data set X, of k cluster and k' known classes respectively.

   [Function]

```
T_METRIC sm::purity
          (const sm::ConfusionMatchingMatrix<T_INSTANCES_CLUSTER_K>
           &aimatchmatrix_confusion)
```

3. **Precision**

   To calculate the *precision* (equation 3.23), it is used the pairs of the R and C partitions, and it is based on the description given in [Faw06].

$$\text{precision} = a/(a + c) \tag{3.23}$$

   Where:

   - a is the number of pairs of data objects belonging to the same class in R and to the same cluster in C.
   - c is the number of pairs of data objects belonging to different classes in R yet to the same cluster in C.

   [Function]

```
T_METRIC sm::precision
          (const ConfusionMatchingMatrix<T_INSTANCES_CLUSTER_K>
           &aimatchmatrix_confusion)
```

4. **Recall**

   To calculate the *recall* (equation 3.24), it is used the pairs of the R and C partitions, and it is based on the description giben in [Faw06].

$$\text{recall} = a/(a + b) \tag{3.24}$$

   Where:

   - a is the number of pairs of data objects belonging to the same class in R and to the same cluster in C.
   - b is the number of pairs of data objects belonging to the same class in R yet to different clusters in C.

   [Function]

```
T_METRIC sm::recall
          (const ConfusionMatchingMatrix<T_INSTANCES_CLUSTER_K>
           &aimatchmatrix_confusion)
```

3.1.3.4 Develop a new measure

The library contains 26 measures used usually in clustering problems. However, new proposals to evaluate clustering algorithms could be developed. This section describes the steps that you should carry out to include a new measure in this library. So that, an illustrative example is specified.

The measure included in this example is WB-Index. WB-Index was proposed by [ZF14] and it is a relevant measure to validate clustering. The WB-Index is defined in equation 3.25.

$$\text{WB-Index}(k) = k \cdot \frac{SS_W}{SS_B} \tag{3.25}$$

Step 1. Identifying primitive functions. The library contains different primitive functions that are common to all measures they can be used to develop a new measure. Any examples of these primitives would be:

a. Radius of cluster

[Function]

```
T_METRIC um::radiusClusterKj
          (const T_CLUSTERIDX                     aicidx_Clusterj,
          const T_FEATURE*                        ait_centroid,
          const ds::PartitionLinked<T_CLUSTERIDX> &aipartlink_memberShip,
          INPUT_ITERATOR                          aiiterator_instfirst,
          const dist::Dist<T_METRIC,T_FEATURE>    &aifunc2p_dist)
```

Find the radius of cluster j, the maximum distance between an instance of the cluster and the centroid

[Function]

```
std::vector<T_METRIC> um::avgRadiusClusterK
          (const mat::MatrixBase<T_FEATURE>    &aimatrixt_centroids,
          INPUT_ITERATOR                       aiiterator_instfirst,
          const INPUT_ITERATOR                 aiiterator_instlast,
          partition::Partition<T_CLUSTERIDX>   &aipartition_clusters,
          const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

Calculate the average radius of clusters

`um::maxRadiusClusterK`,

[Function]

```
std::vector<T_METRIC> um::maxRadiusClusterK
          (const mat::MatrixBase<T_FEATURE>    &aimatrixt_centroids,
          INPUT_ITERATOR                       aiiterator_instfirst,
          const INPUT_ITERATOR                 aiiterator_instlast,
          partition::Partition<T_CLUSTERIDX>   &aipartition_clusters,
          const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

Calculates the maximum radius of a cluster for a partition

b. Diameter of a cluster

[Function]

```
T_METRIC um::diameterClusterKj
          (const T_CLUSTERIDX                     aicidx_Clusterj,
          const ds::PartitionLinked<T_CLUSTERIDX> &aipartlink_memberShip,
          INPUT_ITERATOR                          aiiterator_instfirst,
          const dist::Dist<T_METRIC,T_FEATURE>    &aifunc2p_dist)
```

Find the diameter of cluster j, the maximum distance between two instances of the cluster

c. Distances between objects and centroid

[Function]

```
std::tuple<std::vector<T_METRIC>,std::vector<uintidx>> um::sumDistInstCentInK
          (const mat::MatrixBase<T_FEATURE>    &aimatrixt_centroids,
          INPUT_ITERATOR                       aiiterator_instfirst,
          const INPUT_ITERATOR                 aiiterator_instlast,
          partition::Partition<T_CLUSTERIDX>   &aipartition_clusters,
          const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

Calculate for each cluster, the sum of the distances between objects that belong to the cluster defined by a partition (see [partition::Partition], page 19) and its centroid, as well as the number of objects in each cluster:

$$\text{VectorDist}(j) = \sum_{x_i \in C_j} \|x_i - \mu_j\|$$

,

$$\text{VectorCount}(j) = |C_j|$$

. Where $j = 1, 2, ..., k$, $i = 1, 2, ..., n$, and $\|\cdot\|$ is a distance (see Section 3.1.3.1 [Distances], page 15).

d. Distances between clusters

[Function]

```
T_METRIC um::maxDistCjCjp
          (const mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
          const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

Find the maximum distance beteen the centroids

[Function]

```
T_METRIC um::minDistCjCjp
          (const mat::MatrixRow<T_FEATURE> &aimatrixt_centroids,
          const dist::Dist<T_METRIC,T_FEATURE> &aifunc2p_dist)
```

Find the minimum distance between centroids

e. between-cluster variance `um::ssb`.

[Function]

```
T_METRIC um::ssb
(const mat::MatrixRow<T_FEATURE>          &aimatrixt_centroids,
 const T_FEATURE                          *aiarrayt_meanInstances,
 const std::vector<T_INSTANCES_CLUSTER_K> &aivectort_numInstancesClusterK,
 const dist::Dist<T_METRIC,T_FEATURE>     &aifunc2p_dist)
```

$$SS_B = \sum_{j=i}^{k} |C_j| \|\mu_j - M\|^2$$

A complete list of primitive functions for calculations of measurements can be found in the documentation of API in the `docs` directory.

Step 2. Adding the function to the unsupervised_measures.hpp file or create a new file with a name such as `wb_index.hpp`, with the following structure:

```
#ifndef __WB_INDEX_HPP
#define __WB_INDEX_HPP

#include "unsupervised_measures.hpp"
```

If you prefer that your function belongs to the **um** namespace of unsupervised functions, declare it inside.

```
namespace um {

T_METRIC
WBIndex
(
```

Parameters of the function.

```
)
{
```

Body of the function.

```
}
} /*END namespace um Unsupervised measures*/

#endif /*__WB_INDEX_HPP*/
```

Step 3. Coding the new measure. In this step, it is implemented the function to calculate `WBIndex`:

To standardise the code, the same notation used in the library can be used:

`[a|l|g][i|o][typeData]_[decription]`

The initial letters of the names of the variables have the following meaning:

'a' Specifies that it is a variable that is used as an argument for a function.

'g' Global variable.

'l' Local variable of a function.

'i' Variable required by the function to be processed.

'o' The data generated by the output function.

```
template <typename INPUT_ITERATOR,
          typename T_FEATURE,
          typename T_CLUSTERIDX,
          typename T_METRIC
         >
```

All functions in LEAC are implemented with the generic programming scheme, so the function is parameterized to handle different types of data.

```
T_METRIC
WBIndex
(const mat::MatrixRow<T_FEATURE>       &aimatrixt_centroids,
 INPUT_ITERATOR                        aiiterator_instfirst,
 const INPUT_ITERATOR                  aiiterator_instlast,
 partition::Partition<T_CLUSTERIDX>    &aipartition_clusters,
 const dist::Dist<T_METRIC,T_FEATURE>  &aifunc2p_squaredDist
 )
```

The arguments to the `WBIndex` function are:

aimatrixt_centroids
: Centroids of the cluster, each row of the matrix corresponds to a centroid of a group.

aiiterator_instfirst, *aiiterator_instfirst*
: Iterator of the first and last objects and instances of the container. To store the data set objects, you can use any container, for example, a `std::vector`, a `std::list`.

aipartition_clusters
: A partition of the objects, see [partition::Partition], page 19.

`aifunc2p_squaredDist`
: A distance function, see Section 3.1.3.1 [Distances], page 15.

```
{ //Begin body function

  const uintidx lui_numInstances =
        uintidx(std::distance(aiiterator_instfirst,aiiterator_instlast));

  static T_FEATURE *larray_centroid1 =
    new T_FEATURE[data::Instance<T_FEATURE>::getNumDimensions()];

  T_METRIC  lometric_WBIndex = measuare_undefWBIndex(T_METRIC);
```

Declaration of local variables.

```
  static utils::RunOnce runOnce ([&]() {
     decltype(utils::InstanceDataType().sum(data::Instance<T_FEATURE>::type()))
     *larray_sumFeatureTmp =
         new decltype(utils::InstanceDataType().sum(data::Instance<T_FEATURE>::type()))
         [data::Instance<T_FEATURE>::getNumDimensions()];

      stats::sumFeactures
         (larray_sumFeatureTmp,
          aiiterator_instfirst,
          aiiterator_instlast,
          T_FEATURE(0)
         );

     stats::meanVector
        (larray_centroid1,
         lui_numInstances,
         larray_sumFeatureTmp
         );

         delete [] larray_sumFeatureTmp;
      }
     );
```

Because M is the centroid of all objects in the data set, this does not change for the calculation of SS_B. To have a better performance, you just have to calculate it once. LEAC provides a package called `utils`, which contains `RunOnce` a lambda function, which only runs once for all calls to the function that implements it.

```
#ifdef __VERBOSE_YES
  const char* lpc_labelFunc = "um::WBIndex";
```

```
  ++geiinparam_verbose;
  if ( geiinparam_verbose <= geiinparam_verboseMax ) {
    std::cout
       << lpc_labelFunc
       << ":  IN(" << geiinparam_verbose << ')'
       << "\n\t(input mat::MatrixRow<T_FEATURE>& aimatrixt_centroids["
       << &aimatrixt_centroids << "]\n"
       << "\t input  partition::Partition<>&: aipartition_clusters["
       << &aipartition_clusters << "]\n"
       << "\t input  dist::Dist<T_METRIC,T_FEATURE>  &aifunc2p_squaredDist["
       << &aifunc2p_squaredDist << ']'
       << "\n\t)"
       << std::endl;
  }
#endif //__VERBOSE_YES
```

When it is compiled with the option `DEBUG=yes`, it is possible to track the execution, to detect coding errors and ensure the result of the function. The *geiinparam_verboseMax* is used to determine the functions that are going to be debugged.

```
  //PRECONDITION: Check under what conditions you can
  //     calculate the measure.
  //  If the number of centroids is greater than equal to 2,
  //     it is possible to calculate the WBIndex

  if ( aimatrixt_centroids.getNumRows() > 1 ) {

    std::vector<T_METRIC> lvectorrt_sumDistInstCentInK;
    std::vector<uintidx>  lvectorui_numInstClusterK;

    std::tie
      (lvectorrt_sumDistInstCentInK,
       lvectorui_numInstClusterK) =
      sumDistInstCentInK
      (aimatrixt_centroids,
       aiiterator_instfirst,
       aiiterator_instlast,
       aipartition_clusters,
       aifunc2p_squaredDist
       );

    T_METRIC lmetrict_SSb =
      ssb
      (aimatrixt_centroids,
       larray_centroid1,
       lvectorui_numInstClusterK,
       aifunc2p_squaredDist
       );

    if  ( lmetrict_SSb > 0.0 ) {

      T_METRIC lmetrict_SSw =
         interfacesse::sum
         (lvectorrt_sumDistInstCentInK.data(),
         (uintidx) lvectorrt_sumDistInstCentInK.size()
         );
```

```
      lometric_WBIndex = (lmetrict_SSw / lmetrict_SSb) *
         (T_METRIC) ( aimatrixt_centroids.getNumRows() -1 );
    }
  }



#ifdef __VERBOSE_YES
  if ( geiinparam_verbose <= geiinparam_verboseMax ) {
    std::cout << lpc_labelFunc
      << ": OUT(" << geiinparam_verbose << ')'
      << " lometric_WBIndex = " << lometric_WBIndex
      << std::endl;
  }
  --geiinparam_verbose;
#endif //__VERBOSE_YES



  return lometric_WBIndex;

} //End body function
```

3.1.4 Stop criteria

There is not a stopping criterion in the literature which ensures the convergence in the evolutionary algorithms to an optimal solution. Usually, two stopping criteria are used. In the first, the process is executed for a fixed number of iterations and the best individual/solution obtained is taken to be the optimal one. In the other, the algorithm is terminated if no further improvement in the fitness value of the best individual is observed for a fixed number of iterations, and the best individual obtained is taken to be the optimal one [MC96].

3.1.5 Selection methods

In this step, the individuals of the population are selected in a mating group to apply the crossing and mutation operators. LEAC has avaliable two schemes of individual selection:

1. Roulette wheel. Based on the concept of survival used in natural genetic systems. To apply this selection after having evaluated the fitness function, the probability distribution is calculated with the function:

   [Function]

   ```
   std::vector<T_REAL> prob::makeDistRouletteWheel
             (INPUT_ITERATOR aiiterator_instfirst,
              INPUT_ITERATOR aiiterator_instlast,
              const FITNESSOPERATION fitness_func)
   ```

   See [Example prob::makeDistRouletteWheel], page 99,

   With the probability distribution, the indices of the individuals to be selected are generated:

   [Function]

   ```
   T_INTIDX gaselect::getIdxRouletteWheel
             (const std::vector<T_PROBABILITY> &aivectorrt_probDist,
              const T_INTIDX aiuintidx_begin)
   ```

2. Tournament. This selector carries out several “tournaments” between a small number of individuals specified by the variable *aiuintidx_orderTournament* chosen at random

from the population. Then, the individual with the best fitness of each tournament is selected:

[Function]

```
INPUT_ITERATOR gaselect::tournament
          (const INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const uintidx  aiuintidx_orderTournament,
           const FITNESSOPERATION fitness_func)
```

Since the containers used come from the `STL library`, to store the data, it is possible to reuse the functions provided by the library `<algorithm>` specially designed to be used in ranges of elements, such as `std::max` and `std::sort`.

3.1.6 Crossover operators

LEAC has available two functions to iterate over the population and mating pool obtained after applying the parent selector:

[Function]

```
void gaiterator::crossover
          (INPUT_ITERATOR aiiterator_instfirstParent,
           const INPUT_ITERATOR aiiterator_instlastParent,
           INPUT_ITERATOR aiiterator_instfirstChild,
           const INPUT_ITERATOR aiiterator_instlastChild,
           const GENETIC_OPERATOR genetic_operator)
```

Select a pair of parents and children consecutively from their containers. See [Example gaiterator::crossover], page 100,

[Function]

```
void gaiterator::crossoverRandSelect
          (INPUT_ITERATOR aiiterator_instfirstParent,
           const INPUT_ITERATOR aiiterator_instlastParent,
           INPUT_ITERATOR aiiterator_instfirstChild,
           const INPUT_ITERATOR aiiterator_instlastChild,
           const GENETIC_OPERATOR genetic_operator)
```

Select a pair of parents and children randomly and consecutively respectively from their containers. See [Example gaiterator::crossoverRandSelect], page 114,

Within the iterator function, the crossover operator is applied. LEAC has implemented several operators of crossover and mutation proposed in the literature. These are organized by packages as shown in the Figure 3.4. The way in which genetic operators are classified in LEAC is *cluster-oriented* or *nonoriented operators*. They are also classified according to their coding: *binary*, *integer*, or *real* encoding. For a classification of operators see Hruschka et al. [HCFdC09]. From the point of view of the implementation, it is also possible to classify those that are programmed in a generic way and those that depend on the type of data.

The crossover operators used by the algorithms implemented in section Appendix A [Example source code], page 89, they use `Single-point` and `Two-point` Crossover described below:

[Function]

```
void gagenericop::onePointCrossover
          (gaencode::ChromFixedLength<T_GENE,T_METRIC> &aochrom_child1,
           gaencode::ChromFixedLength<T_GENE,T_METRIC> &aochrom_child2,
           const gaencode::ChromFixedLength<T_GENE,T_METRIC> &aichrom_parent1,
           const gaencode::ChromFixedLength<T_GENE,T_METRIC> &aichrom_parent2)
```

This crossover operator is parameterized for a chromosome of any type of data, internally generates a random number in the interval [1,length of chromosome -2], which is used to make the combination, see [Example gageneticop::onePointCrossover], page 100,

[Function]

```
void gabinaryop::onePointDistCrossover
          (mat::BitMatrix<T_BITSIZE>  &aobitmatrix_child1,
           mat::BitMatrix<T_BITSIZE> &aobitmatrix_child2,
           mat::BitMatrix<T_BITSIZE> &aibitmatrix_parent1,
           mat::BitMatrix<T_BITSIZE> &aibitmatrix_parent2)
```

This is the extension of operator `two-point crossover` for the case of `Bit-Matrix`, see [Example gabinaryop::onePointDistCrossover], page 114,

3.1.7 Mutation operators

Several operators for mutation are proposed in the literature on evolutionary algorithms for clustering. In the Figure 3.4, in the same way that the crossover operators are grouped, the mutation operators are also grouped by packets.

To illustrate how the mutation operator is applied, the two operators that are used in the illustrative examples in Appendix A [Example source code], page 89, are described below.

Bezdek et al. [BBHB94] use a mutation operator to change the one bit from one row to another in an random way in a *crisp matrix*:

[Function]

```
void gabinaryop::bitMutation
          (mat::CrispMatrix<T_BITSIZE,T_CLUSTERIDX> &aiobitcrispmatrix_chrom)
```

See [Example gabinaryop::bitMutation], page 115.

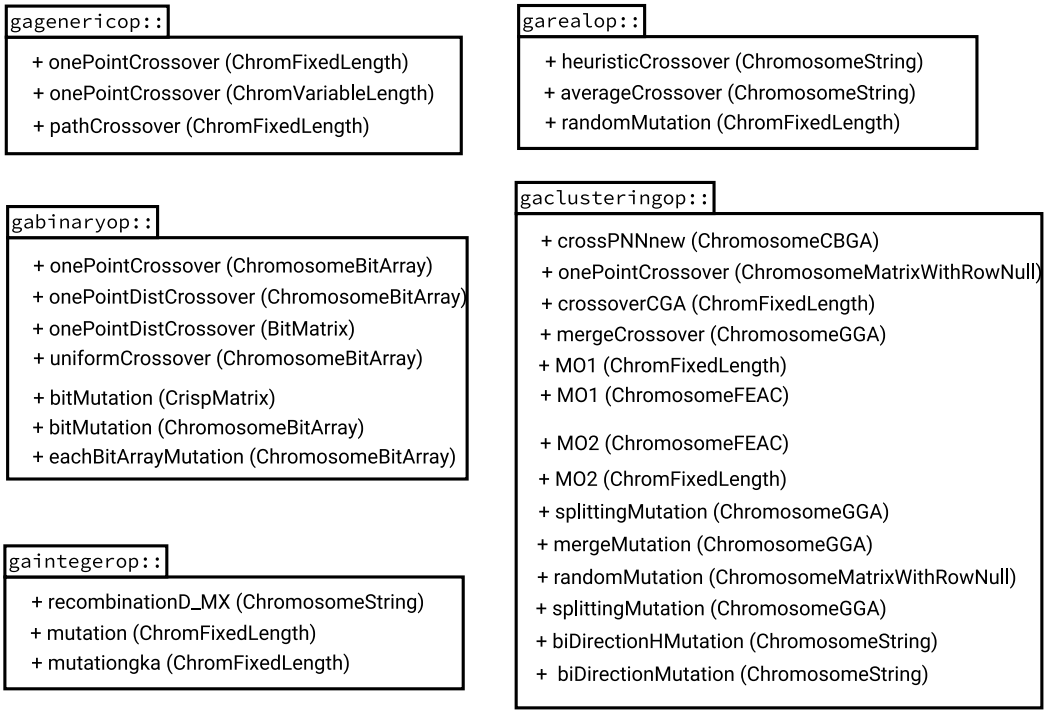

Figure 3.4: Packages of genetic operators provided by LEAC. The type of chromosome received by the operator is indicated in parentheses

Bandyopadhyay and Maulik [BM02a] they propose a mutation operator for chromosomes [centroid-based], page 13. It is located in the file `ga_clustering_operator.hpp` and called here as `gaclusteringop::biDirectionHMutation`:

$$\text{mutate}(g_{jl}) = \begin{cases} g_{jl} + \delta \times (\max(x_l) - g_{jl}) & \text{if } \delta \geq 0, \text{ for } j = 1, 2, .., k \text{ and } l = 1, 2, ...d, \\ g_{jl} + \delta \times (g_{jl} - \min(x_l)) & \text{if } \delta < 0. \end{cases}$$

Where δ is a random number in the interval $[-R, +R]$:

$$R = \begin{cases} \frac{M - M_{min}}{M_{max} - M_{min}} & \text{if } M_{max} > M, \\ 1 & \text{if } M_{min} = M_{max}. \end{cases}$$

M_{min} and M_{max} are the minimum and maximum values of the clustering metric, respectively, in the current population. M is the clustering metric value of the current chromosome that must be mutated.

[Function]

```
void gaclusteringop::biDirectionHMutation
        (gaencode::ChromosomeString<T_GENE,T_METRIC> aochrom_offspring,
         const T_METRIC airt_minObjetiveFunc,
         const T_METRIC airt_maxObjetiveFunc,
         const T_GENE* aiarrayt_minFeatures,
         const T_GENE* aiarrayt_maxFeatures)
```

See [Example gaclusteringop::biDirectionHMutation], page 103,

3.1.8 Updating and replacement methods

In this step, the new individuals resulting from the crossover, the mutation and those who survive without applying an operator, will form the new population.

For most of the algorithms studied in this document, the offspring automatically replace their parents. Then, in the process of crossover, individuals move from the mating pool to the population. For example, in the implementation of the KGA algorithm of [BM02a], the `gaiterator::crossover` iteration function, the input parameter is *lvectorchromfixleng_matingPool* and the output parameter is *lvectorchromfixleng_population*, in this way the replacement is achieved, whether the crossover is done or not by the assignment in the block of `else`, see [Example remplace population], page 100.

Some algorithms select the best from the previous population and the best offspring, both merge to form a new population. For example Bezdek et al. [BBHB94]. See [Example replace the population with the best], page 116.

To assign or copy individuals, the chromosome objects of the class diagram in Figure 3.1, implement assignment operator `(operator=(const class_name &)` and move assignment operator `(operator=(class_name &&)`, as well as their respective constructors, which allows container handling and code readability.

3.1.9 Other parameters

Some EAs for clustering use local search. The `k-means algorithm` is more popular. This is a procedure of fine-tuning of maximum descent. LEAC includes an extensive list of functions for local search, some of which are discussed below:

[Function]

```
void clusteringop::updateCentroids
          (T_CLUSTERIDX &aocidx_numClusterNull,
           mat::MatrixRow<T_FEATURE> &aiomatrixt_centroids,
           mat::MatrixRow<T_FEATURE_SUM> &aomatrixt_sumInstancesCluster,
           std::vector<T_INSTANCES_CLUSTER_K> &aovectort_numInstancesInClusterK,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           const dist::Dist<T_DIST,T_FEATURE> &aifunc2p_dist)
```

In equation 3.2, each point is assigned x_i a the clusters C_j. See [Equation (3.2)], page 13. Then, the centroids $\mu_i^* = 1/n_j \sum_{x_i \in C_j} x_i, j = 1, 2, ..., k$, where n_j is the number of points in cluster C_i are updated. The function returns the new centroids, the sum of instances and their number per cluster. See [Example clusteringop::updateCentroids], page 95,

Krishna and Murty [KM99] propose the use of the `k-means algorithm` as operator:

[Function]

```
T_CLUSTERIDX clusteringop::kmeansoperator
          (T_CLUSTERIDX *aioarraycidx_memberShip,
           mat::MatrixRow<T_FEATURE> &aomatrixt_centroids,
           mat::MatrixRow<T_FEATURE_SUM> &aomatrixt_sumInstancesCluster,
           std::vector<T_INSTANCES_CLUSTER_K> &aovectort_numInstancesInClusterK,
           INPUT_ITERATOR aiiterator_instfirst,
           const INPUT_ITERATOR aiiterator_instlast,
           dist::Dist<T_DIST,T_FEATURE> &aifunc2p_dist)
```

For a given partition in an array of labels, it performs an update using the `k-means algorithm`. Returns the membership labels, centroids, sum of instances and number of instances in each cluster.

Sheng and Liu [SL04] propose a *local heuristic search* for *k-medoids*, it is described below:

Input:

m_j medoids, where $j = 1..k$ and k number of clusters

p is the size of the search subsets (C_{subset})

Output: m_j^* medoids, with SEDmedoid(m_j^*) $\leq$ SEDmedoid(m_j), and SEDmedoid is the equation (3.8).

For each cluster C_j, it is found the most representative object:

1. Assign each object in $x_i \in X$, where X is data set to the cluster C_j with the closest medoid.
2. For each cluster C_j, repeat until the k medoids does not change:
   - Choose a subset $C_{subset} \in C_j$ the corresponds to m_j and its p nearest neighbors of m_j.
   - Calulate the new medoid

$$m_j^* = \underset{x_i \in C_{subset}}{\arg\min} \sum_{x_i' \in C_j} \|x_i - x_i'\|$$

   - if m_j is different from m_j^* replace with the new medoid
3. Repeat step 1 and 2 until k medoids do not change

The function that implements the local heuristic search for *k-medoids* is the following function:

[Function]

```
void clusteringop::updateMedoids
          (uintidx      aoarrayuiidx_medoids,
           T_CLUSTERIDX aicidx_numClusterK,
           uintidx      aiuiidx_nearestNeighborsP,
           mat::MatrixTriang<T_DIST> &aimatrixtriagt_dissimilarity)
```

Update k-medoids, based on [SL04].

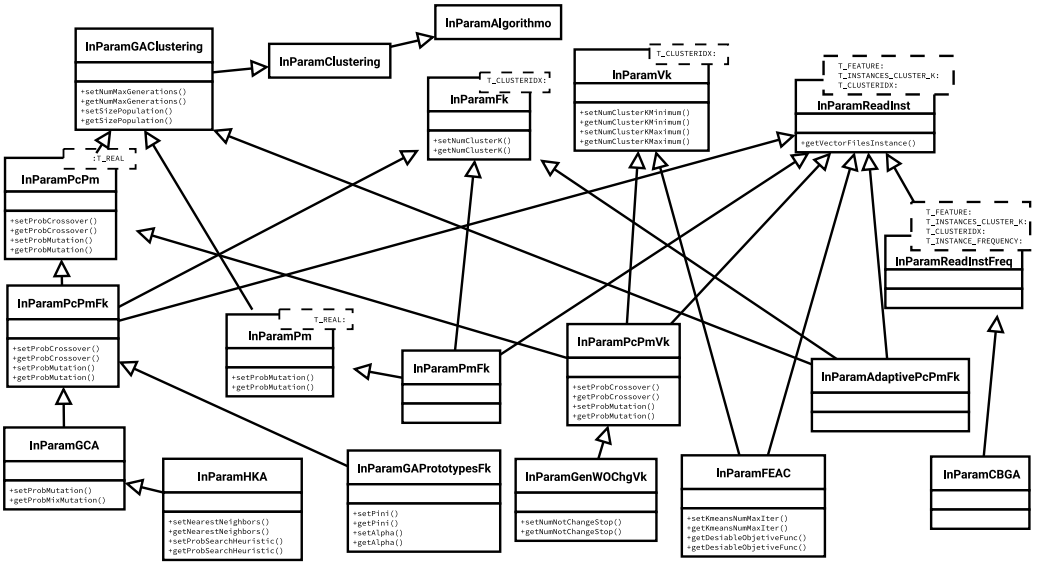

Figure 3.5: Classes used for the input of parameters for the implementation of an algorithm, crossover probability (Pc), mutation probability (Pm), fixed k-clusters (Fk), variable k-clusters (Vk).The classes in the lower level correspond to the specific parameters of some algorithms encoded with LEAC.

3.1.10 Make an executable for a new algorithm

There are two options to make an implementation of a new algorithm. The first, it is simply to include all the necessary operations in the main file. The second option, it is to use the scheme followed in the implementations included in the `eac` directory, you must create a file with a structure similar to the one included in Annex (Section A.1 [KGA algorithm], page 89). In both cases, the configuration scheme of an evolutionary algorithm must be followed see Section 3.1 [Develop a new Evolutionary Algorithm in the library], page 11. The steps necessary to compile the executable file for a new algorithm are described below:

1. Create the source file and include the LEAC library `#include <leac.hpp>`
2. Select the data type of the attributes of the instances of the data set with which you will work, this is independent of the coding of the chromosomes: datatype_instance_real.hpp or datatype_instance_integer.hpp. The files suggest the types of data you can use for the compatibility of variable types, including only one in your source file. '`#include <datatype_instance_real.hpp>`' for real or '`#include <datatype_instance_integer.hpp>`' for integer or define your own data types.
3. Select a class from Figure 3.5 to read the parameters of the new algorithm or define a new class with the parameters specified in the algorithm to be implemented, you can extend from an existing class. For example for `InParamPcPmFk` include the file '`#include <inparam_pcpmfk.hpp>`'.

```
                                                [Constructor on inout::InParamPcPmFk]
InParamPcPmFk<T_CLUSTERIDX,T_REAL,T_FEATURE,T_FEATURE_SUM,T_INSTANCES_CLUSTER_K>
                (const std::string& ais_algorithmoName,
```

```
                const std::string& ais_algorithmoAuthor,
                InParam_algTypeOut aiato_algTypeOut,
                int aii_opNorm)
```

4. Defining an instance of parameter entry class and assign the default values.

```
/*INPUT: PARAMETER
   */
  inout::InParamPcPmFk
    <DATATYPE_CLUSTERIDX,
     DATATYPE_REAL,
     DATATYPE_FEATURE,
     DATATYPE_FEATURE_SUM,
     DATATYPE_INSTANCES_CLUSTER_K
     >
    linparam_ClusteringGA
    ("Acronym of the algorithm",
     "Algorithm Authors",
     inout::CENTROIDS,
     INPARAMCLUSTERING_DISTANCE_EUCLIDEAN
     );

  linparam_ClusteringGA.setNumMaxGenerations(1000);
  linparam_ClusteringGA.setSizePopulation(50);
  linparam_ClusteringGA.setProbCrossover(0.8);
  linparam_ClusteringGA.setProbMutation(0.001);
```

When an instance of the `InParamPcPmFk` object is created, the data types used to perform all the calculations are defined, so it is not necessary to specify the data types for the functions that this `InParamPcPmFk` object is used, allowing you to avoid possible errors or redundancies.

5. Assign the default values or simply use this way to read the parameters, for example:

```
linparam_ClusteringGA.setNumMaxGenerations(1000);
linparam_ClusteringGA.setSizePopulation(50);
linparam_ClusteringGA.setProbCrossover(0.8);
linparam_ClusteringGA.setProbMutation(0.001);
```

6. Optionally, if you wish, you can read the input parameters online using the functions provided in the LEAC library. Declare the sentence '`#include <inparamclustering_getparameter.hpp>`' after the file of the parameter class.

   If you are using a class of the class diagram (Figure 3.5), you have to go to [Step 7], page 45. Otherwise, you have to do the following steps. Define the directive to the preprocessor in the file of your new parameter class. The name of the directive must be different from the ones that are defined, for example:

```
#define __INPARAM_MY_PCPMFK__
```

   If you extend your parameter class from an existing one in Figure 3.5, you must override the definition of the directive that is defined in the base class, for example, instead of simply including the previous statement, you must include the following two statements in your file of parameter class:

```
#undef  __INPARAM_PCPMFK__
#define __INPARAM_MY_PCPMFK__
```

   Include similar code blocks in the inparamclustering_getparameter.hpp file, as shown in the following paragraphs, to print the help and read the parameters of the new algorithm.

a. Find the region of the `inparamclustering_usage` functions, add your directive that was previously defined, and include your definition of the function with the parameter of the new class defined by you (in bold), as it is shown in the following example:

```
#ifdef __INPARAM_MY_PCPMFK__
template<typename T_CLUSTERIDX,
  typename T_REAL,
   typename T_FEATURE,
   typename T_FEATURE_SUM,
   typename T_INSTANCES_CLUSTER_K
   >
void
inparamclustering_usage
(char *argv0,
 InParamMyClassPcPmFk
 <T_CLUSTERIDX,
 T_REAL,
 T_FEATURE,
 T_FEATURE_SUM,
 T_INSTANCES_CLUSTER_K
 >                    &aoipc_inParamClustering
)
#endif
```

b. Search the area to print help messages and write a block of code similar to the following:

```
#ifdef __INPARAM_MY_PCPMFK__
  std::cout << "      --number-clusters[=NUMBER]\n"
            << "                                number of clusters [NUMBER=
            << aoipc_inParamClustering.getNumClusterK() << "]\n";
  std::cout << "      --generations[=NUMBER]  number of generations or iterations\n"
            << "                                 [NUMBER="
            << aoipc_inParamClustering.getNumMaxGenerations()
            << "]\n";
  std::cout << "      --population-size[=NUMBER]\n"
            << "                                size of population [NUMBER="
            << aoipc_inParamClustering.getSizePopulation()
            << "]\n";
  std::cout << "      --crossover-probability[=NUMBER]\n"
            << "                                real number in the interval [0.25, 1]\n"
            << "                                  [NUMBER="
            << aoipc_inParamClustering.getProbCrossover()
            << "]\n";
  std::cout << "      --mutation-probability[=NUMBER]\n"
            << "                                real number in the interval [0, 0.5]\n"
            << "                                  [NUMBER="
            << aoipc_inParamClustering.getProbMutation()
            << "]\n";
#endif
```

c. Find the `inparamclustering_getParameter` functions and define its own function similar to the previous one:

```
#ifdef __INPARAM_MY_PCPMFK__
template<typename T_CLUSTERIDX,
         typename T_REAL,
         typename T_FEATURE,
         typename T_FEATURE_SUM,
         typename T_INSTANCES_CLUSTER_K
```

```
        >
void
inparamclustering_getParameter
(InParamMyClassPcPmFk
 <T_CLUSTERIDX,
 T_REAL,
 T_FEATURE,
 T_FEATURE_SUM,
 T_INSTANCES_CLUSTER_K
 >
 &aoipc_inParamClustering,
 int  argc,
 char **argv
 )
#endif
```

d. In the `inparamclustering_getParameter` function, find the array where the parameter labels are defined and define a new array with the labels of the parameters for the new algorithm, as shown in the following example:

```
#ifdef __INPARAM_MY_PCPMFK__
  const char   *lastr_myInParamPcPmFk[] =
    {"number-clusters",
     "population-size",
     "crossover-probability",
     "mutation-probability",
     "generations",
     (char *) NULL
    };
#endif
```

e. In `long_options` array, define your parameters with the options shown below:

```
#ifdef __INPARAM_MY_PCPMFK__
      {"number-clusters",         required_argument, 0, 0},
      {"population-size",         required_argument, 0, 0},
      {"crossover-probability",   required_argument, 0, 0},
      {"mutation-probability",    required_argument, 0, 0},
      {"generations",             required_argument, 0, 0},
#endif
```

f. Finally, add the necessary code to obtain the parameters:

```
#ifdef __INPARAM_MY_PCPMFK__
      else if ( strcmp /*number-clusters*/
           (long_options[option_index].name,
            lastr_inParamPcPmFk[0] ) == 0 )
        {
          T_CLUSTERIDX lmcidxT_numClusterK;
          liss_stringstream.clear();
          liss_stringstream.str(optarg);
          liss_stringstream >> lmcidxT_numClusterK;
          aoipc_inParamClustering.setNumClusterK(lmcidxT_numClusterK);
        }
      else if ( strcmp /*population-size*/
                (long_options[option_index].name,
                 lastr_inParamPcPmFk[1]) == 0
                )
        {
          liss_stringstream.clear();
          liss_stringstream.str(optarg);
```

```
            liss_stringstream >> luintidx_read;
            aoipc_inParamClustering.setSizePopulation(luintidx_read);
          }
        else if ( strcmp /*crossover-probability*/
                  (long_options[option_index].name,
                   lastr_inParamPcPmFk[2]) == 0
                  )
          {
            T_REAL  lT_readProbabilityCrossover;

            liss_stringstream.clear();
            liss_stringstream.str(optarg);
            liss_stringstream >> lT_readProbabilityCrossover;
            aoipc_inParamClustering.setProbCrossover(lT_readProbabilityCrossover);
          }
        else if ( strcmp /*mutation-probability*/
                  (long_options[option_index].name,
                   lastr_inParamPcPmFk[3]) == 0
                  )
          {
            T_REAL  lT_readProbabilityMutation;

            liss_stringstream.clear();
            liss_stringstream.str(optarg);
            liss_stringstream >> lT_readProbabilityMutation;
            aoipc_inParamClustering.setProbMutation(lT_readProbabilityMutation);
          }
        else if ( strcmp /*generations*/
                  (long_options[option_index].name,
                   lastr_inParamPcPmFk[4]) == 0
                  )
          {
            COMMON_IDOMAIN lT_readNumMaxGenerations;

            liss_stringstream.clear();
            liss_stringstream.str(optarg);
            liss_stringstream >> lT_readNumMaxGenerations;
            aoipc_inParamClustering.setNumMaxGenerations(lT_readNumMaxGenerations);
          }
        else {
          aoipc_inParamClustering.errorArgument
            (argv[0],
             long_options[option_index].name,
             lastr_inParamPcPmFk
             );
        }
    #endif
```

7. If you completed the previous steps, you can now invoke the `inparamclustering_getParameter` function to modify or complete the parameters online:

   ```
   inparamclustering_getParameter(linparam_ClusteringGA, argc, argv);
   ```

   Otherwise, read the parameters as in [Step 5], page 42.

8. Change the seed of random numbers, with some of the following functions. The first is used to generate a new string and the second is used to repeat an experiment with an existing string.

   [Function]

   ```
   std::string randomext::setSeed (const unsigned int aiu_numSeed = 8)
   ```

Generates a random string to use as a seed, it also returns the string to be used in other executions.

[Function]

```
void randomext::setSeed (std::string aistr_seed_seq)
```

When you have a string as a seed, you assign it with this function.

The generation of random numbers is one of the most important aspects in the convergence to a solution through evolutionary algorithms. LEAC uses the improvements incorporated in the C++11 version with STL library, mersenne_twister_engine is a random number engine based on *Mersenne Twister* algorithm. It produces high quality unsigned integer random numbers of type *UIntType* on the interval $[0, 2^w - 1]$.

The file `random_ext.hpp` creates a global object *gmt19937_eng* of type mersenne_twister_engine, this object is used as a parameter to generate random numbers in a probability distribution, necessary for the implementation of several genetic operators. For your own implementations, you can create the object *gmt19937_eng*. For example, first the distribution is instantiated (see [std::uniform_real_distribution], page 91), with the created distribution and with the object *gmt19937_eng* as a parameter, a random number based on the distribution is obtained (see [get a random number], page 100).

9. Read the data set to be processed with any of the following functions:

[Function]

```
std::pair<std::vector<data::Instance<T_FEATURE>* >,
          std::vector<data::Instance<T_FEATURE>* > > inout::dataSetRead
          (inout::InParamReadInst<T_FEATURE,T_INSTANCES_CLUSTER_K,T_CLUSTERIDX>
           &aiipri_inParamReadInst)
```

[Function]

```
std::pair<std::vector<data::Instance<T_FEATURE>* >,
          std::vector<data::Instance<T_FEATURE>* > > inout::dataSetReadWithFreq
          (inout::InParamReadInstFreq
           <T_FEATURE,T_INSTANCES_CLUSTER_K,T_CLUSTERIDX,T_INSTANCE_FREQUENCY>
           &aiipri_inParamReadInstWithFreq)
```

The following example shows how to read a data set, which can have a class attribute and also test data:

```
auto lpairvec_dataset =  inout::dataSetRead(linparam_ClusteringGA);
```

10. Directly, include genetic operators in the main function or invoke directly the function that has the implementation of the new algorithm in the main function. At the end of writing your source code, your `main` function should have something similar to the following code:

```
#include <leac.hpp>
#include <datatype_instance_real.hpp>
#include <inparam_pcpmfk.hpp>
#include <inparamclustering_getparameter.hpp>
#include <outparam_gac.hpp>
#include <instances_read.hpp>

#include "kga_fkcentroid.hpp"

int main(int argc, char **argv)
{
  /*INPUT: PARAMETER
   */
```

```
  inout::InParamPcPmFk
    <DATATYPE_CLUSTERIDX,
     DATATYPE_REAL,
     DATATYPE_FEATURE,
     DATATYPE_FEATURE_SUM,
     DATATYPE_INSTANCES_CLUSTER_K
     >
    linparam_ClusteringGA
    ("KGA",
     "Bandyopadhyay and Maulik 2002",
     inout::CENTROIDS,
     INPARAMCLUSTERING_DISTANCE_EUCLIDEAN
     );

  linparam_ClusteringGA.setNumMaxGenerations(1000);
  linparam_ClusteringGA.setSizePopulation(50);
  linparam_ClusteringGA.setProbCrossover(0.8);
  linparam_ClusteringGA.setProbMutation(0.001);

  inparamclustering_getParameter(linparam_ClusteringGA, argc, argv);

  if ( linparam_ClusteringGA.getRandomSeed().size() == 0 ) {
     std::string lstr_seed_seq = randomext::setSeed();
     linparam_ClusteringGA.setRandomSeed( lstr_seed_seq );
  }
  else {
     randomext::setSeed(linparam_ClusteringGA.getRandomSeed());
  }

  auto lpairvec_dataset =  inout::dataSetRead(linparam_ClusteringGA);

  dist::Euclidean<DATATYPE_REAL,DATATYPE_FEATURE> funct2p_dist;

  inout::OutParamGAC
    <DATATYPE_REAL,
     DATATYPE_CLUSTERIDX>
    loop_outParamGAC(inout::SSE);

  auto lchrom_best =
    eac::kga_fkcentroid
    (loop_outParamGAC,
     linparam_ClusteringGA,
     lpairvec_dataset.first.begin(),
     lpairvec_dataset.first.end(),
     funct2p_dist
     );

  std::cout << "chrom_best: " << lchrom_best << std::endl;

  return 0;
}
```

11. With the source files completed, compile your new algorithm, with the following command:

    ‘`g++ -std=c++11 -D __VERBOSE_YES -I ../include -I ../include_inout/ -fopenmp kga_main.cpp -o kga`’

The '`-D __VERBOSE_YES`' option is optional to debug your program. For the `g++` version on the Mac OS X®, it should be (`>` = 4.8.5), example, use the `g++-mp-5` version.

If you did not install LEAC as described in section Chapter 2 [Get and Install LEAC software], page 5, and you want to compile an evolutionary algorithm using LEAC like the one shown in this section, you only need to install the gcc compiler, [step 3], page 5, for Windows® and [step 7], page 7, for GNU/Linux systems and Mac OS X®.

You can also compile your application with the other evolutionary algorithms provided by LEAC, adding the commands in the Makefile file for your new algorithm.

3.2 Run an Evolutionary Algorithm included in the library

This section shows how to run the algorithms located in the `eac` directory to find a solution to the clustering problem. The algorithms are categorized according to three aspects: the cluster number is fixed or variable, the coding of the solution by the algorithm (see Section 3.1.1 [Encoding criterion], page 11) and the similarity function (see Section 3.1.3.2 [Unsupervised measures], page 18).

To complete the practical examples, you should have completed the installation described in the Chapter 2 [Get and Install LEAC software], page 5, and have access to the `LEAC-1.2/bin` and `LEAC-1.2/data` directory. Add directly to the *PATH* variable, from a terminal (`cmd`), the directory where the binary or executable files are, for example: '`export PATH=$PATH:/home/user/LEAC-1.2/bin`' for GNU/Linux systems and Mac OS X®, or '`SET PATH=%PATH%;C:\LEAC-1.2\bin;`' for Windows® systems. For data set files '`cd c:\LEAC-1.2\data`' for Windows® or '`cd LEAC-1.2/data`' for GNU/Linux. You could have the directory in a different route, but in this case, you have to change the route.

The nomenclature used for the name of the programs is based on the three aspects described above. Name of the algorithm on which the program is based, number of clusters fixed or variable k and the coding used:

```
name_[fk|vk]coding
```

All EAC algorithms are executed from a terminal with online parameters. With the parameter '`--help`', You will get a description of the different options, there are two types of options, those that are common for all the programs and the particular ones of each algorithm, these last ones are shown after the message [Particular options of the algorithm], page 49,

For example, here it is shown the execution of the command: '`kga_fkcentroid --help`'. This is the output of the command:

```
Usage: ./kga_fkcentroid [OPTION]
       About groups of instances for a set K as well as statistics
       of the algorithm used

  -i, --instances=FILE or DIRECTORY
                              file or directory containing data of instances
                                to be clustered
  -x, --select-instances[=PREFIX]
                              if instances is directory search files with
                                prefix for training (eg. iris-10-1tra.dat,
                                iris-10-2tra.dat,... PREFIX=tra.dat)
  -t, --test[=FILE or PREFIX] if instances is directory search files with
                                prefix for test (eg. iris-10-1tst.dat,
```

```
                              iris-10-2tst.dat,... PREFIX=tst.dat),
                              in other case only name file
-b  --format-file[=NAME]      uci, or keel, by default uci
-h, --with-header[=yes/no]    file contains names of instances or a header,
                              by default is no
-u, --number-instances[=NUMBER]
                              the number of instances the file contains
                              instances, if not specified file is obtained
-a, --select-attributes[=ARG]
                              select the attributes to be processed for
                              example, "1-2,4" by default all. Also
                              used to specify the  number of dimensions
                              of the instances, unless specified file is
                              obtained instances
-d, --delimit-attributes=[ARG]
                              separated file by default ","
-c, --class-column[=NUMBER]   input file of instances has a class assigned
                              in the column [NUMBER=undefined]
-e, --cluster-column[=NUMBER]
                              input file of instances has a cluster assigned
                              in the column [NUMBER=undefined]
-l, --idinstances-column[=NUMBER]
                              the input file instance is assigned a column
                              instance identifier [NUMBER=undefined]
-f, --freq-instances-column[=NUMBER]
                              the input file instance is assigned a column
                              frequency instances [NUMBER=undefined]
-r, --number-runs[=NUMBER]    number of runs or repetitions of the algorithm
                              (by default [NUMBER=1])
-R, --runtime-filename=[FILE]
                              out file of times run
-n  --distance[=NAME]         euclidean, euclidean_sq, euclidean_induced,
                              diagonal_induced, or mahalonobis_induced,
                              by default euclidean
-z, --random-seed[=NUMBER]    string with integer number seed by, default
                              is random
-w, --max-execution-time[=NUMBER]
                              real number for max execution time in seconds
                              by default is 36000
-C, --centroids-outfile[=FILE]
                              print centroids,standard output FILE=stdout
    --centroids-format[=yes/no]
                              print the matrices by rows and columns,
                              by default is no
-M, --membership-outfile[=FILE]
                              print membership of the instances,
                                 standard output FILE=stdout
-T, --partitionstable-outfile[=FILE]
                              print partitions table of the instances,
                              standard output FILE=stdout
    --table-format[=yes/no]
                              print the partitions table by rows and
                              columns, by default is no
-P, --gnuplot=FILE            file of  gnuplot to graphics result
                              (compiling only with WITHOUT_PLOT_STAT)
-y, --gnuplot-styles=WORD     plot graphics with: points, lines,
                              linespoints, and dot [ARG=linespoints]
```

```
Particular options of the algorithm KGA
  based on Bandyopadhyay and Maulik 2002
      --number-clusters[=NUMBER]
                              number of clusters [NUMBER=3]
      --generations[=NUMBER]  number of generations or iterations
                               [NUMBER=1000]
      --population-size[=NUMBER]
                              size of population [NUMBER=50]
      --crossover-probability[=NUMBER]
                              real number in the interval [0.25, 1]
                                [NUMBER=0.8]
      --mutation-probability[=NUMBER]
                              real number in the interval [0, 0.5]
                                [NUMBER=0.001]

  -v, --verbose[=NUMBER]      explain what is being done (compiled with
                                VERBOSE=yes)
                              NUMBER=[-1,..,9999] Quiet level -1 not,
                                verbose, default=-1
  -q, --bar-progress          progress bar printing,  default is not
  -?, --help                  help
```

To run any of the programs successfully, the only mandatory parameter is '`-i, --instance`' (data set that should be processed), all other parameters are taken by default proposed by the authors of the algorithms.

For all the evolutionary algorithms studied in this work, the parameters share are:

`--generations`
`--population-size`
: They only vary in the number of generations and the size of population proposed by the different authors.

The following sections describe the evolutionary algorithms currently included in the LEAC library, based on taxonomy proposed by Hruschka et al. [HCFdC09], *k-fixed* vs. *k-variable* and the coding they use to represent the chromosomes, see Table 1.1. The description of each algorithm is based on the distinctive parameters which are significant to run it. For details, it is recommended to consult the included bibliography. We also include practical examples to run a clustering algorithm with real data sets provided by UC Irvine Machine Learning Repository.

3.2.1 Genetic algorithms for fixed k-clusters

3.2.1.1 Based on the centroids

The GAs in this section seek to find the centroids of the cluster for a user-defined k. If you are looking to locate with precision the centroid of the clusters, these algorithms are a good option. They encode the solutions as a string with the coordinates of the centroids consecutively, see [real encoding], page 13. The GAs implemented in this class are listed below:

1. **gas_fkcentroid**

   It is based on [MB00]. It optimizes the SED measure (see [SED], page 18). It uses one point crossover encoded in the function `gagenericop::onePointCrossover` and

a proposed mutation operator encoded in the function `garealop::randomMutation`, both operators apply with fixed probability.

Parameters of the algorithm:

`--crossover-probability[=NUMBER]`
real number in the interval `[0.25, 1]` `[NUMBER=0.8]`

`--mutation-probability[=NUMBER]`
real number in the interval `[0, 0.5]` `[NUMBER=0.001]`

Execution samples:

- 'gas_fkcentroid -i iris.data -a "1-4"'
- 'gas_fkcentroid -i iris.data -a "1-4" -c 5 --number-clusters 3 --generations 100 --population-size 100 --crossover-probability 0.8 --mutation-probability 0.2 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout'

2. **kga_fkcentroid**

It is based on [BM02a]. It optimizes the SED measure (see [SED], page 18). It uses the traditional crossover operator `gagenericop::onePointCrossover` and it proposes a new mutation operator `gaclusteringop::biDirectionHMutation`, used in other algorithms.

Parameters of the algorithm:

`--crossover-probability[=NUMBER]`
real number in the interval `[0.25, 1]` `[NUMBER=0.8]`

`--mutation-probability[=NUMBER]`
real number in the interval `[0, 0.5]` `[NUMBER=0.001]`

Execution sample: see [Illustrative execution samples: Libras Movement Data Set], page 55.

3. **gagr_fkcentroid**

It is based on [CZZ09]. It optimizes the SSE measure (see [SSE], page 18). For the crossover of the chromosomes, it uses two operators `gagenericop::GAGRdist` and `garealop::heuristicCrossover`, and for the mutation, it use the mutation operator defined in `gaclusteringop::biDirectionHMutation`. For the application of the operators, the algorithm uses an adaptive probability. Therefore, the parameters that it receives are only those shared by the evolutionary algorithm `--generations` and `--population-size`.

Execution sample: see [Illustrative execution samples: Wine data set], page 52,

4. **cbga_fkcentroid_int** and **cbga_fkcentroid**

It is based on [FKKN97]. It optimizes the Distortion measure (see [Distortion], page 20). This algorithm was initially applied for the processing of images to work with integers due to the parameterization of the functions in LEAC. It is possible to obtain another version for the domain of the real numbers.

It uses the `gaclusteringop::crossPNNnew` crossing operator and the `clusteringop::randomInitialize` mutation operator. In [FKKN97], they propose different selection methods.

Parameters of the algorithm:

`--mutation-probability[=NUMBER]`
real number in the interval `[0, 1.0] [NUMBER=0.01]`

`--select-method[=NAME]`
roulette, elitist1, elitist2, or zigzag, by default elitist1

`--gla-iterations[=NUMBER]`
number of GLA iterations `[NUMBER=0]`

Execution samples:

- '`cbga_fkcentroid -i iris.data -a "1-4"`'
- '`cbga_fkcentroid -i iris.data -a "1-4" -c 5 --number-clusters 3 --generations 100 --population-size 100 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout`'

Illustrative execution sample: Wine data set

Next, we describe the steps to execute GAGR algorithm based on [CZZ09] and discuss the parameters that can be used to carry out an experimental study.

For the following example, we will analyze the wine data set. First, you must download the wine.data file and store it in the `data` directory, all data sets used in the following illustrative examples should be stored in this directory.

Since the domain of the attributes is different for the wine.data, it is convenient to standardize them, for this, it is used `stdvar_milligan_cooper1988` based on [MC88]. It is available as support for the normalization of the data set. Before executing the commands, you have to make sure you have access to the executable and the data, see [configuration of the PATH variable], page 48.

'`stdvar_milligan_cooper1988 -i wine.data -a "2-14" -c 1 --std-var Z1 > wine_std.data`'

The Wine data set includes 13 variables from column 2 to column 14 and the class on column 1, therefore, the `-a` or `--select-attributes` parameter is `"2-14"`, the class is in column 1, the parameter `-c` or `--class-column` it must be assigned to 1. The transformation that applies to the variables in this case is *z-score* $Z_1 = (x_{il} - \bar{x}_{*l})/s_{*l}$, where x_{il} is the original data value, and $\bar{x}_{*l}$ and s_{*l} are the sample mean and standard deviation, respectively.

Next, algorithm GAGR [CZZ09] will be run, for the normalized data:

'`gagr_fkcentroid -i wine_std.data -a "1-13" -c 14 --number-clusters 3 --print-mulline yes -C stdout --centroids-format yes -M stdout`'

The attributes are now in columns `"1-13"` and the class in column `14`, because the `stdvar_milligan_cooper1988` program in the output file writes the class in the last column. Parameters with uppercase letters are used for the output. '`-C stdout`' indicates that the output of the centroids found by the program is formatted with '`--centroids-format yes`'. The parameter '`-M stdout`' generates a string of the membership labels of the instances in a cluster calculated with equation 3.2.

A possible result for a partition of three clusters ('`--number-clusters 3`') by the GAGR algorithm is:

```
IN:
```

```
    Algorithmo name: GAGR
           Based on: Dong-Xia Chang and Xian-Da Zhang and Chang-Wen Zheng 2009
        Metric used: SSE

           Data set: wine_std.data
Number of instances: 178
         Dimensions: 13

       Random seed: 2330791922 722590507 2437171925 3046485563 2392633958 2970292677
       3353564338 489582404

OUT:

CROMOSOME:BEST:objetive,1274.2,fitness,0.000784804:0.160439,0.88665,0.212095,0.571924,
-0.126608,-0.99909,-1.23221,0.753954,-0.734194,0.955193,-1.17759,-1.28076,-0.396717,
0.894248,-0.293909,0.297414,-0.676197,0.580441,0.882434,0.944615,-0.589229,0.603343,
0.184902,0.44739,0.758496,1.14392,-0.890931,-0.401072,-0.46444,0.103152,-0.429416,
-0.0743665,0.0441158,-0.0771312,-0.0284121,-0.843627,0.404469,0.225602,-0.691161

       Cluster number (K): 3
                      SSE: 1274.2
                      SED: 450.099
                DB-index: 1.41154
              Silhouette: 0.284617
                      VRC: 69.9363
              CS measure: 0.412355
            Dunn's index: 0.232257
     Execution time (seg): 0.303483
Generations find the best: 46


Centroids:

  Col:    0            1            2            3            4
  Row

    0: 0.160439     0.88665      0.212095     0.571924     -0.126608
    1: 0.894248     -0.293909    0.297414     -0.676197    0.580441
    2: -0.890931    -0.401072    -0.46444     0.103152     -0.429416

  Col:    5            6            7            8            9
  Row

    0: -0.99909     -1.23221     0.753954     -0.734194    0.955193
    1: 0.882434     0.944615     -0.589229    0.603343     0.184902
    2: -0.0743665   0.0441158    -0.0771312   -0.0284121   -0.843627

  Col:    10           11           12
  Row

    0: -1.17759     -1.28076     -0.396717
    1: 0.44739      0.758496     1.14392
    2: 0.404469     0.225602     -0.691161

<MEMBERCLUSTERTRAINING,_algorithmo,GAGR,_author,Dong-Xia Chang and Xian-Da Zhang
and Chang-Wen Zheng 2009,_runnig date,20180430:185944,_number run,1,_runnig date,
20180430:185944,_number run,1,_times run,1,_dataset_training,wine_std.data,_outK,3,
PartitionCentroids[50:0x7fffac569a20],length,178>1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,
```

```
1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,
2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,1,2,2,2,2,2,2,2,2,2,0,2,2,2,2,2,2,2,2,2,2,1,2,2,2,2,2,
2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,0,2,2,1,2,2,2,2,2,2,2,2,0,0,0,0,0,0,0,0,0,0,0,
0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
```

The '`-C -M`' uppercase options print the centroids and the membership label of each instance to a cluster, respectively. In this case, the '`stdout`' parameter makes the standard output. The printing format for the centroids is matrixed by the option '`--centroids-format yes`', you can also specify the result in a line of text delimited by special characters, to use the output in another program, as it is shown below.

In addition to the measure of similarity used by the algorithm, the program calculates other ones that can be used to evaluate the goodness of the grouping. See Section 3.1.3.2 [Unsupervised measures], page 18.

To repeat the same result of the program, you can use the '`-z`' option and as parameter the string that was used as seed to generate the random numbers. Now the output will be sent to the `wine_centroids.data` and `wine_membership.data` files, without the option '`--centroids-format yes`', to visualize the results later:

'`gagr_fkcentroid -i wine_std.data -a "1-13" -c 14 --number-clusters 3 --print-mulline yes -C wine_centroids.data -M wine_membership.data -z "2330791922 722590507 2437171925 3046485563 2392633958 2970292677 3353564338 489582404"`'

The program `plot_clustering` is another EAC utility, which allows to visualize a data set, with the results obtained from the different programs. An example of how to use Gnuplot is to use the command: `plot_clustering` with the following parameters:

'`plot_clustering -i wine_std.data -a "1-13" -c 14 --projection pca --centroids-infile wine_centroids.data --member-infile wine_membership.data --graphics-outfile wine_cluster`'

You get the `eps` file `wine_cluster1.eps` and which is shown in Figure 3.6. To see the eps files in the case of Windows®, you can use the see [epsviewer], page 6, program.

You can also omit the option '`--graphics-outfile`' and the drawing can be manipulated interactively in both `2D` and `3D`, you can use the following command:

'`plot_clustering -i wine_std.data -a "1-13" -c 14 --projection pca --centroids-infile wine_centroids.data --member-infile wine_membership.data --x-coord 1 --y-coord 2 --z-coord 3`'

Since the objects in the data set have multiple dimensions, it is advisable to use a Principal Component Analysis (PCA) with the option '`--projection pca`'

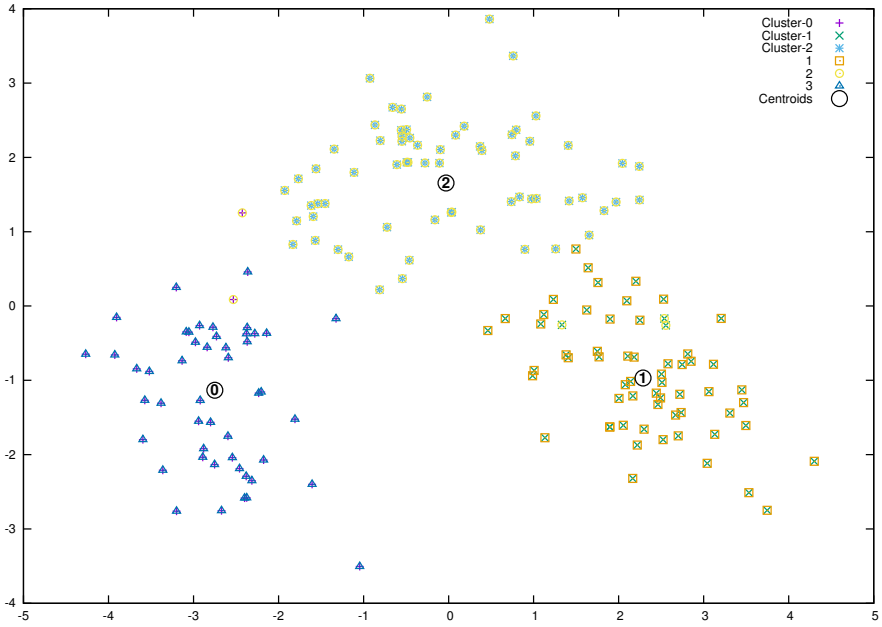

Figure 3.6: Clusters of Wine data set, obtained with `gagr_fkcentroid`

Illustrative execution sample: Libras Movement Data Set

In the following illustrative example, it has two objectives. The first is to obtain the average hand movement of the Libras Movement Data Set, assuming that the data set can be partitioned into 15 clusters. The second objective is to test the quality of the grouping with a set of training data. We will use the KGA algorithm [BM02a]. Before executing the commands, make sure you have access to the executable files and the data, see [configuration of the PATH variable], page 48.

In all programs, it is possible to use part of the data set for *training* and another part for *test*, to make easier to carry out an experimental study. To determine the ownership of the test data, the equation of the nearest centroid-instance is used in equation 3.2.

To demonstrate how to process a data set with training and test data, you can use the movement_libras.data and movement_libras_1.data files.

To obtain better results in the data mining process, it is important to have knowledge about the data set. Libras Movement data set is formed by the coordinates of a two-dimensional curves of the movement of the hand with domain and range to be betweeen $\hat{a}1$ and 1. To have better accuracy, we center to $(0.5, 0, 5)$ each curve of the training data set, with the following awk script:

```
#run:
# 'awk -f movement_libras_trans.awk -F "," -v OFS="," 
   movement_libras.data  > movement_libras_trans.data'

    for(i=1;i< NF;i++) sumcoord1+=$i; i++; sumcoord2+=$i ;
    numpoint = (NF-1) / 2.0;
    xd = 0.5 - sumcoord1/numpoint;
```

```
yd = 0.5 - sumcoord2/numpoint;
sumcoord1=0; sumcoord2=0;
for(i=1;i< NF;i++) $i +=  xd;  i++; $i += yd ;
for(i=1; i<=NF; i++) printf "%s",$i (i==NF?ORS:OFS)
```

The `movement_libras_trans.awk` file of the script can be found in the `data` folder:

'`awk -f movement_libras_trans.awk -F "," -v OFS="," movement_libras.data > movement_libras_trans.data`'

With the transformed data set we apply the KGA algorithm:

'`kga_fkcentroid -i movement_libras_trasn.data -t movement_libras_1.data -a "1-90" -c 91 --print-mulline yes -C c_movement_libras.data -T stdout --table-format yes --number-cluster 15`'

A possible result of the program is the following:

```
IN:
    Algorithmo name: KGA
           Based on: Bandyopadhyay and Maulik 2002
        Metric used: SED

           Data set: movement_libras_trasn.data
Number of instances: 360
         Dimensions: 90

      Data set test: movement_libras_1.data
Number of instances: 45

       Random seed: 2127474194 2277915873 2997828778 567204173 2395445691
       1861208675 35718978 101314263

OUT:

CROMOSOME:BEST:objetive,209.665,fitness,0.00476951:0.545241,0.779453,
0.544903,0.779338,0.542145,0.778586,0.539438,0.776675,0.534216,0.773666,
...
0.462735,0.320573,0.457353,0.311718,0.452307,0.306383,0.451046,0.302055

       Cluster number (K): 15
                      SED: 209.665
                DB-index: 1.15626
              Silhouette: 0.284789
                      VRC: 87.1936
              CS measure: 1.36284
            Dunn's index: 0.0855026

            Test data SED: 52.8738 Has group without objects
      Test data DB-index: 3.59388
    Test data Silhouette: -0.103324
           Test data VRC: 0.721814
    Test data CS measure: 1.76497
  Test data Dunn's index: 0.0650252
   Execution time (seg): 85.0431
Generations find the best: 56


Partition table:
```

Cluster:	0	1	2	3	4
Class					
1:	0	0	10	0	0
2:	0	0	11	0	0
3:	0	0	0	0	0
4:	0	0	0	0	0
5:	0	6	0	0	17
6:	0	0	0	7	0
7:	0	0	0	0	0
8:	14	0	0	0	0
9:	0	0	0	0	0
10:	0	0	0	0	0
11:	11	0	0	0	0
12:	0	0	0	0	0
13:	15	0	0	0	0
14:	0	6	0	14	1
15:	0	0	0	0	0
sum:	40	12	21	21	18

Cluster:	5	6	7	8	9
Class					
1:	0	0	0	8	0
2:	0	0	0	5	0
3:	0	0	23	0	0
4:	0	12	0	0	3
5:	1	0	0	0	0
6:	0	7	0	0	0
7:	0	0	0	0	20
8:	0	0	0	0	0
9:	0	0	0	0	0
10:	7	0	0	0	15
11:	0	0	0	0	0
12:	0	0	0	0	24
13:	0	0	0	0	0
14:	0	0	0	0	3
15:	12	0	0	0	4
sum:	20	19	23	13	69

Cluster:	10	11	12	13	14
Class					
1:	6	0	0	0	0
2:	6	0	0	2	0
3:	0	0	0	1	0
4:	0	0	8	1	0
5:	0	0	0	0	0
6:	0	0	9	1	0
7:	0	0	0	4	0
8:	0	0	0	1	9
9:	0	0	0	24	0
10:	0	0	0	2	0
11:	0	9	0	0	4
12:	0	0	0	0	0
13:	0	7	0	0	2
14:	0	0	0	0	0
15:	0	0	0	0	8

```
    sum: 12          16          17          36          23

Cluster: sum
Class

      1: 24
      2: 24
      3: 24
      4: 24
      5: 24
      6: 24
      7: 24
      8: 24
      9: 24
     10: 24
     11: 24
     12: 24
     13: 24
     14: 24
     15: 24
    sum: 360

            Rand index: 0.915877
               Purity: 0.552778
            Precision: 0.385553
               Recall: 0.527295


Partition table test:

Cluster: 0           1           2           3           4
Class

      1: 0           0           2           0           0
      2: 0           0           1           0           0
      3: 0           0           0           0           0
      4: 0           0           0           0           0
      5: 0           1           0           0           2
      6: 0           0           0           0           0
      7: 0           0           0           0           0
      8: 1           0           0           0           0
      9: 0           0           0           0           0
     10: 0           0           0           0           0
     11: 1           0           0           0           0
     12: 0           0           0           0           0
     13: 0           0           0           0           0
     14: 0           0           0           0           0
     15: 0           0           0           0           0
    sum: 2           1           3           0           2

Cluster: 5           6           7           8           9
Class

      1: 0           0           0           1           0
      2: 0           0           0           2           0
      3: 0           0           3           0           0
      4: 0           1           0           0           0
      5: 0           0           0           0           0
```

```
      6: 0            2            0            0            0
      7: 0            0            0            0            3
      8: 0            0            0            0            0
      9: 0            0            0            0            0
     10: 0            0            0            0            3
     11: 0            0            0            0            0
     12: 0            0            0            0            3
     13: 0            0            0            0            0
     14: 0            0            0            0            3
     15: 0            0            0            0            3
    sum: 0            3            3            3            15

Cluster: 10           11           12           13           14
Class

      1: 0            0            0            0            0
      2: 0            0            0            0            0
      3: 0            0            0            0            0
      4: 0            0            2            0            0
      5: 0            0            0            0            0
      6: 0            0            1            0            0
      7: 0            0            0            0            0
      8: 0            0            0            0            2
      9: 0            0            0            3            0
     10: 0            0            0            0            0
     11: 0            2            0            0            0
     12: 0            0            0            0            0
     13: 0            3            0            0            0
     14: 0            0            0            0            0
     15: 0            0            0            0            0
    sum: 0            5            3            3            2

Cluster: sum
Class

      1: 3
      2: 3
      3: 3
      4: 3
      5: 3
      6: 3
      7: 3
      8: 3
      9: 3
     10: 3
     11: 3
     12: 3
     13: 3
     14: 3
     15: 3
    sum: 45

    Test data Rand index: 0.879798
        Test data Purity: 0.577778
     Test data Precision: 0.227941
        Test data Recall: 0.688889
```

With the option '`-T, --partitionstable-outfile`', you get the confusion matrix and with the '`-t`' option for training and test. As well as, it is shown measures related to the previous classification of the objects, called supervised measures.

The centroids, besides serving to represent the centers of the clusters, also have a meaning that depends on the domain of the problem. In the libras data set, centroids represent the mean movement of the hand in a two-dimensional curve made in a period of time. The centroids obtained in the execution are shown in Figure 3.7.

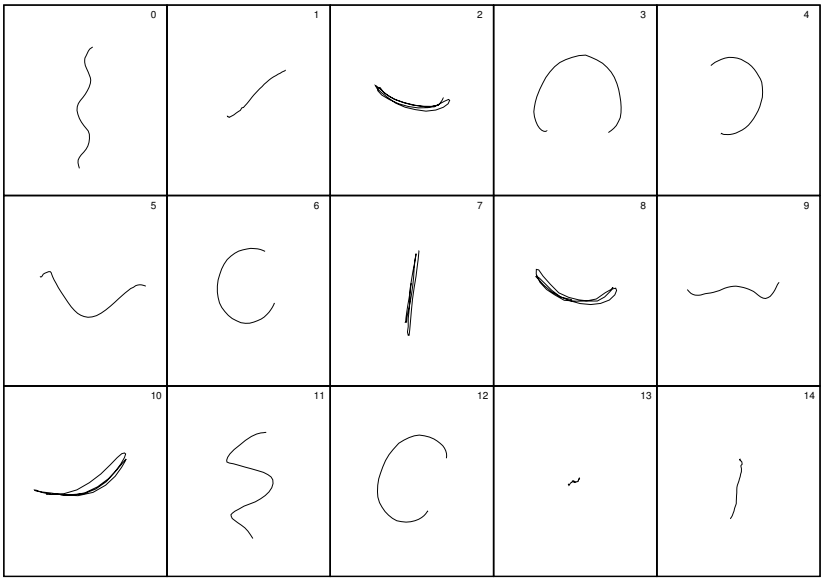

Figure 3.7: Average of the movements of the libras data set obtained with the program `kga_fkcentroid`

3.2.1.2 Based on cluster label

The GAs in this section use the coding described in [string-of-group-numbers encoding], page 12. The algorithms included in LEAC are the following:

1. **gaclustering_fklabel**

   It is based on [MC96]. It optimizes the SED measure (see [SED], page 18). It uses the operator `gagenericop::onePointCrossover` and `gaintegerop::mutation` (change a random gene). The classification of these operators can be considered *object-oriented*, that randomly they move objects among clusters. They propose a small population size, which makes a guided exploration around the best solution, with a fixed crossing probability and a mutation probability with a default value high 0.5 and decreasing in each generation until reaching $1/n$.

   Parameters of the algorithm:

   `--crossover-probability[=NUMBER]`
   real number in the interval `[0.25, 1]` `[NUMBER=0.8]`

`--mutation-probability[=NUMBER]`
real number in the interval `[0, 0.5]` `[NUMBER=0.5]`

Execution samples:

- 'gaclustering_fklabel -i iris.data -a "1-4"'
- 'gaclustering_fklabel -i iris.data -a "1-4" -c 5 --number-clusters 3 --generations 10000 --population-size 6 --crossover-probability 0.8 --mutation-probability 0.5 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout'

2. **gka_fklabel**

   It is based on [KM99]. It optimizes the TWCV measure (see [TWCV], page 18). The authors of this algorithm propose not to use the crossover operator, instead they use the `k-means algorithm`. LEAC implements several variants of the `k-means algorithm`, including the algorithm used by this algorithm ([clusteringop::kmeansoperator], page 39). Mutation operator changes an gene value depending on the distances of the cluster centroids from the corresponding instance. It can be assigned to another group by the following probability distribution associated with each gene.

   Parameters of the algorithm:

   `--mutation-probability[=NUMBER]`
   real number in the interval `[0, 1.0]` `[NUMBER=0.05]`

   Execution sample:

   'gka_fklabel -i iris.data -a "1-4" -c 5 --number-clusters 3 --generations 200 --population-size 50 --mutation-probability 0.05 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout'

3. **igka_fklabel** is based on [LLF+04b], and **fgka_fklabel** is based on [LLF+04a]. These two proposals are inspired by [KM99]. They optimize the TWCV measure (see [TWCV], page 18). Define a legality ratio $e(Ch_i)$ for each Ch_i chromosome, associate with the number of non-empty clusters in the solution obtained by Ch_i divided by number of clusters k. $e(Ch_i)$ is legal if $e(Ch_i) = 1$, and illegal, otherwise. The legality ratio together with the value of TWCV define the fitness function that will guide the evolution of the algorithm.

   Parameters of the algorithm:

   `--mutation-probability[=NUMBER]`
   real number in the interval `[0, 1.0]` `[NUMBER=0.05]`

   Execution sample:

   'igka_fklabel -i iris.data -a "1-4" -c 5 --number-clusters 3 --generations 200 --population-size 50 --mutation-probability 0.05 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout'

3.2.1.3 Based on the most representative

These algorithms attempt to partition the data by assigning each object to a representative and then optimizing a unsupervised measures (Section 3.1.3.2 [Unsupervised measures], page 18).

1. **gaprototypes_fkmedoid**

   It is based on [KB97]. It optimizes the J_1 measure (see [J_1], page 21). It uses a binary encoding, see [Binary encoding for medoid-based], page 14.

   Parameters of the algorithm:

   `--crossover-probability[=NUMBER]`
   : real number in the interval `[0.25, 1]` `[NUMBER=0.5]`

   `--mutation-probability[=NUMBER]`
   : real number in the interval `[0, 0.5]` `[NUMBER=0.015]`

   `--probability-ini[=NUMBER]`
   : real number in the interval `[0.01, 0.1]` depending n and k, if -1 is eq k/n `[NUMBER=-1]`

   `--alpha[=NUMBER]`
   : real number `alpha > 0` to force the algorithm desired number cluster `[NUMBER=10]`

   The parameter `--probability-ini` serves for the initialization of the chromosomes, each gene in a chromosome has the value 1 with a especified probability `--probability-ini`. The genetic operators used are `gabinaryop::uniformCrossover` where the parent chromosomes swap their i-th genes with a certain probability (`--crossover-probability`) and `gabinaryop::eachBitArrayMutation` where each gene de each offspring chromosome alternates with a specified probability (`--mutation-probability`). To avoid the generating invalid offspring for fixed k, the parameters must be adjusted together with `--alpha`.

   Execution sample:

   ‘`gaprototypes_fkmedoid -i iris.data -a "1-4" -c 5 --number-clusters 3 --generations 500 --population-size 20 --crossover-probability 0.5 --mutation-probability 0.015 --probability-ini 0.02 --alpha 100 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout`’

2. **gca_fkmedoid**

   It is based on [LDK93], optimize to SEDmedoid (see [SEDmedoid], page 20). Individuals are coded as string of integers of length k. Each integer number of the string corresponds to the index of the most representative instance of the cluster. This algorithm uses two new genetic operators *mix subset recombination* D_MX and *point mutation*, D_PM. D serves to remind the fact that direct encoding rather than binary. In the LEAC library they are coded with the `gaintegerop::recombinationD_MX` and `gaintegerop::mutationD_PM` functions.

   Parameters of the algorithm:

   `--mix-recombination-probability[=NUMBER]`
   : real number in the interval `[0.5, 0.9]` `[NUMBER=0.9]`

   `--point-mutation-probability[=NUMBER]`
   : real number in the interval `[0.2, 0.4]` `[NUMBER=0.4]`

   `--mix-mutation-probability[=NUMBER]`
   : real number in the interval `[0, 0.125]` `[NUMBER=0.125]`

The first two parameters establish the frequency of application of genetic operators D_MX and D_PM. The third parameter adds new material in the application of D_MX.

Execution sample:

'`gca_fkmedoid -i iris.data -a "1-4" -c 5 --number-clusters 3 --generations 200 --population-size 200 --mix-recombination-probability 0.9 --point-mutation-probability 0.4 --mix-mutation-probability 0.125 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout`'

3. **hka_fkmedoid**

   It is based on [SL04]. It optimizes the SEDmedoid measure (see [SEDmedoid], page 20). This algorithm is inspired in [LDK93]. It contains one step of a `local heuristic search` to accelerate convergence and it proposes a heuristic search operator equivalent to `k-means algorithm`, but for medoids. The local heuristic search is implemented in the `clusteringop::updateMedoids` function. See [local heuristic search], page 39.

   Parameters of the algorithm:

   `--mix-recombination-probability[=NUMBER]`
   real number in the interval `[0.5, 0.9]` `[NUMBER=0.95]`

   `--point-mutation-probability[=NUMBER]`
   real number in the interval `[0.2, 0.4]` `[NUMBER=0.02]`

   `--mix-mutation-probability[=NUMBER]`
   real number in the interval `[0, 0.125]` `[NUMBER=0.05]`

   `--order-tournament[=NUMBER]`
   order of tournament `[NUMBER=2]`

   `--nearest-neighbors[=NUMBER]`
   number of the nearest neighbors (p) `[NUMBER=3]`

   `--search-heuristic-probability[=NUMBER]`
   real number in the interval `[0.0, 1.0]` `[NUMBER=0.2]`

   Execution sample: see [Illustrative execution samples: Iris Data Set], page 63.

Illustrative execution sample: Iris Data Set

As an illustrative example of algorithms that find the most representative instances for each cluster, we describe the `hka_fkmedoid` program based on the HKA algorithm [SL04]. Before executing the commands, you have to make sure you have access to the executable files and the data, see [configuration of the PATH variable], page 48.

Now, let's illustrate how to find the most representative instances of the iris.data. You can run the program with the following parameters:

'`hka_fkmedoid -i iris.data -a "1-4" -c 5 --number-clusters=3 --print-mulline yes -C c_hka_iris.dat -M m_hka_iris.dat`'

A possible output from this running would be:

```
IN:
    Algorithmo name: HKA
           Based on: Weiguo Sheng and Xiaohui Liu
        Metric used: SED
```

```
           Data set: iris.data
Number of instances: 150
         Dimensions: 4

       Random seed: 4253005715 70818531 1631842517 1223368670 2252683652
       1178029056 3404574059 1048346743

OUT:

CROMOSOME:BEST:objetive,98.2137,fitness,0.0101819:7,78,112

       Cluster number (K): 3
                      SED: 98.2137
                DB-index: 0.811606
              Silhouette: 0.552592
                      VRC: 494.895
              CS measure: 0.155418
            Dunn's index: 0.0988074
     Execution time (seg): 0.072937
Generations find the best: 69
```

For this execution, the most representative instances for each Iris cluster are:

ID	SepalLength	SepalWidth	PetalLength	PetalWidth	Class
7	5	3.4	1.5	0.2	Iris-setosa
78	6	2.9	4.5	1.5	Iris-versicolor
112	6.8	3	5.5	2.1	Iris-virginica

To visualize the results:

'`plot_clustering -i iris.data -a "1-4" -c 5 --centroids-infile c_hka_iris.dat --member-infile m_hka_iris.dat --centroids-title "Medoid" --graphics-outfile hka_iris`'

Graphically, the prototypes and groups are shown in Figure 3.8.

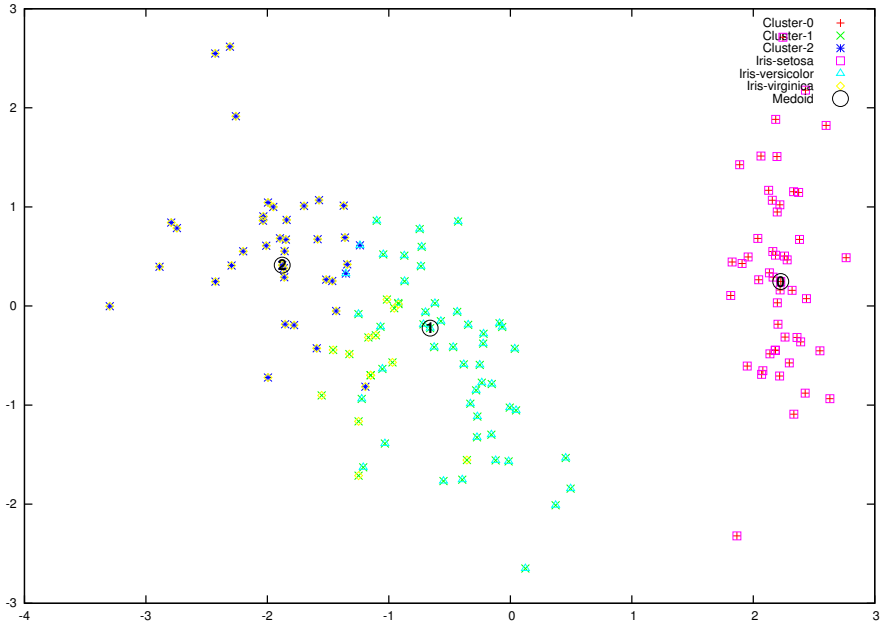

Figure 3.8: The most representative instances of the Iris data set obtained with the program '`hka_fkmedoid`'

3.2.2 Genetic algorithms for variable k-clusters

The GAs described in the following sections obtain both the best cluster number (k^*) and its content.

The common parameters in these algorithms are:

`--k-minimum[=NUMBER]`
: number of clusters by default `[NUMBER=2]`

`--k-maximum[=NUMBER]`
: Some authors leave it to the user's criteria, others propose a predetermined value based on the size of the data set, such as $n/2$ or $n^{1/2}$, most agree with the latter.

3.2.2.1 Based on the centroids

The GAs in this section use a real encoding (see [real encoding], page 13) with some variant to allow the search of the optimum k. The algorithms included in LEAC are the following:

1. **gcuk_vkcentroid**

   It is based on [BM02b]. It optimizes the SSE measure [DB], page 22. Individuals are coded as strings of real numbers that represent the coordinates of the centroids combined with `#` symbols that allow the diversity of chromosomes with different k. Genetic operators used are `gaclusteringop::onePointCrossover` and `gaclusteringop::randomMutation`.

   Parameters of the algorithm:

`--crossover-probability[=NUMBER]`
real number in the interval `[0.25, 1]` `[NUMBER=0.8]`

`--mutation-probability[=NUMBER]`
real number in the interval `[0, 0.5]` `[NUMBER=0.001]`

Execution sample: see [Illustrative execution samples: Zoo Data Set], page 66.

2. **tgca_vkcentroid**

It is based on [HT12]. It optimizes the VRC measure ([VRC], page 25). First, TGCA focuses on the search of the best number of clusters, and then gradually transfers towards finding the globally optimal cluster centers. Furthermore, a maximum attribute range partition approach is used in the population initialization so as to overcome the sensitivity of clustering algorithms to initial partitions [HT12].

Parameters of the algorithm:

`--num-subpopulations-cross[=NUMBER]`
number of subpopulations for parallel crossover. It must be less than half the size compared to the population [NUMBER=4]

`--crossover-probability[=NUMBER]`
real number in the interval [0.25, 1] [NUMBER=0.8]

`--kmeans-iterations[=NUMBER]`
maximum number of iterations for k-means algorithm [NUMBER=100]

`--kmeans-threshold[=NUMBER]`
threshold value for k-means algorithm [NUMBER=0]

Execution sample:

‘`tgca_vkcentroid -i iris.data -a "1-4" -c 5 --population-size 200 --num-subpopulations-cross 4 --crossover-probability 0.8 --generations 200 --kmeans-iterations 100 --kmeans-threshold 0 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout`’

Illustrative execution sample: Zoo Data Set

Next, it is shown an example of the `gcuk_vkcentroid` algorithm using Zoo data set. The zoo.data has 7 classes with 17 attributes. All attributes are binary, with the exception of number 14, which can be seen as nominal. Before executing the commands, you have to make sure you have access to the executable files and the data, see [configuration of the PATH variable], page 48.

To process it, the data set can be transformed into binary with the following `awk` script:

```
#run:
# awk -f zoo_binary.awk -F ',' -v OFS=','  zoo.data > zoo_bin.csv
BEGIN {
    h1 = "animalname";
    h2 = "hair";
    h3 = "feathers";
    h4 = "eggs";
    h5 = "milk";
    h6 = "airborne";
    h7 = "aquatic";
```

```
    h8 = "predator";
    h9 = "toothed";
    h10 = "backbone";
    h11 = "breathes";
    h12 = "venomous";
    h13 = "fins";
    h14 = "legs_0,legs_2,legs_4,legs_5,legs_6,legs_8";
    h15 = "tail";
    h16 = "domestic";
    h17 = "catsize";
    h18 = "type";
    print h1,h2,h3,h4,h5,h6,h7,h8,h9,h10,h11,h12,h13,h14,h15,h16,h17,h18;
}
{
# legs:Numeric (set of values: 0,2,4,5,6,8)
    if ( $14 == 0)
        $14 = "1,0,0,0,0,0";
    else if ($14 == 2)
        $14 = "0,1,0,0,0,0";
    else if ($14 == 4)
        $14 = "0,0,1,0,0,0";
    else if ($14 == 5)
        $14 = "0,0,0,1,0,0";
    else if ($14 == 6)
        $14 = "0,0,0,0,1,0";
    else if ( $14 == 8)
        $14 = "0,0,0,0,0,1";
    print $1,$2,$3,$4,$5,$6,$7,$8,$9,$10,$11,$12,$13,$14,$15,$16,$17,$18
}
```

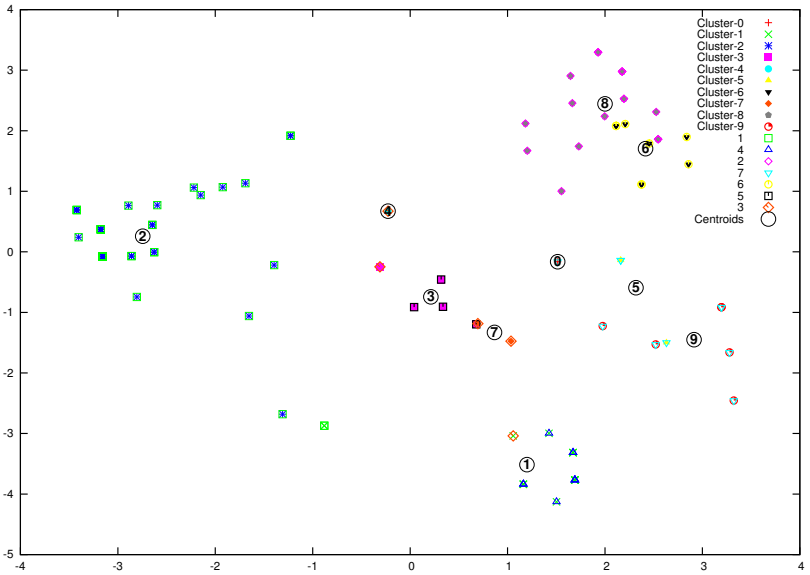

Figure 3.9: Clusters obtained in the data set Zoo with `gcuk_vkcentroid`

'`awk -f zoo_binary.awk -F ',' -v OFS=',' zoo.data > zoo_bin.csv`'

```
  'gcuk_vkcentroid -i zoo_bin.csv -h yes -a "2-22" -c 23 --k-minimum=2
--k-maximum=20 --print-mulline yes -C c_zoo_gcuk.data -M m_zoo_gcuk.data -T
stdout --table-format yes'
     IN:
         Algorithmo name: GCUK
                Based on: Bandyopadhyay and Maulik 2002
             Metric used: DB-index

                Data set: zoo_bin.csv
     Number of instances: 101
              Dimensions: 21

            Random seed: 728997733 111590912 682175903 3140775393 958797699
            412503851 3032481805 703125621

     OUT:

     CROMOSOME:BEST:rows,9,columns,21>0,1,1,0,0.8,0.3,0.45,0,1,1,0,0,0,1,0,0,0,0,
     1,0.15,0.3;0,0,0,0,0,0,1,0,0,1,1,0,0,0,0,0,0,1,1,0,0;0.0588235,0,0.764706,
     0.176471,0,1,0.764706,1,1,0.176471,0.117647,0.941176,1,0,0,0,0,0,0.941176,
     0.0588235,0.411765;1,0,0.0263158,1,0.0526316,0.0789474,0.5,0.973684,1,1,0,
     0.0263158,0,0.184211,0.815789,0,0,0,0.868421,0.210526,0.763158;0,0,1,0,0,0.8,
     0.8,1,1,1,0.2,0,0,0,1,0,0,0,0.4,0,0;0.4,0,1,0,0.6,0,0.1,0,0,1,0.2,0,0.2,0,0,
     0,0.8,0,0,0.1,0;0,0,1,0,0,0,0,0,1,1,0,0,0,0,1,0,0,0,1,0,1;0,0,1,0,0,0,1,1,1,
     1,0.5,0,1,0,0,0,0,0,1,0,0;0,0,1,0,0,0.857143,1,0,0,0,0.142857,0,0.285714,0,
     0.142857,0.142857,0.285714,0.142857,0,0,0.142857

            Cluster number (K): 9
                      DB-index: 0.855135
                           SED: 98.3379
                    Silhouette: 0.355542
                           VRC: 26.5558
                    CS measure: 1.72969
                  Dunn's index: 0.57735
          Execution time (seg): 0.354636
     Generations find the best: 53


     Partition table:

     Cluster: 0            1            2            3            4
     Class

           1: 0            0            3            38           0
           4: 0            0            13           0            0
           2: 20           0            0            0            0
           7: 0            1            0            0            0
           6: 0            0            0            0            0
           5: 0            0            0            0            4
           3: 0            0            1            0            1
         sum: 20           1            17           38           5

     Cluster: 5            6            7            8            sum
     Class

           1: 0            0            0            0            41
           4: 0            0            0            0            13
           2: 0            0            0            0            20
```

```
   7: 2          0          0          7          10
   6: 8          0          0          0          8
   5: 0          0          0          0          4
   3: 0          1          2          0          5
 sum: 10         1          2          7          101

          Rand index: 0.956238
              Purity: 0.930693
           Precision: 0.932188
              Recall: 0.875956
```

$$C = \begin{bmatrix} & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \text{hair} & 0.00 & 0.00 & 0.06 & 1.00 & 0.00 & 0.40 & 0.00 & 0.00 & 0.00 \\ \text{feathers} & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ \text{eggs} & 1.00 & 0.00 & 0.76 & 0.03 & 1.00 & 1.00 & 1.00 & 1.00 & 1.00 \\ \text{milk} & 0.00 & 0.00 & 0.18 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ \text{airborne} & 0.80 & 0.00 & 0.00 & 0.05 & 0.00 & 0.60 & 0.00 & 0.00 & 0.00 \\ \text{aquatic} & 0.30 & 0.00 & 1.00 & 0.08 & 0.80 & 0.00 & 0.00 & 0.00 & 0.86 \\ \text{predator} & 0.45 & 1.00 & 0.76 & 0.50 & 0.80 & 0.10 & 0.00 & 1.00 & 1.00 \\ \text{toothed} & 0.00 & 0.00 & 1.00 & 0.97 & 1.00 & 0.00 & 0.00 & 1.00 & 0.00 \\ \text{backbone} & 1.00 & 0.00 & 1.00 & 1.00 & 1.00 & 0.00 & 1.00 & 1.00 & 0.00 \\ \text{breathes} & 1.00 & 1.00 & 0.18 & 1.00 & 1.00 & 1.00 & 1.00 & 1.00 & 0.00 \\ \text{venomous} & 0.00 & 1.00 & 0.12 & 0.00 & 0.20 & 0.20 & 0.00 & 0.50 & 0.14 \\ \text{fins} & 0.00 & 0.00 & 0.94 & 0.03 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ \text{legs 0} & 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.20 & 0.00 & 1.00 & 0.29 \\ \text{legs 2} & 1.00 & 0.00 & 0.00 & 0.18 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ \text{legs 4} & 0.00 & 0.00 & 0.00 & 0.82 & 1.00 & 0.00 & 1.00 & 0.00 & 0.14 \\ \text{legs 5} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.14 \\ \text{legs 6} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.80 & 0.00 & 0.00 & 0.29 \\ \text{legs 8} & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.14 \\ \text{tail} & 1.00 & 1.00 & 0.94 & 0.87 & 0.40 & 0.00 & 1.00 & 1.00 & 0.00 \\ \text{domestic} & 0.15 & 0.00 & 0.06 & 0.21 & 0.00 & 0.10 & 0.00 & 0.00 & 0.00 \\ \text{catsize} & 0.30 & 0.00 & 0.41 & 0.76 & 0.00 & 0.00 & 1.00 & 0.00 & 0.14 \end{bmatrix} \quad W = \begin{bmatrix} 0.20 \\ 0.01 \\ 0.17 \\ 0.38 \\ 0.05 \\ 0.10 \\ 0.01 \\ 0.02 \\ 0.07 \end{bmatrix}$$

Figure 3.10: Zoo Clusters with `gcuk_vkcentroid`

From the run of the algorithm, 9 clusters were obtained using the *DB-index* similarity measure, with very good measured values obtained. For this data set, it is possible to use the centroids to obtain an association between items in the same row ([AIS93], [HPY00]) as it is shown in the Figure 3.10 and the summary in the Table 3.1.

'`plot_clustering -i zoo_bin.csv -h yes -a "2-22" -c 23 --centroids-infile c_zoo_gcuk.data --member-infile m_zoo_gcuk.data --graphics-outfile zoo_gcuk`'

C_j	W_j	**Frequent dimension**	**Outliers**
0	20%	95-100%: feathers eggs backbone breathes legs 2 tail 80-90%: airborne	
1	1%	90-100%: predator breathes venomous legs 8 tail	
2	17%	90-100%: aquatic backbone fins legs 0 tail	{eggs hair domestic}
3	38%	90-100%: hair milk toothed backbone breathes legs 4	{eggs airborne fins legs 2}
4	5%	90-100%: eggs toothed backbone breathes legs 4 80-90%: aquatic predator	
5	10%	90-100%: eggs breathes 80-90%: legs 6	{legs 6 domestic}
6	1%	90-100%: eggs backbone breathes legs 4 tail catsize	
7	2%	90-100%: eggs predator toothed backbone breathes legs 0 tail	
8	7%	90-100%: eggs predator 80-90%: aquatic	{aquatic venomous legs 4 legs 5 legs 8 catsize }

Table 3.1: Zoo clusters summary table

3.2.2.2 Based on cluster label

The GAs in this section are coded as a string of group numbers (see [string-of-group-numbers encoding], page 12) with some variant to allow the search of the optimum k. The algorithms included in LEAC are the following:

1. **gga_vklabeldbindex** and **gga_vklabelsilhouette**

   It is based on [ABSSJF+12]. It optimizes the SSE measure [DB], page 22, and [Silhouette], page 22. Chromosome is formed by two sections [*element* | *group*]. The element section where each position (gene) indicates the cluster of that object. The group section corresponds to the alphabet of possible values of the genes $\{1, 2, 3, ..., k\}$. An island model is used, where the following operators are used: `gaclusteringop::mergeCrossover`, `gaclusteringop::mergeMutation` and `gaclusteringop::splittingMutation` are applied.

   Parameters of the algorithm:

   `--sub-population-size[=NUMBER]`
   : size of sub-populations (islands) `[NUMBER=20]`

   `--number-island[=NUMBER]`
   : number of sub-populations or islands `[NUMBER=4]`

   `--pe[=NUMBER]`
   : probability of migration good individuals between islands `[0,1]` `[NUMBER=0.5]`

   `--pci[=NUMBER]`
   : initial probability crossover, real number in the interval `[0,1]` must be high in the first stages `[NUMBER=0.8]`

`--pcf[=NUMBER]`
: final probability crossover, real number in the interval `[0,1]` must moderate in the last stages `[NUMBER=0.4]`

`--pci[=NUMBER]`
: initial probability mutation, real number in the interval `[0,1]` is smaller in the first generations `[NUMBER=0.05]`

`--pcf[=NUMBER]`
: final probability mutation, real number in the interval `[0,1]` is larger in the last ones `[NUMBER=0.2]`

`--pbi[=NUMBER]`
: initial probability local search, real number in the interval `[0,1]` must be high in the first stages `[NUMBER=0.1]`

`--pbf[=NUMBER]`
: final probability local search, real number in the interval `[0,1]` must moderate in the last stages `[NUMBER=0.05]`

Execution sample: see [Illustrative execution samples: Ionosphere Data Set], page 73.

2. **cga_vklabel**

   It is based on [HE03]. It optimizes the Silhouette measure (see [Silhouette], page 22). Chromosome is represented as a string of label of $(n + 1)$ positions. Each position corresponds to an instance, i.e., the i-th position (gene) represents the $(n + 1)$ object, whereas the last gene represents the number of clusters (k). Crossover operator combines clustering solutions coming from different chromosome (`gaclusteringop::crossoverCGA`). Two operators for mutation are used in MO_1 (`gaclusteringop::MO1`) and MO_2 (`gaclusteringop::MO1`). MO_1 works only on genotypes that encode more than two clusters. It eliminates a randomly chosen cluster, placing its objects to the nearest remaining clusters (according to their centroids). MO_2 divides a randomly selected cluster into two new ones. The first cluster is formed by the objects closer to the original centroid, whereas the other cluster is formed by those objects closer to the farthest object from the centroid. The `cga_vklabel` does not employ crossover and mutation probabilities, that is, after the roulette wheel selection process, the designed operators are applied in some selected genotypes. This strategy considers that 50% of the selected genotypes are crossed-over, 25% are mutated by MO_1 and 25% are mutated by MO_2 [HE03].

   Execution sample:

   ‘`cga_vklabel -i iris.data -a "1-4" -c 5 --generations 200 --population-size 20 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout`’

3. **eac_vklabel**

   It is based on [HCdC06]. It optimizes the Simplified silhouette (see [Simplified silhouette], page 23). Chromosome is represented as a string of label of n. Each position corresponds to an instance, i.e., the i-th position (gene) represents the n object, whereas the last gene represents the number of clusters k. Two Mutation operators are used: MO_1 and MO_2 similar to [HE03]. Also `k-means` operator is applied.

   Parameters of the algorithm:

`--desiable-objfunc[=NUMBER]`
: value desiable of objetive function (eg. silhouette `[-1,1]` rand index[0,1]) `[NUMBER=1]`

`--kmeans-iterations[=NUMBER]`
: maximum number of iterations for k-means algorithm `[NUMBER=5]`

`--kmeans-difference[=NUMBER]`
: maximum absolute difference between centroids in two consecutive iterations is less than or equal to `[NUMBER=0.001]`

Execution sample:

```
'cga_vklabel -i iris.data -a "1-4" -c 5 --generations 200 --population-size
200 --crossover-probability 0.5 --mutation-probability 0.25
--print-mulline yes -C stdout -T stdout --table-format yes -M stdout'
```

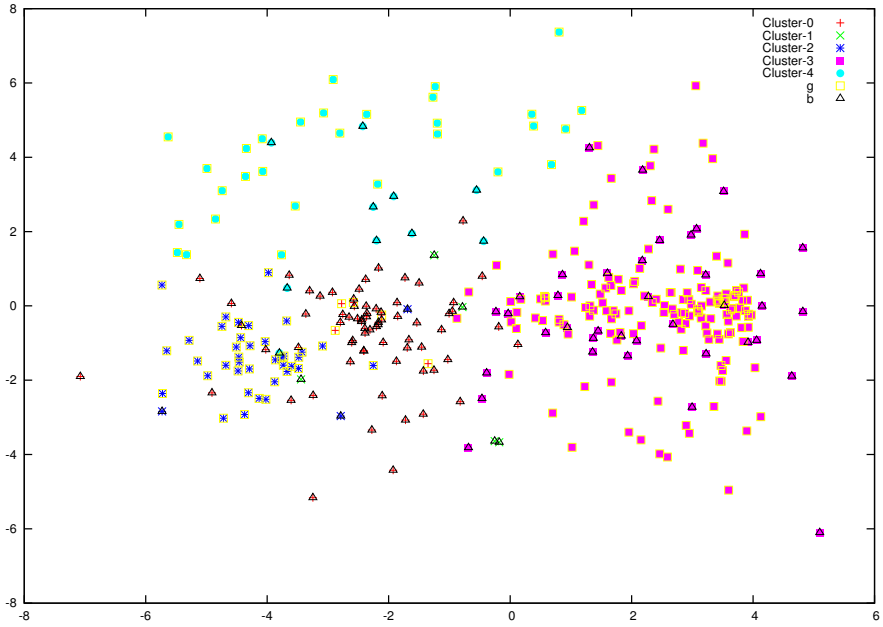

Figure 3.11: Clusters obtained with `gga_vklabelsilhouette`

4. **feac_vklabel**, and its variants **eaci_vklabel**, **eacii_vklabel** and **eaciii_vklabel**

   It is based on [ACH06]. It optimizes the Simplified silhouette [Simplified silhouette], page 23. Chromosome is represented as a string of label of n. Each position corresponds to an instance, i.e., the i-th position (gene) represents the n object, whereas the last gene represents the number of clusters k. For implementation purposes, the chromosome includes the centroids associated with the string of group numbers encoding `gaencode::ChromosomeFEAC`. Operator of crossover does not use. Mutation two operators for mutation MO_1 (`gaclusteringop::MO1`) and MO_2 (`gaclusteringop::MO2`) similar to [HCdC06]. In addition, a `k-means` operator is applied (`gaclusteringop::kmeansfeac`). The only difference between `eaci_vklabel`

and FEAC `feac_vklabel` is rate of each mutation operator according to its performance during the *evolutionary search*.

Parameters of the algorithm:

`--desiable-objfunc[=NUMBER]`
: value desiable of objetive function (eg. silhouette `[-1,1]` rand index `[0,1]`) `[NUMBER=1]`

`--kmeans-iterations[=NUMBER]`
: maximum number of iterations for k-means algorithm `[NUMBER=5]`

`--kmeans-difference[=NUMBER]`
: maximum absolute difference between centroids in two consecutive iterations is less than or equal to `[NUMBER=0.001]`

Execution sample:

'`feac_vklabel -i iris.data -a "1-4" -c 5 --generations 500 --population-size 20 --kmeans-iterations 5 --kmeans-difference 0.001 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout`'

Illustrative execution sample: Ionosphere Data Set

As an illustrative example, the Ionosphere data set is processed with the algorithm `gga_vklabelsilhouette`. This data set has the complexity that the instances of different classes overlap. For this case, the see [silhouette], page 22, metric is appropriate. Before executing the commands, make sure you have access to the executable programs and the data, see [configuration of the PATH variable], page 48.

'`gga_vklabelsilhouette -i ionosphere.data -a "1-34" -c 35 -M m_gga_ionosphere.data -T stdout --table-format yes`'

```
IN:
    Algorithmo name: GGA_SILHOUETTE
           Based on: Agustin-Blas L.E. and Salcedo-Sanz S. and
           Jimenez-Fernandez S. and Carro-Calvo L. and Del Ser J.
           and Portilla-Figueras, J.A.
        Metric used: Silhouette

           Data set: ionosphere.data
Number of instances: 351
         Dimensions: 34

       Random seed: 389887919 3739475900 1204968903 2830340246 1365531614
       2641306820 2495066055 1120010892

OUT:

CROMOSOME:BEST:objetive,0.320094,fitness,0.3200943,0,3,1,3,0,3,1,3,0,3,3,3,
3,3,0,3,0,3,4,3,0,3,0,3,3,3,0,3,1,3,3,3,3,3,3,3,4,3,3,4,2,4,3,3,4,3,0,3,0,3,
0,2,0,3,0,3,0,3,0,3,0,3,2,3,3,3,3,2,3,3,1,4,0,3,3,3,4,4,4,3,3,4,4,3,3,3,3,3,
4,3,0,3,0,3,4,4,4,0,3,3,3,0,3,3,3,0,3,0,3,3,4,3,4,0,3,3,3,0,3,3,3,0,3,0,3,3,
3,0,3,3,3,3,4,3,4,2,3,0,3,0,3,3,0,3,0,0,3,3,3,0,3,0,2,0,3,0,2,0,2,0,3,0,2,3,
2,0,2,0,3,0,3,0,3,0,3,0,3,0,3,0,3,3,2,0,2,1,3,0,0,0,3,0,3,3,3,0,3,3,3,0,
3,0,3,0,3,0,3,0,3,0,3,3,2,3,4,4,4,0,4,3,4,0,4,0,2,3,3,0,3,0,3,3,3,4,3,0,3,0,
3,0,3,3,3,0,3,0,2,0,2,0,2,2,2,3,3,3,3,3,4,4,4,4,4,4,3,3,3,3,3,3,3,3,3,3,3,4,
4,4,4,4,2,0,3,3,3,3,3,3,3,3,3,3,3,4,2,2,2,2,2,3,3,3,3,3,4,4,2,2,2,3,3,2,2,2,
```

```
3,3,3,3,3,3,3,2,2,2,2,2,3,3,3,3,3,3,3,2,2,2,2,0,3,3,3,3,3,3,3,3,3,3|0,1,2,3,4

       Cluster number (K): 5
               Silhouette: 0.320094
                      SED: 705.646
                DB-index: 1.93699
                      VRC: 54.7797
              CS measure: 1.9306
            Dunn's index: 0.0709856
     Execution time (seg): 3.59483
Generations find the best: 77


Partition table:

Cluster: 0            1            2            3            4
Class

      g: 5            0            38           152          30
      b: 70           5            3            38           10
    sum: 75           5            41           190          40

Cluster: sum
Class

      g: 225
      b: 126
    sum: 351

               Rand index: 0.612291
                   Purity: 0.840456
                Precision: 0.707252
                   Recall: 0.477702
```

'`plot_clustering -i ionosphere.data -a "1-34" -c 35 --member-infile m_gga_ionosphere.data --graphics-outfile gga_ionosphere`'

3.2.2.3 Based on other encoding schemes

1. **gaclustering_vktreebinary**

   It is based on [CdLM03]. It optimizes VRC measure (see [VRC], page 25). Adopt an encoding scheme based on minimum spanning tree (MST), the tree nodes represent the n instances of the data set and the edges $(n-1)$ correspond to the nearest instances. The algorithm first calculates the MST and creates the partitions of the data set by preserving or deleting the edges, represented by a binary string. The value 0 means that the corresponding edge remains, while the value 1 means that it is deleted. The number of elements with value 1 is equal to $(k\hat{a}1)$, where k is the number of clusters.

   Parameters of the algorithm:

   `--notchangestop[=NUMBER]`
   : after a number x of iteratios, the best chromosome does not change. (We have fixed x = 3) `[NUMBER=3]`.

   `--crossover-probability[=NUMBER]`
   : real number in the interval `[0.25, 1]` `[NUMBER=0.8]`

`--mutation-probability[=NUMBER]`
real number in the interval `[0, 0.5]` `[NUMBER=0.008]`

Execution sample: see [Illustrative execution samples: Ecoli Data Set], page 75.

2. **clustering_vksubclusterbinary**

It is based on [TY01]. It optimizes intra-cluster and inter-cluster distance measure (see [Intra-cluster and inter-cluster distance], page 25). It uses a binary coding scheme centroid-based (see [Centroid-based binary encoding], page 13), with traditional genetic operators, `gabinaryop::onePointDistCrossover` and `gabinaryop::bitMutation`. It also uses a *heuristic strategy* to find a "good grouping".

Parameters of the algorithm:

`--u-parameter[=NUMBER]`
parameter u `[NUMBER=1.4]`

`--lambda[=NUMBER]`
parameter lambda `[NUMBER=0.125]`

`--w1[=NUMBER]`
smallest value w1 `[NUMBER=1]`

`--w2[=NUMBER]`
largest value w2 `[NUMBER=3]`

`--crossover-probability[=NUMBER]`
real number in the interval `[0.25, 1]` `[NUMBER=0.8]`

`--mutation-probability[=NUMBER]`
real number in the interval `[0, 0.5]` `[NUMBER=0.05]`

Execution sample:

‘`clustering_vksubclusterbinary -i iris.data -a "1-4" -c 5 --u-parameter 1.4 --lambda 0.125 --w1 1 --w2 3 --generations 100 --population-size 50 --crossover-probability 0.8 --mutation-probability 0.5 --print-mulline yes -C stdout -T stdout --table-format yes -M stdout`’

Illustrative execution sample: Ecoli Data Set

As an illustrative example, the Ecoli data set is processed, in order to obtain a cluster number automatically and compare it with the classification proposed in the data set. Before executing the commands, make sure you have access to the executable files and the data, see [configuration of the PATH variable], page 48.

‘`gaclustering_vktreebinary -i ecoli.data -a "2-8" -c 9 -d " " --print-mulline yes -C ecoli_centroids.data -M ecoli_membership.data -G ecoli_tree.data -T stdout --table-format yes --generations=500 --notchangestop=100`’

```
IN:
    Algorithmo name: GA_CASILLAS2003
           Based on: Casillas and Gonzalez and Martinez 2003
        Metric used: Variance Ratio Criterion

           Data set: ecoli.data
Number of instances: 336
```

```
          Dimensions: 7

        Random seed: 3034846250 3476018755 2194011041 1038797822 4055928898
        2745797188 3302303888 3051852958

OUT:

CROMOSOME:BEST:objetive,215.739,fitness,215.739,0000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000000000
0000000000010000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000000010

       Cluster number (K): 3
 Variance Ratio Criterion: 215.739
                      SED: 80.6089
                DB-index: 0.976877
              Silhouette: 0.39575
              CS measure: 0.0297727
            Dunn's index: 0.038597
     Execution time (seg): 12.9314
Generations find the best: 10


Partition table:

Cluster: 0            1            2            sum
Class

     cp: 142          0            1            143
     im: 7            68           2            77
    imS: 0            1            1            2
    imL: 0            2            0            2
    imU: 1            34           0            35
     om: 0            1            19           20
    omL: 0            5            0            5
     pp: 5            1            46           52
    sum: 155          112          69           336

              Rand index: 0.86672
                  Purity: 0.761905
               Precision: 0.687857
                  Recall: 0.927444
```

And the results can be visualized with the following command (Figure 3.12):

```
'plot_clustering -i ecoli.data -a "2-8" -c 9 -d " " --centroids-infile
ecoli_centroids.data --member-infile ecoli_membership.data --graph-infile
ecoli_tree.data --graphics-outfile ecoli_tree --centroids-size 1.5
--member-size 0.5 --size-instance 0.6'
```

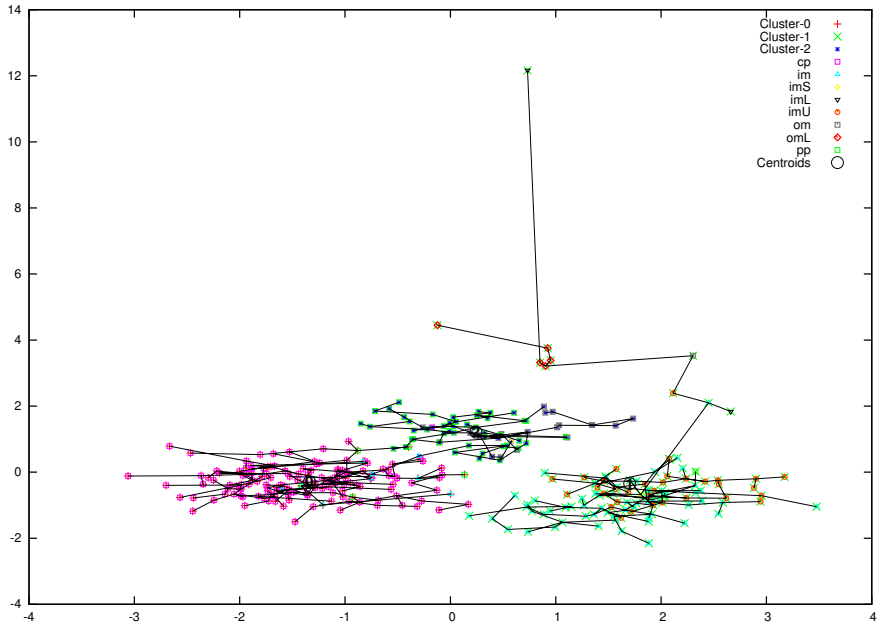

Figure 3.12: Minimum spanning tree (MST) and clusters obtained with `gaclustering_vktreebinary` program for the ecoli data set

3.3 Carry out an experimental study with Evolutionary algorithms included in the library

An experimental study between algorithms includes a combination of algorithms and problems that require a heavy computational work. This library has been designed to use a script and facilitate the task of carrying out an exhaustive experimental study. Moreover, it is allowed that the script can be batch-executed in a cluster of computers to speed up the computation time. The library allows the researcher to apply the same sequence of experiments and analyse to large batteries of problems and focus his attention on a summary of results.

Figure 3.13 shows the sequence of steps that should be given to carry out a comparative study between different proposals included in the library.

1. The first step considers the selection and preparation of data set. In this step can be selected any data set of the well-known UCI repository. Then, it can be selected seven different normalization procedures of the attributes [MC88] and finally, a k-fold cross validation method can be selected on each data set. These steps together with commands and scripts used are detailed in section [Selection and preparation of data set], page 78.
2. The second step considers the design and running of experiments. In this step is indicated the different data sets (processed in the previous step) and the different algorithms that want to be included in the experimental study. In section [Design and

execution of experiments], page 82, it is specified a script where all information can be specified and run easily.

3. The third step considers the processing of the results obtained in the previous step. In this step, it is used the result files obtained in the previous step and it is obtained average values of each measure and applied a statistical test to compare results. For statistical test is used R software, in this section is detailed the scripts necessary to carry out the statistical tests and analysis of results.

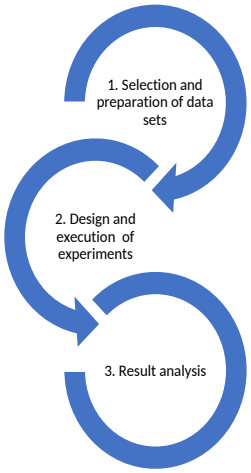

Figure 3.13: Sequence of steps to carry out a comparative study between different proposals included in the LEAC library

3.3.1 Selection and preparation of data set

The fundamental purpose of selection and preparation of data sets includes to obtain, normalize and apply cross validation methods on data sets that are going to be used in experimental study.

3.3.1.1 Obtaining data sets

Data sets can be download of the UCI Machine Learning Repository [DG17]. There are other sites that provide data sets `https://sci2s.ugr.es/keel/datasets.php` [AFFL+11]. Really, a classic `csv` format can be used in this library.

3.3.1.2 Preparation data sets

This step includes to select the attributes and indicate a normalization process to numerical attributes.

The library contains the `stdvar_milligan_cooper1988` program based on [MC88] which allows to select attributes and class (in the event that it is available) and to transform the data set so that the different numerical attributes have the same weight. There are seven transformation methods ($Z1$, $Z2$, $Z3$, $Z4$, $Z5$, $Z6$ or $Z7$) or no transformation $Z0$ [MC88].

3.3.1.3 Using k-fold cross validation

It is very usual to use a cross validation method in exhaustive experimental study, therefore, it is included as a step of preparation of data set.

To carry out the *k-fold* cross validation, it is used the file `kfold.R`, located in the `data` directory of the library. This script is written in `R` and it is necessary to indicate the data set that you want to make the partitions. The parameters of use are:

'`Rscript kfold.R dataset k-fold`'

`dataset` is the file that contains the data set.

`k-folds` is the number of *k-folds*, if it is not specified is set by default to '`10`'.

3.3.1.4 Illustrative example

It is detailed an example using the different steps that have to be carried out. First, these ten datasets have to be download of the UCI Machine Learning Repository [DG17]: iris, wine, sonar, glass, spect, ecoli, haberman, ionosphere, hayes-roth and zoo. Then, they have to be located in fold `data` in the library (see [Directory system of LEAC], page 5).

Then, the next commands have to be run to carried out each step described previously.[1]

a. iris.data
   - Add the names of the attributes, from the terminal with the following script in perl:
     '`perl -i.bk -pe "s/^/SepalLength,SepalWidth,PetalLength,PetalWidth, Class\n/ if($.==1)" iris.data`'
   - `running stdvar_milligan_cooper1988` application for normalize to $Z5$:
     '`stdvar_milligan_cooper1988 -i iris.data -a "1-4" -c 5 -h yes --std-var Z5 > iris_z5.data`'
   - Make the *k-fold* files:
     '`Rscript kfold.R iris_z5.data 10`',

b. wine.data
   - Add the names of the attributes, from the terminal with the following script in perl:
     '`perl -i.bk -pe "s/^/Alcohol,MalicAcid,Ash,AlcalinityAsh,Magnesium, TotalPhenols,Flavanoids,NonflavanoidPhenols,Proanthocyanins, ColorIntensity,Hue,OD280_OD315,Proline\n/ if($.==1)" wine.data`'
   - `running stdvar_milligan_cooper1988` application for normalize to $Z5$:
     '`stdvar_milligan_cooper1988 -i wine.data -a "2-13" -c 1 -h yes --std-var Z5 > wine_z5.data`'
   - Make the *k-fold* files:
     '`Rscript kfold.R wine_z5.data`'

[1] To facilitate the work, you can download the data set and create the *k-fold* files with the script `tendatasetdemo.pl` automatically, in the terminal and in the directory `data` and type the command '`perl tendatasetdemo.pl`', this script is only used for the preparation of the data sets used in this illustrative example.

c. sonar.all-data
   - Add the names of the attributes, from the terminal with the following script in perl: '`perl -i.bk -pe "s/^/ X1,X2,X3,X4,X5,X6,X7,X8,X9,X10,X11,X12,X13,X14,X15, X16,X17,X18,X19,X20,X21,X22,X23,X24,X25,X26,X27,X28,X29,X30,X31,X32, X33,X34,X35,X36,X37,X38,X39,X40,X41,X42,X43,X44,X45,X46,X47,X48,X49, X50,X51,X52,X53,X54,X55,X56,X57,X58,X59,X60,Class \n/ if($.==1)" sonar.all-data`'
   - `running stdvar_milligan_cooper1988` application for normalize to $Z5$: '`stdvar_milligan_cooper1988 -i sonar.all-data -a "1-60" -c 61 -h yes --std-var Z5 > sonar_z5.data`'
   - Make the *k-fold* files: '`Rscript kfold.R sonar_z5.data`'

d. glass.data
   - Add the names of the attributes, from the terminal with the following script in perl: '`perl -i.bk -pe "s/^/Id,RI,Na,Mg,Al,Si,K,Ca,Ba,Fe,TypeGlass\n/ if($.==1)" glass.data`'
   - `running stdvar_milligan_cooper1988` application for normalize to $Z5$: '`stdvar_milligan_cooper1988 -i glass.data -a "2-10" -c 11 -h yes --std-var Z5 > glass_z5.data`'
   - Make the *k-fold* files: '`Rscript kfold.R glass_z5.data` '

e. Download SPECT.train and SPECT.test. This file is divided in training and test in UCI repository. Therefore, they have to be united using the next command: '`cat SPECT.train SPECT.test > spect.data`'
   - Add the names of the attributes, from the terminal with the following script in perl: '`perl -i.bk -pe "s/^/DIAGNOSIS,F1,F2,F3,F4,F5,F6,F7,F8,F9,F10,F11,F12, F13,F14,F15,F16,F17,F18,F19,F20,F21,F22\n/ if($.==1)" spect.data`'
   - `running stdvar_milligan_cooper1988` application for normalize to $Z5$: '`stdvar_milligan_cooper1988 -i spectf.data -a "2-23" -c 1 -h yes --std-var Z5 > spect_z5.data`'
   - Make the *k-fold* files: '`Rscript kfold.R spect_z5.data`'

f. haberman.data
   - Add the names of the attributes, from the terminal with the following script in perl: '`perl -i.bk -pe "s/^/Age,PatientsYear,Nodes,Survival\n/ if($.==1)" haberman.data`'
   - `running stdvar_milligan_cooper1988` application for normalize to $Z5$: '`stdvar_milligan_cooper1988 -i haberman.data -a "1-3" -c 4 -h yes --std-var Z5 > haberman_z5.data`'
   - Make the *k-fold* files: '`Rscript kfold.R haberman_z5.data`'

g. ecoli.data
   - Add the names of the attributes, from the terminal with the following script in perl:
     'perl -i.bk -pe "s/^/name mcg gvh lip chg aac alm1 alm2 class\n/ if($.==1)" ecoli.data'
   - running stdvar_milligan_cooper1988 application for normalize to $Z5$:
     'stdvar_milligan_cooper1988 -i ecoli.data -d " " -a "2-8" -c 9 -h yes --std-var Z5 > ecoli_z5.data'
   - Make the *k-fold* files:
     'Rscript kfold.R ecoli_z5.data'

h. ionosphere.data
   - Add the names of the attributes, from the terminal with the following script in perl:
     'perl -i.bk -pe "s/^/ X1,X2,X3,X4,X5,X6,X7,X8,X9,X10,X11,X12,X13,X14,X15, X16,X17,X18,X19,X20,X21,X22,X23,X24,X25,X26,X27,X28,X29,X30,X31,X32, X33,X34,Class\n/ if($.==1)" ionosphere.data'
   - running stdvar_milligan_cooper1988 application for normalize to $Z5$:
     'stdvar_milligan_cooper1988 -i ionosphere.data -a "1,3-34" -c 35 -h yes --std-var Z5 > ionosphere_z5.data'
   - Make the *k-fold* files:
     'Rscript kfold.R ionosphere_z5.data'

i. Download hayes-roth.data and hayes-roth.test
   Adding a name column to test file, so that the two files have the same number of attributes: 'sed -i "N;s/^/1,/" hayes-roth.test'
   . This file is divided in training and test in UCI repository. Therefore, they have to be united using the next command: 'cat hayes-roth.data hayes-roth.test > hayes_roth.data'
   - Add the names of the attributes, from the terminal with the following script in perl:
     'perl -i.bk -pe "s/^/name,hobby,age,educational,marital,class\n/ if($.==1)" hayes_roth.data'
   - running stdvar_milligan_cooper1988 application for normalize to $Z5$:
     'stdvar_milligan_cooper1988 -i hayes_roth.data -a "3-5" -c 6 -h yes --std-var Z5 > hayes_roth_z5.data'
   - Make the *k-fold* files:
     'Rscript kfold.R hayes_roth_z5.data'

j. zoo.data'
   - Add the names of the attributes, from the terminal with the following script in perl:
     'perl -i.bk -pe "s/^/animalname,hair,feathers,eggs,milk,airborne, aquatic,predator,toothed,backbone,breathes,venomous,fins,legs, tail,domestic,catsize,type\n/ if($.==1)" zoo.data'
   - running stdvar_milligan_cooper1988 application for normalize to $Z5$:
     'stdvar_milligan_cooper1988 -i zoo.data -a "2-17" -c 18 -h yes --std-var Z5 > zoo_z5.data'

– Make the *k-fold* files:
'`Rscript kfold.R zoo_z5.data`'

3.3.2 Design and execution of experiments

The fundamental purpose of design and execution of experiments is to specify the different data and algorithms that are going to be included in the experimental study.

The execution of an exhaustive experimental study requires a large computation time. For this reason, you can take advantage of the resources you can use GNU parallel. It is a shell tool to execute jobs in parallel to one or more computers. GNU parallel is contained in most distribution of GNU/Linux systems or you can also install it manually, downloading it from the official page.

To facilitate the task of carrying out a batch run, the run_alg_kfold.sh[2] script, which is located in the `bin` directory of the library, can be used for the execution of experiments.

3.3.2.1 Illustrative example

In the example shown, it is considered the ten data sets prepared in the previous section and six algorithms included in the library (`fgka_fklabel`, `gagr_fkcentroid`, `hka_fkmedoid`, `gaclustering_fklabel`, `gka_fklabel` and `kga_fkcentroid`).

First you have to configure the run_alg_kfold.sh file. If you have another location for the installation directory, dataset location, and output directory for the **k-fold experimental study**, you can modify the following three variables:

`PATH_ALGORITHMS==~/LEAC-1.2/bin`
: Set the path where the binary files of the LEAC algorithms are located in in your computer's file system (see [Directory system of LEAC], page 5).

`PATH_DATASETS=~/dataset`
: Set the path to locate the data set in your computer's file system (see [Directory system of LEAC], page 5).

`PATH_KFOLD_TEST_OUT=~/LEAC-1.2/kfix_kfold_test`
: Set the path where the k-fold experimental study output files will be stored

The following two variables of the run_alg_kfold.sh file are used to specify the dataset and algorithm to be analyzed, you can use '`#`' at the beginning of a line to omit some dataset or algorithm or you can also add some of your own.

`DATASET_ARRAY`
: Include the data sets with their parameters:

```
DATASET_ARRAY=(
"iris_z5"        "-b uci -h yes -a \"1-4\"  -c 5  --number-clusters=3"
"wine_z5"        "-b uci -h yes -a \"1-12\" -c 13 --number-clusters=3"
"sonar_z5"       "-b uci -h yes -a \"1-60\" -c 61 --number-clusters=2"
"glass_z5"       "-b uci -h yes -a \"1-9\"  -c 10 --number-clusters=7"
```

[2] Another option is to manually run each algorithm with each *k-fold* of the data set and obtain the execution files with the measurements, with the example '`kga_fkcentroid -i ~/leac/data/iris_z5/iris_z5-10-1tra.dat -t ~/leac/data/iris_z5/iris_z 5-10-1tst.dat -b uci -h yes -a "1-4" -c 5 --number-clusters=3 -r 1 -R kga_fkcentroid_iris_z5_1_run.csv -C kga_fkcentroid_iris_z5_1_centroids.dat -M kga_fkcentroid_iris_z5_1_membership.dat -T kga_fkcentroid_iris_z5_1_partitionstable.dat`' command. But this is a tedious job

```
"spect_z5"       "-b uci -h yes -a \"1-22\" -c 23 --number-clusters=2"
"haberman_z5"    "-b uci -h yes -a \"1-3\"  -c 4  --number-clusters=2"
"ecoli_z5"       "-b uci -h yes -a \"1-7\"  -c 8  --number-clusters=8"
"ionosphere_z5"  "-b uci -h yes -a \"1-33\" -c 34 --number-clusters=2"
"hayes_roth_z5"  "-b uci -h yes -a \"1-3\"  -c 4  --number-clusters=3"
"zoo_z5"         "-b uci -h yes -a \"1-16\" -c 17 --number-clusters=7"
)
```

the parameters are those used by the programs to read the data set, see Section 3.2 [Run an Evolutionary Algorithm included in the library], page 48)

`ALGORITHMS_ARRAY`

Include algorithms that are going to be evaluated with their parameters or a null string to take the default parameters:

```
ALGORITHMS_ARRAY=(
"kga_fkcentroid"  ""
"fgka_fklabel"    ""
"hka_fkmedoid"    ""
"gka_fklabel"     ""
"gaclustering_fklabel"  ""
"gagr_fkcentroid" "--generations=200"
)
```

To see the meaning of the parameters see Section 3.2 [Run an Evolutionary Algorithm included in the library], page 48).

Now you need to run the scripts `run_alg_kfold.sh`, for example you can type the following command in a terminal: (you must give execution permission to the file '`chmod u+x ~/LEAC-1.2/bin/bin/run_alg_kfold.sh`'):

'`parallel -j4 ~/LEAC-1.2/bin/run_alg_kfold.sh 10 ::: {1..200} > test_run.log&`'

`-j4` The number of jobs will be done in parallel, it is recommended to use the number of processors or cores of the computer used to perform the experimental study.

`../eac/run_alg_kfold.sh`
The path of the file `run_alg_kfold.sh`.

`10` the number of *k-fold* used, if it is not specified by default it is 10

`{1..200}` The interval is the number of repetitions for each *k-fold*, for the case of `{1..200}`, it is equivalent to 20 executions because each data set is run 10 times. You can see results quickly using `{1..40}` is equivalent to 4 executions for each *k-fold*. But, in order to obtain a value that converges with the average of the metrics, you should use about `{1..200}` or more.

`test_run.log`
A file name to store the output of the runs of the methods.

A directory is automatically created for each algorithm where the output files are stored.

For the illustrative example, we obtain: `fgka_fklabel_test`, `gagr_fkcentroid_test` `hka_fkmedoid_test`, `gaclustering_fklabel_test`, `gka_fklabel_test` and `kga_fkcentroid_test`

3.3.3 Result analysis

The fundamental purpose of result analysis is to obtain a summary of the average values of the different measures considered. Concretely, it is obtained 30 measured used in clustering. Also, it is possible to carry out a statistical test using R sofware with the results obtained.

3.3.3.1 Obtaining the average values for the different measures for each algorithm

Included in the experimental study in the directory `test`, you have to run the script:

'`sh ../eac/average_kfold.sh directory numberOfRuns kfoldUsed`'

`directory`
: The first parameter is one of the directories with the output files. Remember that it was created a directory for each algorithm. In the example previous, it can be used: `kga_fkcentroid_test`.

`numberOfRuns`
: This value corresponds to the repetitions made in the previous step, only it is used to check if all the executions were made. If it is a smaller number, a warning will be shown indicating that the number of executions is lower. If this is the case, the script `run_alg_kfold.sh` from the previous step can be executed once more.

`kfoldUsed`
: An integer with the *k-fold* used, if it is not specified by default is '`10`'

For the illustrative example, you can go to the directory `test` and execute the following commands:

```
'sh ../eac/average_kfold.sh kga_fkcentroid_test 4'
'sh ../eac/average_kfold.sh fgka_fklabel_test 4'
'sh ../eac/average_kfold.sh gagr_fkcentroid_test 4'
'sh ../eac/average_kfold.sh hka_fkmedoid_test 4'
'sh ../eac/average_kfold.sh gaclustering_fklabel_test 4'
'sh ../eac/average_kfold.sh gka_fklabel_test 4'
```

3.3.3.2 Applying statistical test

It is used R software to carry out the statistical test. Thus, a large number of tests are available. In this example, it is used friedman test, a non parametric test, widely used in the comparison between different evolutionary algorithms. Moreover, the output are `csv` files with information of all measures, therefore, you can process this these with other tools to obtain an analysis.

In order to carry a stastical test, it is necessary to do the next steps:

a. In the directory of `metric_average`, you must join the same measures for all the algorithms, for this the following script is used:

   '`perl ../../eac/join_metrics.pl *_metric.csv`'

   The result is a file for each metric obtained by the algorithm and the data set. For example, for the metric *silhouette*, you get the file `silhouette_table.csv` which contains:

   ```
   DATASET,FGKA,GA,GAGR,GKA,HKA,KGA
   ```

```
ecoli_z5,0.214,0.165,0.182,0.209,0.201,0.206
glass_z5,0.352,0.196,0.275,0.335,0.308,0.321
haberman_z5,0.382,0.382,0.376,0.382,0.367,0.382
hayes_roth_z5,0.221,0.227,0.239,0.23,0.244,0.252
ionosphere_z5,0.301,0.299,0.301,0.301,0.3,0.296
iris_z5,0.464,0.437,0.464,0.459,0.423,0.444
sonar_z5,0.151,0.143,0.15,0.151,0.135,0.144
spect_z5,0.17,0.147,0.17,0.171,0.149,0.13
wine_z5,0.257,0.257,0.256,0.257,0.254,0.258
zoo_z5,0.253,0.251,0.251,0.235,0.245,0.265
```

b. To apply the Friedman test, you have to use the script `friedman.R` based in [CS16]. In particular, execute the following command:

'`Rscript ../../eac/friedman.R db_index_table.csv db_index > test_db_index.log`'

Or you can also execute the script for all the metrics:

'`sh ../../eac/scrip_friedman.sh`'

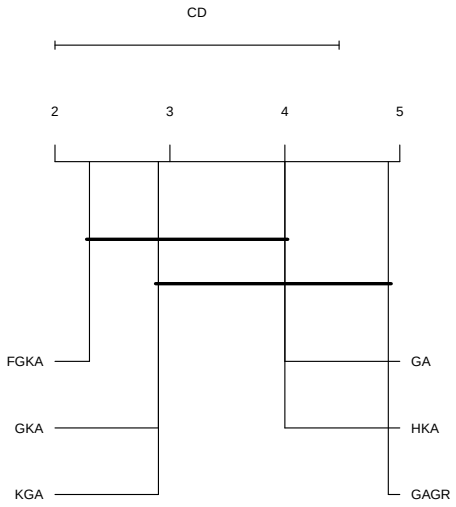

Figure 3.14: Each algorithm is placed in an axis according to its average ranking for `DB-Index`

The output is a file for each metric which, you can use to study significant differences between the different methods. The five files obtained are:

`db_index.log`
: It contains numerical information of the Friedman test

`db_index_nemeny_matrix.tex`
: In this table there are significant differences between two algorithms, if the number is in bold.

`db_index_nemeny_plot.pdf`
: In this plot each algorithm is placed in an axis according to its average ranking. Then, those algorithms that show no significant differences are grouped together using a horizontal line. The plot also shows the size of the critical difference required for considering two algorithms as significantly different [CS16]. See Figure 3.14.

`db_index_ranking.csv`
: The rankings of the algorithms in a simplified `csv` file.

`db_index_ranking_graph_friedman.pdf`
: The ranking plotted as a graph, when the algorithms are not connected, there are significant differences between them. See Figure 3.15.

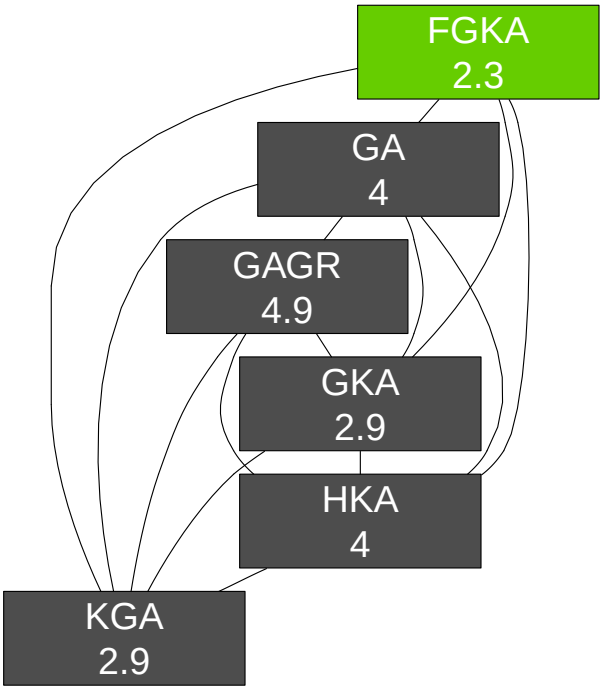

Figure 3.15: Example of algorithm graph for `DB-Index`

4 Reporting Bugs

If you find a bug in LEAC, please send electronic mail to hermes@uaz.edu.mx.

Appendix A Example source code

The following source code show the use of the LEAC library. The files are in `eac` directory.

A.1 KGA algorithm

The following encoded algorithm is the KGA (`kga_fkcentroid.hpp`), described in the paper [BM02a].

```
/*! \file kga_fkcentroid.hpp
 *
 * \brief KGA \cite Bandyopadhyay:Maulik:GAclustering:KGA:2002
 *
 * \details This file is part of the LEAC.\n\n
 * Implementation of the KGA algorithm based on the paper:\n
 * S. Bandyopadhyay and U. Maulik. An evolutionary technique based\n
 * on k-means algorithm for optimal clustering in rn. Inf. Sci. Appl.,\n
 * 146(1-4):221-237, 2002.\n
 * URL: http://www.sciencedirect.com/science/article/pii/S0020025502002086,\n
 * <a href="http://dx.doi.org/10.1016/S0020-0255(02)00208-6">
 * doi:http://dx.doi.org/10.1016/S0020-0255(02)00208-6</a>\n.
 * \n
 * Library Evolutionary Algorithms for Clustering (LEAC) is a library\n
 * for the implementation of evolutionary algorithms\n
 * focused on the partition type clustering problem. Based on the\n
 * current standards of the <ahref="http://en.cppreference.com">C++</a>
 * language, as well as on Standard\n
 * Template Library <a href="http://en.cppreference.com/w/cpp/container">STL</a>
 * and also  <a href="http://www.openblas.net/">OpenBLAS</a> to have a better performance.\n
 * \version 1.0
 * \date 2017-2018
 * \authors Hermes Robles-Berumen <hermes@uaz.edu.mx>\n
 * Sebastian Ventura <sventura@uco.es>\n
 * Amelia Zafra <azafra@uco.es>\n
 * <a href="http://www.uco.es/kdis/">KDIS</a>
 * \copyright <a href="https://www.gnu.org/licenses/gpl-3.0.en.html">GPLv3</a> license
 */

#ifndef __KGA_FKCENTROID_HPP__
#define __KGA_FKCENTROID_HPP__

#include <vector>
#include <algorithm>

#include <leac.hpp>
#include "inparam_pcpmfk.hpp"
#include "outparam_gac.hpp"

#include "plot_runtime_function.hpp"

/*! \namespace eac
  \brief Evolutionary Algorithms for Clustering
  \details Implementation of evolutionary algorithms used to solve the clustering problem

  \version 1.0
  \date   2017-2018
  \copyright GPLv3 license
*/
```

```
namespace eac {

/*! \fn gaencode::ChromFixedLength<T_FEATURE,T_REAL> kga_fkcentroid
    (inout::OutParamGAC<T_REAL,T_CLUSTERIDX> &aoop_outParamGAC,
    inout::InParamPcPmFk<T_CLUSTERIDX,T_REAL,T_FEATURE,T_FEATURE_SUM,T_INSTANCES_CLUSTER_K>
    &aiinp_inParamPcPmFk,
    const INPUT_ITERATOR aiiterator_instfirst,
    const INPUT_ITERATOR aiiterator_instlast,
    const dist::Dist<T_REAL,T_FEATURE> &aifunc2p_dist)
  \brief  KGA \cite Bandyopadhyay:Maulik:GAclustering:KGA:2002
  \details Implementation of the KGA algorithm based on
  \cite Bandyopadhyay:Maulik:GAclustering:KGA:2002.
  \returns A partition of a data set, encoded on a chromosome where
    each gene is the coordinate of a centroid. Base to following equation:
  \f[
  x_i \in C_j \leftrightarrow  \| x_i - \mu_j \|  \beginarraycmin\\  k \endarray
  \| x_i - \mu_k \|,\; j=1,2,..k,
  \f]
  where \f$mu_j\f$, represents the centroid of cluster \f$C_j\f$
  \param aoop_outParamGAC a inout::OutParamGAC with the
    output parameters of the algorithm
  \param aiinp_inParamPcPmFk a inout::InParamPcPmFk parameters
    required by the algorithm
  \param aiiterator_instfirst an InputIterator to the initial
    positions of the sequence of instances
  \param aiiterator_instlast an InputIterator to the final positions
    of the sequence of instances
  \param aifunc2p_dist an object of type dist::Dist to calculate distances
*/
template < typename T_FEATURE,
           typename T_REAL,
           typename T_FEATURE_SUM,
           typename T_INSTANCES_CLUSTER_K,
           typename T_CLUSTERIDX, //-1, 0, 1, .., K
           typename INPUT_ITERATOR
           >
gaencode::ChromFixedLength<T_FEATURE,T_REAL>
kga_fkcentroid
(inout::OutParamGAC
 <T_REAL,
 T_CLUSTERIDX>                       &aoop_outParamGAC,
 inout::InParamPcPmFk
 <T_CLUSTERIDX,
 T_REAL,
 T_FEATURE,
 T_FEATURE_SUM,
 T_INSTANCES_CLUSTER_K>              &aiinp_inParamPcPmFk,
 const INPUT_ITERATOR                aiiterator_instfirst,
 const INPUT_ITERATOR                aiiterator_instlast,
 const dist::Dist<T_REAL,T_FEATURE>  &aifunc2p_dist
 )
{
  const uintidx lconstui_numClusterFixedK =
    (uintidx) aiinp_inParamPcPmFk.getNumClusterK();
```

Defines the size of the chromosome. Specifically, each chromosome is described by a sequence of $length(Ch) = l \times k$ real-valued numbers where l is the dimension of the instances,

and k is the number of clusters [BM02a]. That is to say, the chromosome of the algorithm is written as (4.2) (see [centroid-based], page 13)

```
  /*ASSIGN SIZE FOR ALL CHROMOSOMES
   */
  gaencode::ChromFixedLength<T_FEATURE,T_REAL>::setStringSize
    ( lconstui_numClusterFixedK * data::Instance<T_FEATURE>::getNumDimensions() );


  gaencode::ChromFixedLength<T_FEATURE,T_REAL> lochromfixleng_best;

  /*VARIABLE NEED FOR POPULATION AND MATINGPOOL GENETIC
   */

  /*POPULATION CREATE
   */
  std::vector<gaencode::ChromFixedLength<T_FEATURE,T_REAL> >
    lvectorchromfixleng_population
    (aiinp_inParamPcPmFk.getSizePopulation());

  /*CREATE SPACE FOR STORE MATINGPOOL
   */
  std::vector<gaencode::ChromFixedLength<T_FEATURE,T_REAL> >
    lvectorchromfixleng_matingPool
    (aiinp_inParamPcPmFk.getSizePopulation());

  std::uniform_real_distribution<T_REAL> uniformdis_real01(0,1);

#ifdef __VERBOSE_YES

  /*ID PROC
   */
  geverboseui_idproc = 1;

  ++geiinparam_verbose;
  const char* lpc_labelAlgGA = "kga_fkcentroid";
  if ( geiinparam_verbose <= geiinparam_verboseMax ) {
    std::cout
      << lpc_labelAlgGA
      << ":  IN(" << geiinparam_verbose << ")\n"
      << "\t(output Chromosome: lochromfixleng_best["
      << &lochromfixleng_best << "]\n"
      << "\t output outparam::OutParamGAC&: "
      << "aoop_outParamGAC["
      << &aoop_outParamGAC << "]\n"
      << "\t input  InParamPcPmFk&: "
      <<"aiinp_inParamPcPmFk["
      << &aiinp_inParamPcPmFk << "]\n"
      << "\t input aiiterator_instfirst[" << *aiiterator_instfirst << "]\n"
      << "\t input aiiterator_instlast[" <<  &aiiterator_instlast << "]\n"
      << "\t input  dist::Dist<T_REAL,T_FEATURE> &aifunc2p_dist["
      << &aifunc2p_dist << ']'
      << "\n\t\tPopulation size = "
      << aiinp_inParamPcPmFk.getSizePopulation()
      << "\n\t\tProbCrossover = "
      << aiinp_inParamPcPmFk.getProbCrossover()
      << "\n\t\tProbMutation  = "
      << aiinp_inParamPcPmFk.getProbMutation()
```

```
      << "\n\t)"
      << std::endl;
  }
#endif /*__VERBOSE_YES*/

  runtime::ListRuntimeFunction<COMMON_IDOMAIN>
    llfh_listFuntionHist
    (aiinp_inParamPcPmFk.getNumMaxGenerations(),
     "Iterations",
     "Clustering metrics"
     );

  /*DECLARATION OF VARIABLES: COMPUTING STATISTICAL AND METRIC OF THE ALGORITHM*/
#ifndef __WITHOUT_PLOT_STAT
  std::ofstream               lfileout_plotStatObjetiveFunc;
  runtime::RuntimeFunctionValue<T_REAL> *lofh_SSE = NULL;
  runtime::RuntimeFunctionStat<T_REAL>
    *lofhs_statObjectiveFunc[STATISTICAL_ALL_MEASURES];
  std::vector<T_REAL>         lvectorT_statfuncObjetiveFunc;

  if ( aiinp_inParamPcPmFk.getWithPlotStatObjetiveFunc() ) {

    lvectorT_statfuncObjetiveFunc.reserve
      ( aiinp_inParamPcPmFk.getSizePopulation());
    //DEFINE FUNCTION
    lofh_SSE  = new runtime::RuntimeFunctionValue<T_REAL>
      ("SSE",
       aiinp_inParamPcPmFk.getAlgorithmoName(),
       RUNTIMEFUNCTION_NOT_STORAGE
       );

    llfh_listFuntionHist.addFuntion(lofh_SSE);

    //DEFINE FUNCTION STATISTICAL
    for  (int li_i = 0; li_i < STATISTICAL_ALL_MEASURES; li_i++) {
      lofhs_statObjectiveFunc[li_i] =
        new runtime::RuntimeFunctionStat<T_REAL>
        ( (char) li_i,
          aiinp_inParamPcPmFk.getAlgorithmoName(),
          RUNTIMEFUNCTION_NOT_STORAGE
        );
      llfh_listFuntionHist.addFuntion(lofhs_statObjectiveFunc[li_i]);
    }

    //OPEN FILE STRORE FUNCTION
    aoop_outParamGAC.setFileNameOutPlotStatObjetiveFunc
      (aiinp_inParamPcPmFk.getFileNamePlotStatObjetiveFunc(),
       aiinp_inParamPcPmFk.getTimesRunAlgorithm()
       );

    lfileout_plotStatObjetiveFunc.open
      (aoop_outParamGAC.getFileNameOutPlotStatObjetiveFunc().c_str(),
       std::ios::out | std::ios::app
       );

    lfileout_plotStatObjetiveFunc.precision(COMMON_COUT_PRECISION);

    //FUNCTION HEADER
```

```
    lfileout_plotStatObjetiveFunc
      <<  llfh_listFuntionHist.getHeaderFuntions()
      << "\n";
  }

#endif /*__WITHOUT_PLOT_STAT*/

  /*WHEN CAN MEASURE STARTS AT ZERO INVALID OFFSPRING
   */
  aoop_outParamGAC.setTotalInvalidOffspring(0);

  /*OUT: GENETIC ALGORITHM CHARACTERIZATION*/
  runtime::ExecutionTime let_executionTime = runtime::start();

  T_FEATURE *larray_maxFeactures =
    new T_FEATURE[data::Instance<T_FEATURE>::getNumDimensions()];

  T_FEATURE *larray_minFeactures =
    new T_FEATURE[data::Instance<T_FEATURE>::getNumDimensions()];

  stats::maxFeatures
    (larray_maxFeactures,
     aiiterator_instfirst,
     aiiterator_instlast
     );

  stats::minFeatures
    (larray_minFeactures,
     aiiterator_instfirst,
     aiiterator_instlast
     );
```

Population initialization. Chosen distict points from the data set are used to initialize the K cluster centers encoded in each choromosome. This is similar to the initialization of the centers in K-Means algorithm. This process is repeated for each chromosome in the population [BM02a]

```
  {/*BEGIN INITIALIZE POPULATION P(t)*/

#ifdef __VERBOSE_YES
    geverbosepc_labelstep = "(0) POPULATION INITIAL";
    ++geiinparam_verbose;
    if ( geiinparam_verbose <= geiinparam_verboseMax ) {
      std::cout
        << geverbosepc_labelstep
        << ": IN(" << geiinparam_verbose << ')'
        << std::endl;
    }
#endif /*__VERBOSE_YES*/

    for ( auto& lchromfixleng_iter: lvectorchromfixleng_population ) {

      /*DECODE CHROMOSOME
       */
      mat::MatrixRow<T_FEATURE>
        lmatrixrowt_centroidsChrom
        (lconstui_numClusterFixedK,
         data::Instance<T_FEATURE>::getNumDimensions(),
         lchromfixleng_iter.getString()
```

```
        );

      clusteringop::randomInitialize
        (lmatrixrowt_centroidsChrom,
         aiiterator_instfirst,
         aiiterator_instlast
        );

      lchromfixleng_iter.setFitness
        (-std::numeric_limits<T_REAL>::max());
      lchromfixleng_iter.setObjetiveFunc
        (std::numeric_limits<T_REAL>::max());

    }

#ifdef __VERBOSE_YES
    if ( geiinparam_verbose <= geiinparam_verboseMax ) {
      std::cout
       << geverbosepc_labelstep
       << ": OUT(" << geiinparam_verbose << ')'
       << std::endl;
    }
    --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

  } /*END INITIALIZE POPULATION P(t)*/

while ( 1 ) {

    /*BEGIN ITERATION
     */
    llfh_listFuntionHist.increaseDomainUpperBound();
```

Clustering. In this step, clusters are formed according to the center encoded in the chromosome. This is done by assigning each point $x_i, i = 1, 2, ..., n$ to one of the clusters Cj with center z_i^*, such that

$$\|x_i - \mu_j\| \leq \|x_i - \mu'_j\|,\ j' = 1, 2, ..., k,\ and\ j \neq j'$$

. All ties are resolved arbitrarily. As like the K-Means algorithm, for each cluster C_i, its new center μ^* is computed as $\mu_i^* = 1/n_j \sum_{x_i \in C_j} x_i,\ j = 1, 2, ..., k$, where n_j is the number of points in cluster C_i. These μ^* now replace the preious μ_i's in the chromosome [BM02a].

```
    {/*BEGIN CLUSTERING*/
#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "A. THE CLUSTERS ARE FORMED";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ":  IN(" << geiinparam_verbose << ')'
          << std::endl;
     }
#endif /*__VERBOSE_YES*/

      for ( auto& liter_iChrom: lvectorchromfixleng_population ) {
```

```
          /*DECODE CHROMOSOME*/
          mat::MatrixRow<T_FEATURE>
            lmatrixrowt_centroidsChrom
              (lconstui_numClusterFixedK,
               data::Instance<T_FEATURE>::getNumDimensions(),
               liter_iChrom.getString()
              );

          mat::MatrixRow<T_FEATURE_SUM>
            llmatrixrowt_sumInstancesCluster
              (lconstui_numClusterFixedK,
               data::Instance<T_FEATURE>::getNumDimensions(),
               T_FEATURE_SUM(0)
              );

          std::vector<T_INSTANCES_CLUSTER_K>
            lvectort_numInstancesInClusterK
              (lconstui_numClusterFixedK,
               T_INSTANCES_CLUSTER_K(0)
              );

          T_CLUSTERIDX lmcidx_numClusterNull;


          clusteringop::updateCentroids
            (lmcidx_numClusterNull,
             lmatrixrowt_centroidsChrom,
             llmatrixrowt_sumInstancesCluster,
             lvectort_numInstancesInClusterK,
             aiiterator_instfirst,
             aiiterator_instlast,
             aifunc2p_dist
            );
      }
#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

    } /*END CLUSTERING*/

    /*FITNESS FUNCTION
```

Fitness function computation. For each chromosome, the clusters formed in the previous step are utilized computing the clustering metric, SSE, as follows:

$$SSE = \sum_{j=1}^{k} \sum_{x_i \in C_j} ||x_i - \mu_j||$$

The fitness function of a chromosome is defined as $1/SSE$. Therefore, maximization of the fitness function will lead to minimization of the clustering metric SSE [BM02a].

```
    { /*BEGIN COMPUTED METRIC M AND FITNESS*/
```

```
#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "B. COMPUTED METRIC M AND FITNESS";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": IN(" << geiinparam_verbose << ')'
          << std::endl;
      }
#endif /*__VERBOSE_YES*/

      long ll_invalidOffspring = 0;

      for ( auto& lchromfixleng_iter: lvectorchromfixleng_population ) {

        /*DECODE CHROMOSOME*/
        mat::MatrixRow<T_FEATURE>
          lmatrixrowt_centroidsChrom
            (lconstui_numClusterFixedK,
             data::Instance<T_FEATURE>::getNumDimensions(),
             lchromfixleng_iter.getString()
            );

        std::pair<T_REAL,bool> lpair_SSE =
          um::SSE
            (lmatrixrowt_centroidsChrom,
             aiiterator_instfirst,
             aiiterator_instlast,
             aifunc2p_dist
            );

        lchromfixleng_iter.setObjetiveFunc(lpair_SSE.first);
        lchromfixleng_iter.setFitness(1.0 / lpair_SSE.first);
        lchromfixleng_iter.setValidString(lpair_SSE.second);

        if ( lchromfixleng_iter.getValidString() == false )
          ++ll_invalidOffspring;

#ifndef __WITHOUT_PLOT_STAT
        lvectorT_statfuncObjetiveFunc.push_back
          (lchromfixleng_iter.getObjetiveFunc());
#endif /*__WITHOUT_PLOT_STAT*/

      } //End for

      aoop_outParamGAC.sumTotalInvalidOffspring
        (ll_invalidOffspring);

#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/
```

```
    } /*END COMPUTED METRIC M AND FITNESS*/
```

Elitism. Has been implemented in each generation by replacing the worst chromosome of the population with the best one seen up to the previous generation [BM02a].

```
    { /*BEGIN ELITISM REPLACING THE WORST CHROMOSOME*/
#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "ELITISM REPLACING THE WORST CHROMOSOME";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": IN(" << geiinparam_verbose << ')'
          << std::endl;
      }
#endif /*__VERBOSE_YES*/

      auto lit_chromMin =
        std::min_element
          (lvectorchromfixleng_population.begin(),
           lvectorchromfixleng_population.end(),
           [](const gaencode::ChromFixedLength<T_FEATURE,T_REAL>& x,
              const gaencode::ChromFixedLength<T_FEATURE,T_REAL>& y
             )
           { return x.getFitness() < y.getFitness(); }
          );

      if ( lit_chromMin->getFitness() < lochromfixleng_best.getFitness() ) {
        *lit_chromMin = lochromfixleng_best;
      }

#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

    } /*END ELITISM REPLACING THE WORST CHROMOSOME*/
```

The best string or chromosome seen up to the last generation provides the solution to the clustering problem [BM02a].

```
    { /*BEGIN PRESERVING THE BEST STRING*/


      auto lchromfixleng_iterMax  =
        std::max_element
          (lvectorchromfixleng_population.begin(),
           lvectorchromfixleng_population.end(),
           [](const gaencode::ChromFixedLength<T_FEATURE,T_REAL>& x,
              const gaencode::ChromFixedLength<T_FEATURE,T_REAL>& y
           )
            {  return x.getFitness() < y.getFitness(); }
          );
```

```
#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "ELITISM PRESERVING THE BEST";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": IN(" << geiinparam_verbose << ")\tmax fitness = "
          << lchromfixleng_iterMax->getFitness()
          << std::endl;
      }
#endif /*__VERBOSE_YES*/

      if ( lochromfixleng_best.getFitness() <
           lchromfixleng_iterMax->getFitness() ) {

        /*CHROMOSOME ONE WAS FOUND IN THIS ITERATION*/
        lochromfixleng_best  = *lchromfixleng_iterMax;

        aoop_outParamGAC.setIterationGetsBest
          (llfh_listFuntionHist.getDomainUpperBound());
        aoop_outParamGAC.setRunTimeGetsBest
          (runtime::elapsedTime(let_executionTime));
      }

#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

    } /*END PRESERVING THE BEST STRING*/


    /*MEASUREMENT BEST: COMPUTING STATISTICAL AND METRIC OF THE
      ALGORITHM
    */
#ifndef __WITHOUT_PLOT_STAT
    if ( aiinp_inParamPcPmFk.getWithPlotStatObjetiveFunc() ) {

      lofh_SSE->setValue(lochromfixleng_best.getObjetiveFunc());

      functionhiststat_evaluateAll
        (lofhs_statObjectiveFunc,
         lvectorT_statfuncObjetiveFunc
         );
      lfileout_plotStatObjetiveFunc << llfh_listFuntionHist;
      lvectorT_statfuncObjetiveFunc.clear();
    }
#endif /*__WITHOUT_PLOT_STAT*/

    /*TERMINATION CRITERION
      3.1.5 TERMINATION CRITERION
      [BM02a]     */
#ifdef __VERBOSE_YES
```

```
    /*ID PROC
     */
    ++geverboseui_idproc;

    ++geiinparam_verbose;
    if ( geiinparam_verbose <= geiinparam_verboseMax ) {
      std::cout
        << "TERMINATION CRITERION ATTAINED?: "
        << llfh_listFuntionHist.getDomainUpperBound()
        << std::endl;
    }
    --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

    if ( !(llfh_listFuntionHist.getDomainUpperBound()
           < aiinp_inParamPcPmFk.getNumMaxGenerations() )
         )
      break;
    /*3.1.4 GENETIC OPERATIONS
      [BM02a]      */
```

Selection. The selection process selects chromosomes from the mating pool directed by the survival of the fittest concept of natural genetic systems. In the proportional selection strategy adopted in this paper, a chromosome is assigned a number of copies, which is proportional to its fitness in the population [BM02a].

```
    { /*BEGIN SELECTION*/
#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "SELECTION";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": IN(" << geiinparam_verbose << ')'
          << std::endl;
      }
#endif /*__VERBOSE_YES*/


      const std::vector<T_REAL>&& lvectorT_probDistRouletteWheel =
        prob::makeDistRouletteWheel
        (lvectorchromfixleng_population.begin(),
         lvectorchromfixleng_population.end(),
         [](const gaencode::ChromFixedLength<T_FEATURE,T_REAL>&
            lchromfixleng_iter) -> T_REAL
         {
           return lchromfixleng_iter.getFitness();
         }
         );

      /*COPY POPULATION TO STRING POOL FOR ROULETTE WHEEL
       */
      for ( auto& lchromfixleng_iter: lvectorchromfixleng_matingPool ) {

        uintidx lstidx_chrom =
          gaselect::getIdxRouletteWheel
          (lvectorT_probDistRouletteWheel,
           uintidx(0)
           );
```

```
        lchromfixleng_iter = lvectorchromfixleng_population.at(lstidx_chrom);
      }

#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

    } /*END SELECTION*/
```

Crossover. It is a probabilistic process that exchanges information between two parent chromosomes for generating two offspring. Here, single-point crossover with a fixed crossover probability of p_c is used. For chromosomes of length $l \times k$, a random integer, called the crossover point, is generated in the range $[1, l-1]$. The portions of the chromosomes lying to the right of the crossover point are exchanged to produce two offspring [BM02a].

```
    { /*BEGIN CROSSOVER*/
#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "CROSSOVER";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout << geverbosepc_labelstep
                  << ": IN(" << geiinparam_verbose << ')'
                  << std::endl;
      }
#endif /*__VERBOSE_YES*/

      long ll_invalidOffspring = 0;

      gaiterator::crossover
        (lvectorchromfixleng_matingPool.begin(),
         lvectorchromfixleng_matingPool.end(),
         lvectorchromfixleng_population.begin(),
         lvectorchromfixleng_population.end(),
         [&](const gaencode::ChromFixedLength<T_FEATURE,T_REAL>&
             aichrom_parent1,
             const gaencode::ChromFixedLength<T_FEATURE,T_REAL>&
             aichrom_parent2,
             gaencode::ChromFixedLength<T_FEATURE,T_REAL>&
             aochrom_child1,
             gaencode::ChromFixedLength<T_FEATURE,T_REAL>&
             aochrom_child2
             )
         {


           if ( uniformdis_real01(gmt19937_eng) <
                aiinp_inParamPcPmFk.getProbCrossover()  ) {


             gagenericop::onePointCrossover
               (aochrom_child1,
                aochrom_child2,
```

```
        aichrom_parent1,
        aichrom_parent2
        );

      /*DECODE CHROMOSOME CHILD1*/
      mat::MatrixRow<T_FEATURE>
        lmatrixrowt_centroidsChromChild1
        (lconstui_numClusterFixedK,
         data::Instance<T_FEATURE>::getNumDimensions(),
         aochrom_child1.getString()
         );

      std::pair<T_REAL,bool>
        lpair_SSE1 =
        um::SSE
        (lmatrixrowt_centroidsChromChild1,
         aiiterator_instfirst,
         aiiterator_instlast,
         aifunc2p_dist
         );
      aochrom_child1.setObjetiveFunc(lpair_SSE1.first);
      aochrom_child1.setFitness(1.0 / lpair_SSE1.first);
      aochrom_child1.setValidString(lpair_SSE1.second);

      if ( aochrom_child1.getValidString() == false )
        ++ll_invalidOffspring;

      /*DECODE CHROMOSOME CHILD1*/
      mat::MatrixRow<T_FEATURE>
        lmatrixrowt_centroidsChromChild2
        (lconstui_numClusterFixedK,
         data::Instance<T_FEATURE>::getNumDimensions(),
         aochrom_child2.getString()
         );

      std::pair<T_REAL,bool>
        lpair_SSE2 =
        um::SSE
        (lmatrixrowt_centroidsChromChild2,
         aiiterator_instfirst,
         aiiterator_instlast,
         aifunc2p_dist
         );

      aochrom_child2.setObjetiveFunc(lpair_SSE2.first);
      aochrom_child2.setFitness(1.0 / lpair_SSE2.first);
      aochrom_child2.setValidString(lpair_SSE2.second);

      if ( aochrom_child2.getValidString() == false )
        ++ll_invalidOffspring;

    } //if  Crossover
    else {
      aochrom_child1 =  aichrom_parent1;
      aochrom_child2 =  aichrom_parent2;
    }
  }
  );
```

```
      aoop_outParamGAC.sumTotalInvalidOffspring
        (ll_invalidOffspring);

#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

    } /*END CROSSOVER*/
```

Mutation. Each *liter_Chrom* chromosome undergoes mutation with a fixed probability p_m (*lr_mutationProbability*). Let M_{min} (*lchrom_minObjFunc*) and M_{max} (*lrt_maxClusteringMetric*) be the minimum and maximum values of the clustering metric, respectively, in the current population. See [Definition gaclusteringop::biDirectionHMutation], page 38,

```
    { /*BEGIN MUTATION*/
#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "MUTATION";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout << geverbosepc_labelstep
                  << ": IN(" << geiinparam_verbose << ')'
                  << std::endl;
      }
#endif /*__VERBOSE_YES*/

      auto lchrom_minObjFunc  =
        std::min_element
        (lvectorchromfixleng_population.begin(),
         lvectorchromfixleng_population.end(),
         [](const gaencode::ChromFixedLength<T_FEATURE,T_REAL>& x,
            const gaencode::ChromFixedLength<T_FEATURE,T_REAL>& y
            )
         {  return x.getObjetiveFunc() < y.getObjetiveFunc(); }
         );
      T_REAL  lrt_minClusteringMetric =
        lchrom_minObjFunc->getObjetiveFunc();

      auto lchrom_maxObjFunc  =
        std::max_element
        (lvectorchromfixleng_population.begin(),
         lvectorchromfixleng_population.end(),
         [](const gaencode::ChromFixedLength<T_FEATURE,T_REAL>& x,
            const gaencode::ChromFixedLength<T_FEATURE,T_REAL>& y
            )
         {  return x.getObjetiveFunc() < y.getObjetiveFunc(); }

         );

      T_REAL lrt_maxClusteringMetric =
        lchrom_maxObjFunc->getObjetiveFunc();
```

```
      for ( auto& lchromfixleng_iter: lvectorchromfixleng_population ) {

        if ( uniformdis_real01(gmt19937_eng)
             < aiinp_inParamPcPmFk.getProbMutation() )
          { //IF MUTATION
            gaclusteringop::biDirectionHMutation
              (lchromfixleng_iter,
               lrt_minClusteringMetric,
               lrt_maxClusteringMetric,
               larray_minFeactures,
               larray_maxFeactures
               );
            lchromfixleng_iter.setFitness
              (-std::numeric_limits<T_REAL>::max());
            lchromfixleng_iter.setObjetiveFunc
              (std::numeric_limits<T_REAL>::max());
          } //END IF MUTATION
      }
#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

    } /*END MUTATION*/


  } /*END EVOLUTION While*/

  /*FREE MEMORY
   */
  delete [] larray_maxFeactures;
  delete [] larray_minFeactures;

  runtime::stop(let_executionTime);
  aoop_outParamGAC.setNumClusterK
    (aiinp_inParamPcPmFk.getNumClusterK());
  aoop_outParamGAC.setMetricFuncRun
    (lochromfixleng_best.getObjetiveFunc());
  aoop_outParamGAC.setAlgorithmRunTime
    (runtime::getTime(let_executionTime));
  aoop_outParamGAC.setFitness
    (lochromfixleng_best.getFitness());
  aoop_outParamGAC.setNumTotalGenerations
    (llfh_listFuntionHist.getDomainUpperBound());

#ifndef __WITHOUT_PLOT_STAT
  if ( aiinp_inParamPcPmFk.getWithPlotStatObjetiveFunc() ) {
    runtime::plot_funtionHist
      (llfh_listFuntionHist,
       aiinp_inParamPcPmFk,
       aoop_outParamGAC
       );
  }
```

```
#endif /*__WITHOUT_PLOT_STAT*/

#ifdef __VERBOSE_YES
  if ( geiinparam_verbose <= geiinparam_verboseMax ) {
    geverbosepc_labelstep = lpc_labelAlgGA;
    std::cout
      << lpc_labelAlgGA
      << ": OUT(" << geiinparam_verbose << ")\n";
    lochromfixleng_best.print();
    std::cout << std::endl;
  }
  --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

  return lochromfixleng_best;

} /* END kga_fkcentroid */

} /*END eac */

#endif /*__KGA_FKCENTROID_HPP__*/
```

A.2 GA algorithm

```
/*! \file gaclustering_fkcrispmatrix.hpp
 *
 * \brief GA CLUSTERING \cite Bezdek:etal:GAclustering:GA:1994
 *
 * \details This file is part of the LEAC.\n\n
 * Implementation of the GA algorithm based on the paper:\n
 * J.C. Bezdek, S. Boggavarapu, L.O. Hall, and A. Bensaid.\n
 * Genetic algorithm guided clustering. In Evolutionary Computation,\n
 * 1994. IEEE World Congress on Computational Intelligence., Proceed-\n
 * ings of the First IEEE Conference on, pages 34â39 vol.1, Jun 1994.\n
 * <a href="http://dx.doi.org/10.1109/ICEC.1994.350046">doi:10.1109/ICEC.1994.350046</a>\n.
 * \n
 * Library Evolutionary Algorithms for Clustering (LEAC) is a library\n
 * for the implementation of evolutionary algorithms\n
 * focused on the partition type clustering problem. Based on the\n
 * current standards of the <a href="http://en.cppreference.com">C++</a>
 * language, as well as on Standard\n
 * Template Library <a href="http://en.cppreference.com/w/cpp/container">STL</a>
 * and also  <a href="http://www.openblas.net/">OpenBLAS</a> to have a better performance.\n
 * \version 1.0
 * \date 2017-2018
 * \authors Hermes Robles-Berumen <hermes@uaz.edu.mx>\n
 * Sebastian Ventura <sventura@uco.es>\n
 * Amelia Zafra <azafra@uco.es>\n
 * <a href="http://www.uco.es/kdis/">KDIS</a>
 * \copyright <a href="https://www.gnu.org/licenses/gpl-3.0.en.html">GPLv3</a> license
 */

#ifndef __GACLUSTERING_FKCRISPMATRIX_HPP__
#define __GACLUSTERING_FKCRISPMATRIX_HPP__
```

```
#include <iostream>
#include <iomanip>
#include <vector>

#include <leac.hpp>

#include "plot_runtime_function.hpp"
#include "inparam_withoutpcpmfk.hpp"
#include "outparam_gac.hpp"

/*! \namespace eac
  \brief Evolutionary Algorithms for Clustering
  \details Implementation of evolutionary algorithms used to solve the clustering problem

  \version 1.0
  \date   2015-2017
  \copyright GPLv3 license
*/

namespace eac {

/*! \fn gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>
gaclustering_fkcrispmatrix
(inout::OutParamGAC<T_REAL,T_CLUSTERIDX> &aoop_outParamGAC,
inout::InParamWithoutPcPm<T_CLUSTERIDX,T_BITSIZE,T_FEATURE,
T_FEATURE_SUM,T_INSTANCES_CLUSTER_K> &aiinp_inParamWithoutPcPmFk,
const INPUT_ITERATOR aiiterator_instfirst,
const INPUT_ITERATOR aiiterator_instlast, dist::Dist<T_REAL,T_FEATURE> &aifunc2p_dist)
  \brief  gaclustering_fkcrispmatrix
  \details GA clustering based on [BBHB94]   Returns a crisp matrix, which encodes a partition of a data
  \param aoop_outParamGAC a inout::OutParamGAC that contains
  information relevant to program execution
  \param aiinp_inParamWithoutPcPmFk a inout::InParamWithoutPcPm with
  the input parameters for the program configuration
  \param aiiterator_instfirst an InputIterator to the initial positions of the
   sequence of instances
  \param aiiterator_instlast an InputIterator to the final positions of the
  sequence of instances
  \param aipartition_clusters a partition of instances in clusters
  \param aifunc2p_dist an object of type dist::Dist to calculate distances
*/

template < typename T_BITSIZE,
           typename T_REAL,
           typename T_FEATURE,
           typename T_FEATURE_SUM,
           typename T_INSTANCES_CLUSTER_K, //0, 1, .., N
           typename T_CLUSTERIDX,          //-1, 0, 1, .., K
           typename INPUT_ITERATOR
   >
gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>
gaclustering_fkcrispmatrix
(inout::OutParamGAC
 <T_REAL,
 T_CLUSTERIDX>                &aoop_outParamGAC,
 inout::InParamWithoutPcPm
 <T_CLUSTERIDX,
 T_BITSIZE,
```

```
 T_FEATURE,
 T_FEATURE_SUM,
 T_INSTANCES_CLUSTER_K>       &aiinp_inParamWithoutPcPmFk,
 const INPUT_ITERATOR         aiiterator_instfirst,
 const INPUT_ITERATOR         aiiterator_instlast,
 dist::Dist<T_REAL,T_FEATURE> &aifunc2p_dist
 )
{
#ifdef __VERBOSE_YES
  /*ID PROC
   */
  geverboseui_idproc = 1;

  ++geiinparam_verbose;
  const char* lpc_labelAlgGA = "gaclustering_fkcrispmatrix";
  if ( geiinparam_verbose <= geiinparam_verboseMax ) {
    std::cout
      << lpc_labelAlgGA
      << "  IN(" << geiinparam_verbose << ")\n"
      << "\t(output outparam::OutParamGAC&: aoop_outParamGAC["
      << &aoop_outParamGAC << "]\n"
      << "\t input  InParamClusteringBezdekGA1994&: aiinp_inParamWithoutPcPmFk["
      << &aiinp_inParamWithoutPcPmFk << "]\n"
      << "\t input aiiterator_instfirst[" << *aiiterator_instfirst << "]\n"
      << "\t input aiiterator_instlast[" <<  &aiiterator_instlast << "]\n"
      << "\t input  dist::Dist<T_REAL,T_FEATURE>  &aifunc2p_dist["
      << &aifunc2p_dist << ']'
      << "\n\t\tPopulation size = "
      << aiinp_inParamWithoutPcPmFk.getSizePopulation()
      << "\n\t\tMatingPool size = "
      << aiinp_inParamWithoutPcPmFk.getSizeMatingPool()
      << "\n\t\t Generations  = "
      << aiinp_inParamWithoutPcPmFk.getNumMaxGenerations()
      << "\n\t\trandom-seed = "
      << aiinp_inParamWithoutPcPmFk.getRandomSeed()
      << "\n\t)"
      << std::endl;
  }
#endif /*__VERBOSE_YES*/

  const uintidx  luintidx_numClusterK =
    (uintidx) aiinp_inParamWithoutPcPmFk.getNumClusterK();
  const uintidx  luintidx_numIntances =
    uintidx(std::distance(aiiterator_instfirst,aiiterator_instlast));

  /*CONVERT INSTANCES TO FORMAT MATRIX
   */
  mat::MatrixRow<T_FEATURE>&& lmatrixt_y =
    data::toMatrixRow
    (aiiterator_instfirst,
     aiiterator_instlast
     );

  std::uniform_int_distribution<T_CLUSTERIDX> uniformdis_mmcidx0K
    (0,aiinp_inParamWithoutPcPmFk.getNumClusterK()-1);


  gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>
```

```
    lochrombitcrispmatrix_best(luintidx_numClusterK,luintidx_numIntances);

  /*STL container for storing the chromosome population
   */
  std::vector<gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>* >
    lvectorchrombitcrispmatrix_population;

  /*Vector for matingpool
   */
  std::vector<gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>* >
    lvectorchrombitcrispmatrix_matingPool;

  /*Vector for temporary storage when applying generic operators
   */
  std::vector<gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>* >
    lvectorchromfixleng_childR;

  if ( aiinp_inParamWithoutPcPmFk.getSizePopulation()
       <= aiinp_inParamWithoutPcPmFk.getSizeMatingPool() )
    throw std::invalid_argument
      ("gaclustering_fkcrispmatrix: "
       "size population should be greater than size matingpool"
       );

  runtime::ListRuntimeFunction<COMMON_IDOMAIN>
    llfh_listFuntionHist
    (aiinp_inParamWithoutPcPmFk.getNumMaxGenerations(),
     "Iterations",
     "Clustering metrics"
     );

  /*Declaration of variables: computing statistical
    and metric of the algorithm
   */
#ifndef __WITHOUT_PLOT_STAT
  std::ofstream               lfileout_plotStatObjetiveFunc;
  runtime::RuntimeFunctionValue<T_REAL> *lofh_J1 = NULL;
  runtime::RuntimeFunctionValue<T_INSTANCES_CLUSTER_K>
    *lofh_misclassified = NULL; /*function extra*/
  runtime::RuntimeFunctionStat<T_REAL>
    *lofhs_statObjectiveFunc[STATISTICAL_ALL_MEASURES];
  std::vector<T_REAL>       lvectorT_statfuncObjetiveFunc;

  if ( aiinp_inParamWithoutPcPmFk.getWithPlotStatObjetiveFunc() ) {

    lvectorT_statfuncObjetiveFunc.reserve
      ( aiinp_inParamWithoutPcPmFk.getSizePopulation());
    //Variable to monitor in the execution of the program
    lofh_J1  = new runtime::RuntimeFunctionValue<T_REAL>
      ("J1",
       aiinp_inParamWithoutPcPmFk.getAlgorithmoName(),
       RUNTIMEFUNCTION_NOT_STORAGE
       );

    llfh_listFuntionHist.addFuntion(lofh_J1);

    if ( aiinp_inParamWithoutPcPmFk.getClassInstanceColumn()  ) {
      lofh_misclassified =
```

```
        new runtime::RuntimeFunctionValue<T_INSTANCES_CLUSTER_K>
        ("Misclassified",
         aiinp_inParamWithoutPcPmFk.getAlgorithmoName(),
         RUNTIMEFUNCTION_NOT_STORAGE
         );
      llfh_listFuntionHist.addFuntion(lofh_misclassified);
    }

    //Statistics of variable J1 in runtime
    for  (int li_i = 0; li_i < STATISTICAL_ALL_MEASURES; li_i++) {
      lofhs_statObjectiveFunc[li_i] =
        new runtime::RuntimeFunctionStat
        <T_REAL>
        ( (char) li_i,
          aiinp_inParamWithoutPcPmFk.getAlgorithmoName(),
          RUNTIMEFUNCTION_NOT_STORAGE
          );
      llfh_listFuntionHist.addFuntion(lofhs_statObjectiveFunc[li_i]);
    }

    //OPEN FILE STRORE FUNCTION
    aoop_outParamGAC.setFileNameOutPlotStatObjetiveFunc
      (aiinp_inParamWithoutPcPmFk.getFileNamePlotStatObjetiveFunc(),
       aiinp_inParamWithoutPcPmFk.getTimesRunAlgorithm()
       );

    lfileout_plotStatObjetiveFunc.open
      (aoop_outParamGAC.getFileNameOutPlotStatObjetiveFunc().c_str(),
       std::ios::out | std::ios::app
       );

    lfileout_plotStatObjetiveFunc.precision(COMMON_COUT_PRECISION);

    //Header function
    lfileout_plotStatObjetiveFunc
      <<  llfh_listFuntionHist.getHeaderFuntions()
      << "\n";
  }
#endif /*__WITHOUT_PLOT_STAT*/


  runtime::ExecutionTime let_executionTime  = runtime::start();

  /*Create space for store population
   */
  lvectorchrombitcrispmatrix_population.reserve
    (aiinp_inParamWithoutPcPmFk.getSizePopulation() + 1);
  for (uintidx lui_i = 0;
       lui_i < aiinp_inParamWithoutPcPmFk.getSizePopulation();
       lui_i++)
    {
      lvectorchrombitcrispmatrix_population.push_back
        (new gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>
         (luintidx_numClusterK,luintidx_numIntances)
         );
    }

  /*Space for store matingpool
   */
```

```
  lvectorchrombitcrispmatrix_matingPool.reserve
    (aiinp_inParamWithoutPcPmFk.getSizeMatingPool());

  /*Space for chromosomes R
   */
  lvectorchromfixleng_childR.reserve
    (aiinp_inParamWithoutPcPmFk.getSizeMatingPool() + 1 );
```

Initialization of population. Initial population of size P, consisting of U matrices is pseudo randomly generated such that each has one at least one 1 in every row $\sum_{j=1}^{n} U_{ij} \geq 1 \forall i$) and each column sums to 1, i.e. $\sum_{i=1}^{c} U_{ij} = 1, \forall j$. The partly random initialization is obtained as follows. For each cluster center v_i, it is chosen the k^{th} element of the cluster center to be the k^{th} feature of a randomly chosen pattern to be clustered. This is done for each of the s elements of a cluster center. The process is repeated for each cluster center. An initial U matrix is then generated from the cluster centers.

For a GA of population P (the population size), U matrices are generated in this manner [BBHB94].

```
{/*BEGIN INITIALIZE POPULATION*/

#ifdef __VERBOSE_YES
    geverbosepc_labelstep = "POPULATION INITIALIZATION";
    ++geiinparam_verbose;
    if ( geiinparam_verbose <= geiinparam_verboseMax ) {
      std::cout
        << geverbosepc_labelstep
        << ":  IN(" << geiinparam_verbose << ')'
        << std::endl;
    }
#endif /*__VERBOSE_YES*/

    mat::MatrixRow<T_FEATURE>
      lmatrixt_v
      ( luintidx_numClusterK,
        data::Instance<T_FEATURE>::getNumDimensions()
        );

    for ( auto lchrombitcrispmatrix_iter: lvectorchrombitcrispmatrix_population) {

      clusteringop::randomInitialize
        (lmatrixt_v,
         aiiterator_instfirst,
         aiiterator_instlast
         );

      clusteringop::getPartition
        (*lchrombitcrispmatrix_iter,
         lmatrixt_y,
         lmatrixt_v,
         aifunc2p_dist
         );

      T_REAL lT_j1 =
        um::j1
        (*lchrombitcrispmatrix_iter,
         lmatrixt_v,
         aiiterator_instfirst,
```

```
          aiiterator_instlast,
          aifunc2p_dist
          );

      lchrombitcrispmatrix_iter->setObjetiveFunc(lT_j1);

    }

#ifdef __VERBOSE_YES
    if ( geiinparam_verbose <= geiinparam_verboseMax ) {
      std::cout
        << geverbosepc_labelstep
        << ": OUT(" << geiinparam_verbose << ')'
        << std::endl;
    }
    --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

  } /*END INITIALIZE POPULATION*/
```

The U matrices are sorted by J_1 value.

```
{/*BEGIN POPULATION SORT BY J_1*/

#ifdef __VERBOSE_YES
    geverbosepc_labelstep = "SORT POPULATION";
    ++geiinparam_verbose;
    if ( geiinparam_verbose <= geiinparam_verboseMax ) {
      std::cout
        << geverbosepc_labelstep
        << ":  IN(" << geiinparam_verbose << ')'
        << std::endl;
    }
#endif /*__VERBOSE_YES*/


    std::sort
      (lvectorchrombitcrispmatrix_population.begin(),
       lvectorchrombitcrispmatrix_population.end(),
       [](const gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>* x,
          const gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>* y
          )
       {  return x->getObjetiveFunc() < y->getObjetiveFunc(); }
       );


#ifdef __VERBOSE_YES

    ++geiinparam_verbose;
    if ( geiinparam_verbose <= geiinparam_verboseMax ) {

      for ( auto lchrombitcrispmatrix_iter: lvectorchrombitcrispmatrix_population) {

        lchrombitcrispmatrix_iter->print
          (std::cout,
           geverbosepc_labelstep,
           ',',
           ';'
           );
        std::cout << '\n';
```

```
      }
    }
    --geiinparam_verbose;

    if ( geiinparam_verbose <= geiinparam_verboseMax ) {
      std::cout
        << geverbosepc_labelstep
        << ": OUT(" << geiinparam_verbose << ')'
        << std::endl;
    }
    --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

  } /*END POPULATION SORT BY J_1*/


  while( true ) {

    {/*BEGIN PRESERVING THE CHROMOSOME BEST
      */
#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "ELITISM PRESERVING THE BEST";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ":  IN(" << geiinparam_verbose << ')'
          << std::endl;
      }
#endif /*__VERBOSE_YES*/

      if ( lvectorchrombitcrispmatrix_population[0]->getObjetiveFunc()
           < lochrombitcrispmatrix_best.getObjetiveFunc() ) {
        lochrombitcrispmatrix_best =
          *lvectorchrombitcrispmatrix_population[0];
         /*A better chromosome is found in this iteration
          */
        aoop_outParamGAC.setIterationGetsBest
          (llfh_listFuntionHist.getDomainUpperBound());
        aoop_outParamGAC.setRunTimeGetsBest
          (runtime::elapsedTime(let_executionTime));
      }

#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

    } /*END PRESERVING THE CHROMOSOME BEST*/

    /*COMPUTING STATISTICAL OF THE ALGORITHM
     */
#ifndef __WITHOUT_PLOT_STAT
```

```
if ( aiinp_inParamWithoutPcPmFk.getWithPlotStatObjetiveFunc() ) {

  for ( auto lchrombitcrispmatrix_iter:
          lvectorchrombitcrispmatrix_population) {
    lvectorT_statfuncObjetiveFunc.push_back
      (lchrombitcrispmatrix_iter->getObjetiveFunc());
  }

  lofh_J1->setValue
    (lvectorchrombitcrispmatrix_population[0]->getObjetiveFunc());

  if ( lofh_misclassified != NULL ) {

    partition::PartitionCrispMatrix
      <T_BITSIZE,T_CLUSTERIDX>
      lpartitionCrispMatrix_classifierU
      (*lvectorchrombitcrispmatrix_population[0]);


    sm::ConfusionMatchingMatrix<T_INSTANCES_CLUSTER_K>&&
      lmatchmatrix_confusion =
      sm::getConfusionMatrix
      (aiiterator_instfirst,
       aiiterator_instlast,
       lpartitionCrispMatrix_classifierU,
       [](const data::Instance<T_FEATURE>* aiinst_iter )
       -> T_INSTANCES_CLUSTER_K
       {
         return  T_INSTANCES_CLUSTER_K(1);
       },
       [](const data::Instance<T_FEATURE>* aiinst_iter )
       -> T_CLUSTERIDX
       {
         data::InstanceClass
           <T_FEATURE,
            T_INSTANCES_CLUSTER_K,
            T_CLUSTERIDX>
           *linstclass_iter =
           (data::InstanceClass
            <T_FEATURE,
            T_INSTANCES_CLUSTER_K,
            T_CLUSTERIDX>*)
           aiinst_iter;

         return linstclass_iter->getClassIdx();

       }
       );
    lofh_misclassified->setValue
      (lmatchmatrix_confusion.getMisclassified());
  }
  functionhiststat_evaluateAll
    (lofhs_statObjectiveFunc,
     lvectorT_statfuncObjetiveFunc
     );
  lfileout_plotStatObjetiveFunc << llfh_listFuntionHist;
  lvectorT_statfuncObjetiveFunc.clear();
```

```
    }
#endif /*__WITHOUT_PLOT_STAT*/


#ifdef __VERBOSE_YES

    /*ID PROC
     */
    ++geverboseui_idproc;

    ++geiinparam_verbose;
    if ( geiinparam_verbose <= geiinparam_verboseMax ) {
      std::cout
        << "END ITERATION: "
        << llfh_listFuntionHist.getDomainUpperBound()
        << "\tobjetivoFunc = "
        << lochrombitcrispmatrix_best.getObjetiveFunc()
        << std::endl;
    }
    --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

    /*Termination criterion attained?
     */
    if ( (llfh_listFuntionHist.getDomainUpperBound()
          >= aiinp_inParamWithoutPcPmFk.getNumMaxGenerations()) ||
         (runtime::elapsedTime(let_executionTime) >
          aiinp_inParamWithoutPcPmFk.getMaxExecutiontime())
         )
      break;
```

Selection. R matrices with the lowest J_1, values are choses to reproduce [BBHB94].

```
    {/*BEGIN SELECTION
      */
      auto ichrom_population = lvectorchrombitcrispmatrix_population.begin();

      for (uintidx lui_i = 0;
           lui_i < aiinp_inParamWithoutPcPmFk.getSizeMatingPool();
           lui_i++)  {
        lvectorchrombitcrispmatrix_matingPool.push_back
          (*ichrom_population);
        ++ichrom_population;
      }

    }/*END SELECTION*/
```

Crossover operator. The crossover point and number of columns in the two U matrices chosen for reproduction are randomly chosen. The columns of the matrices are combined to create the children matrices [BBHB94].

```
    {/*BEGIN CROSSOVER OPERATORS*/

#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "CROSSOVER OPERATORS";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
```

```
          << geverbosepc_labelstep
          << ":  IN(" << geiinparam_verbose << ')'
          << std::endl;
      }
#endif /*__VERBOSE_YES*/

      for (uintidx lui_i = 0;
           lui_i < aiinp_inParamWithoutPcPmFk.getSizeMatingPool();
           lui_i++) {
        lvectorchromfixleng_childR.push_back
          (new gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>
           (luintidx_numClusterK,luintidx_numIntances)
           );
      }

      gaiterator::crossoverRandSelect
      (lvectorchrombitcrispmatrix_matingPool.begin(),
       lvectorchrombitcrispmatrix_matingPool.end(),
       lvectorchromfixleng_childR.begin(),
       lvectorchromfixleng_childR.end(),
       [&](gaencode::ChromosomeCrispMatrix
           <T_BITSIZE,T_CLUSTERIDX,T_REAL>* aichrom_parent1,
           gaencode::ChromosomeCrispMatrix
           <T_BITSIZE,T_CLUSTERIDX,T_REAL>* aichrom_parent2,
           gaencode::ChromosomeCrispMatrix
           <T_BITSIZE,T_CLUSTERIDX,T_REAL>* aochrom_child1,
           gaencode::ChromosomeCrispMatrix
           <T_BITSIZE,T_CLUSTERIDX,T_REAL>* aochrom_child2
           )
       {

         gabinaryop::onePointDistCrossover
           (*aochrom_child1,
            *aochrom_child2,
            *aichrom_parent1,
            *aichrom_parent2
            );

         aochrom_child1->setObjetiveFunc(std::numeric_limits<T_REAL>::max());
         aochrom_child2->setObjetiveFunc(std::numeric_limits<T_REAL>::max());

       }
       );

      lvectorchrombitcrispmatrix_matingPool.clear();

#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

    }/*END CROSSOVER OPERATORS*/
```

Mutation. It consists of randomly choosing an element of a column to have the value 1, such that it is a different element than the one currently having a value of 1 [BBHB94].

```
    {/*BEGIN MUTATION OPERATOR*/
#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "MUTATION OPERATOR";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ":  IN(" << geiinparam_verbose << ')'
          << std::endl;
      }
#endif /*__VERBOSE_YES*/

      for ( auto ichrom_childR: lvectorchromfixleng_childR ) {
        gabinaryop::bitMutation(*ichrom_childR);
      }

#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/
    } /*END MUTATION OPERATOR*/
```

Evaluate J_1 for childr

```
    {/*BEGIN EVALUATE J1 FOR CHILDR*/
#ifdef __VERBOSE_YES
      geverbosepc_labelstep = "EVALUATE J1 FOR CHILDR";
      ++geiinparam_verbose;
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ":  IN(" << geiinparam_verbose << ')'
          << std::endl;
      }
#endif /*__VERBOSE_YES*/

      mat::MatrixRow<T_FEATURE>
        lmatrixt_v
        (luintidx_numClusterK,
         data::Instance<T_FEATURE>::getNumDimensions()
         );

      mat::MatrixRow<T_FEATURE_SUM>
        lmatrixT_sumWX
        (lmatrixt_v.getNumRows(),
         lmatrixt_v.getNumColumns()
         );
      std::vector<T_INSTANCES_CLUSTER_K>
        lvectorT_sumWik(lmatrixt_v.getNumRows());

      for ( auto ichrom_childR: lvectorchromfixleng_childR ) {
```

```
          /*Calculate the centroid associated with U_i
           */
          clusteringop::getCentroids
            (lmatrixt_v,
             lmatrixT_sumWX,
             lvectorT_sumWik,
             *ichrom_childR,
             lmatrixt_y
             );

          T_REAL lT_j1 =
            um::j1
            (*ichrom_childR,
             lmatrixt_v,
             aiiterator_instfirst,
             aiiterator_instlast,
             aifunc2p_dist
             );

          ichrom_childR->setObjetiveFunc(lT_j1);

        }

#ifdef __VERBOSE_YES
        if ( geiinparam_verbose <= geiinparam_verboseMax ) {
          std::cout
            << geverbosepc_labelstep
            << ": OUT(" << geiinparam_verbose << ')'
            << std::endl;
        }
        --geiinparam_verbose;
#endif /*__VERBOSE_YES*/
      } /*END EVALUATE J1 FOR CHILDR*/
```

Replace. The R and U matrices are added to the population with the $P - R$. U matrices with the greatest J_1 values dropped from the population [BBHB94].

```
      { /*BEGIN ADD P-R U MATRICES TO POPULATION*/
#ifdef __VERBOSE_YES
        geverbosepc_labelstep = "ADD P-R U MATRICES TO POPULATION";
        ++geiinparam_verbose;
        if ( geiinparam_verbose <= geiinparam_verboseMax ) {
          std::cout
            << geverbosepc_labelstep
            << ":  IN(" << geiinparam_verbose << ')'
            << std::endl;
        }
#endif /*__VERBOSE_YES*/

        std::sort
          (lvectorchromfixleng_childR.begin(),
           lvectorchromfixleng_childR.end(),
           [](const gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>* x,
              const gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>* y
              )
           {  return x->getObjetiveFunc() < y->getObjetiveFunc(); }
           );

        std::vector<gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>* >
```

```
        lvectorchrombitcrispmatrix_tmpL;

      lvectorchrombitcrispmatrix_tmpL.swap(lvectorchrombitcrispmatrix_population);

      /*Insert a sentinel to merge the two vectors
       */
      lvectorchrombitcrispmatrix_tmpL.push_back
        (new gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>());
      lvectorchromfixleng_childR.push_back
        (new gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>());

      lvectorchrombitcrispmatrix_population.reserve
        (aiinp_inParamWithoutPcPmFk.getSizePopulation() + 1);

      uintidx luintidx_l = 0;
      uintidx luintidx_r = 0;

      for (uintidx lui_i = 0;
           lui_i < aiinp_inParamWithoutPcPmFk.getSizePopulation();
           lui_i++)
        {

          if (  lvectorchrombitcrispmatrix_tmpL[luintidx_l]->getObjetiveFunc() <
                lvectorchromfixleng_childR[luintidx_r]->getObjetiveFunc() )
            {

#ifdef __VERBOSE_YES
              ++geiinparam_verbose;
              if ( geiinparam_verbose <= geiinparam_verboseMax ) {
                std::cout
                  << " lvectorchrombitcrispmatrix_population[" << lui_i <<  ']'
                  << " <--  lvectorchrombitcrispmatrix_tmpL[" << luintidx_l << ']'
                  << '[' << & lvectorchrombitcrispmatrix_population[luintidx_l] << ']'
                  << " Fitness: "
                  <<  lvectorchrombitcrispmatrix_tmpL[luintidx_l]->getObjetiveFunc()
                  << '\n';
              }
              --geiinparam_verbose;
#endif //__VERBOSE_YES

              lvectorchrombitcrispmatrix_population.push_back
                (lvectorchrombitcrispmatrix_tmpL[luintidx_l]);
              lvectorchrombitcrispmatrix_tmpL[luintidx_l] = NULL;
              ++luintidx_l;

            }
          else {

#ifdef __VERBOSE_YES
            ++geiinparam_verbose;
            if ( geiinparam_verbose <= geiinparam_verboseMax ) {
              std::cout
                << " lvectorchrombitcrispmatrix_population[" << lui_i <<  ']'
                << " <--  lvectorchromfixleng_childR[" << luintidx_r << ']'
                << "[" << & lvectorchrombitcrispmatrix_population[luintidx_r] << ']'
                << " Fitness: "
                <<  lvectorchromfixleng_childR[luintidx_r]->getObjetiveFunc()
                << '\n';
```

```
            }
            --geiinparam_verbose;
#endif //__VERBOSE_YES

            lvectorchrombitcrispmatrix_population.push_back
              (lvectorchromfixleng_childR[luintidx_r]);
            lvectorchromfixleng_childR[luintidx_r] = NULL;
            ++luintidx_r;

          }

        }

      for (uintidx lui_i = 0;
           lui_i < lvectorchromfixleng_childR.size();
           ++lui_i) {
        if ( lvectorchromfixleng_childR[lui_i] != NULL )
          delete lvectorchromfixleng_childR[lui_i];
      }
      lvectorchromfixleng_childR.clear();

      for (uintidx lui_i = 0;
           lui_i < lvectorchrombitcrispmatrix_tmpL.size();
           ++lui_i) {
        if ( lvectorchrombitcrispmatrix_tmpL[lui_i] != NULL )
          delete lvectorchrombitcrispmatrix_tmpL[lui_i];
      }
      lvectorchrombitcrispmatrix_tmpL.clear();

#ifdef __VERBOSE_YES
      if ( geiinparam_verbose <= geiinparam_verboseMax ) {
        std::cout
          << geverbosepc_labelstep
          << ": OUT(" << geiinparam_verbose << ')'
          << std::endl;
      }
      --geiinparam_verbose;
#endif /*__VERBOSE_YES*/
    } /*END ADD P-R U MATRICES TO POPULATION*/

    /*The reproduction and survival of fittest process
      continues for some set number of generations
    */

    llfh_listFuntionHist.increaseDomainUpperBound();

  } /*while*/

  /*FREE MEMORY*/
  {/*BEGIN FREE MEMORY OF POPULATION*/

#ifdef __VERBOSE_YES
    geverbosepc_labelstep = "DELETEPOPULATION";
    ++geiinparam_verbose;
    if ( geiinparam_verbose <= geiinparam_verboseMax ) {
      std::cout
        <<  geverbosepc_labelstep
        << ":  IN(" << geiinparam_verbose << ')'
```

```
        << std::endl;
    }
#endif /*__VERBOSE_YES*/

    for (uintidx lui_i = 0;
         lui_i < lvectorchrombitcrispmatrix_population.size();
         ++lui_i) {
      delete lvectorchrombitcrispmatrix_population[lui_i];
    }

#ifdef __VERBOSE_YES
    if ( geiinparam_verbose <= geiinparam_verboseMax ) {
      std::cout
        << geverbosepc_labelstep
        << ": OUT(" << geiinparam_verbose << ')'
        << std::endl;
    }
    --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

  }/*END FREE MEMORY OF POPULATION*/

  runtime::stop(let_executionTime);
  aoop_outParamGAC.setNumClusterK
    (aiinp_inParamWithoutPcPmFk.getNumClusterK());
  aoop_outParamGAC.setMetricFuncRun
    (lochrombitcrispmatrix_best.getObjetiveFunc());
  aoop_outParamGAC.setAlgorithmRunTime
    (runtime::getTime(let_executionTime));

  aoop_outParamGAC.setFitness
    (lochrombitcrispmatrix_best.getObjetiveFunc());
  aoop_outParamGAC.setNumTotalGenerations
    (llfh_listFuntionHist.getDomainUpperBound());

  /*FREE: COMPUTING STATISTICAL AND METRIC OF THE ALGORITHM
   */
#ifndef __WITHOUT_PLOT_STAT

  if ( aiinp_inParamWithoutPcPmFk.getWithPlotStatObjetiveFunc() ) {
    plot_funtionHist
      (llfh_listFuntionHist,
       aiinp_inParamWithoutPcPmFk,
       aoop_outParamGAC
       );
  }

#endif /*__WITHOUT_PLOT_STAT*/



#ifdef __VERBOSE_YES
  geverbosepc_labelstep = lpc_labelAlgGA;
  if ( geiinparam_verbose <= geiinparam_verboseMax ) {
    std::cout
      << lpc_labelAlgGA
      << " OUT(" << geiinparam_verbose << ")\n";
    std::setprecision(COMMON_COUT_PRECISION);
```

```
    mat::MatrixRow<T_FEATURE>
      lmatrixt_vBestChrom
      ( luintidx_numClusterK,
        data::Instance<T_FEATURE>::getNumDimensions()
        );

    mat::MatrixRow<T_FEATURE_SUM>
      lmatrixT_sumWX
      (lmatrixt_vBestChrom.getNumRows(),
       lmatrixt_vBestChrom.getNumColumns()
       );

    std::vector<T_INSTANCES_CLUSTER_K>
      lvectorT_sumWik(lmatrixt_vBestChrom.getNumRows());

    clusteringop::getCentroids
      (lmatrixt_vBestChrom,
       lmatrixT_sumWX,
       lvectorT_sumWik,
       lochrombitcrispmatrix_best,
       lmatrixt_y
       );

    lochrombitcrispmatrix_best.print
      (std::cout,
       geverbosepc_labelstep,
       ',',
       ';'
       );

    std::cout << '\n';
    um::j1
      (lochrombitcrispmatrix_best,
       lmatrixt_vBestChrom,
       aiiterator_instfirst,
       aiiterator_instlast,
       aifunc2p_dist
       );

    std::cout << std::endl;

    std::setprecision(COMMON_VERBOSE_COUT_PRECISION);

  }
  --geiinparam_verbose;
#endif /*__VERBOSE_YES*/

  return lochrombitcrispmatrix_best;

} /*END gaclustering_fkcrispmatrix */

} /*END namespace alg*/

#endif /*__GACLUSTERING_FKCRISPMATRIX_HPP__*/
```

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Appendix C Concept index