Library Evolutionary Algorithms for Clustering (LEAC)

Hermes Robles-Berumen,
Amelia Zafra,
Habib M. Fardoun,
Sebastian Ventura.

This user guide is for Library LEAC (version 1.8, 7 March 2016), and documents commands for clustering analysis.

Table of Contents

1 Introduction

Library Evolutionary Algorithms for Clustering (LEAC) is a library for the implementation of evolutionary algorithms to solve the problem of *partitional clustering*, the purpose is to find an optimal partition of a dataset 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 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.

LEAC library it is based on a *layered software architecture* and is conceptually composed of four layers, each of which consists of a set of related packets as shown in the Figure 1.1. The description of each layer is described below:

Algorithm

It consists of evolutionary algorithms, which use the layer based on the operator EA.

EA Implement what you need to configure GA: encoding criterion, initialization of population, criterion for selecting parents, crossover and mutation operators. Along with the support of the lower layers to achieve scheme of evolution.

Clustering

It refers to the domain of the problem and implements all specic clustering operators, such as, supervised and unsupervised performance measures and clustering operators based on centroids, crispmatrix or medoids. It is the layer referring to the domain of the problem.

Performance

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

---

[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
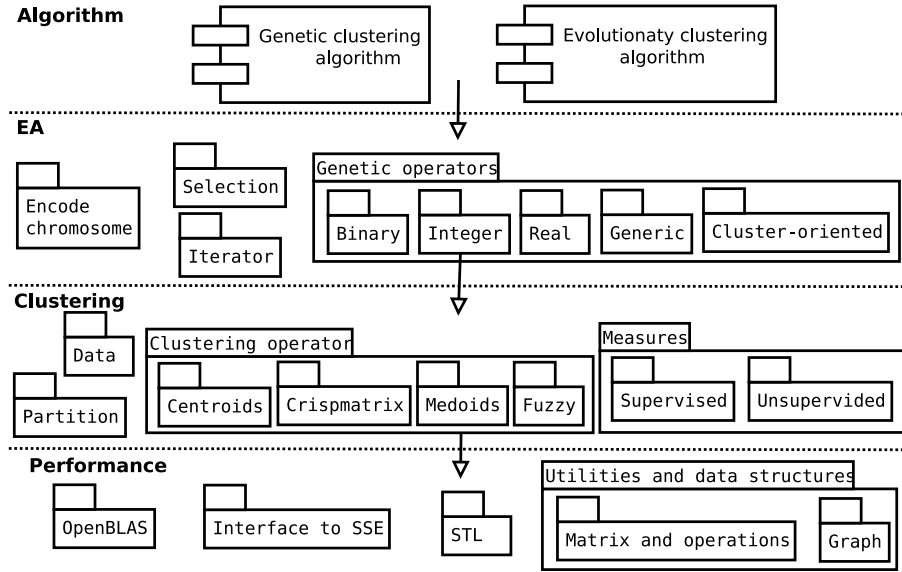
Figure 1.1: *Layered software architecture* of LEAC library

Encode	Fixed-K	Variable-K
	`gaclustering_fklabel`, MC96	`gga_vklabeldbindex` and `gga_vklabelsilhouette`, ABSSJF+12
	`gka_fklabel`, KM99	
	`igka_fklabel`, LLF+04b	`cga_vklabel`, HE03
Label	`fgka_fklabel`, LLF+04a	`eac_vklabel`, HCdC06
		`eaci_vklabel`, `eacii_vklabel`, `eaciii_vklabel` and `feac_vklabel`, ACH06
Crisp matrix	`gaclustering_fkcrispmatrix`, BBHB94	
	`gas_fkcentroid`, MB00	`gcuk_vkcentroid`, BM02b
	`kga_fkcentroid`, BM02a	`tgca_vkcentroid`, HT12
Centroids	`gagr_fkcentroid`, CZZ09	
	`cbga_fkcentroid_int` and `cbga_fkcentroid`, FKKN97	
Medoid	`gaprototypes_fkmedoid`, KB97	
	`hka_fkmedoid`, SL04	
	`gca_fkmedoid`, LDK93	
Tree		`gaclustering_vktreebinary`, CdLM03
Sub-cluster		`clustering_vksubclusterbinary`, TY01

Table 1.1: List of evolutionary algorithms implemented with the LEAC library, described by the taxonomy proposed by HCFdC09

LEAC is a modular library which make easier to develop new evolutionary algorithm proposals for solving the partitional clustering. Moreover, it contains the most representative proposals of Evolutionary Algorithms for partitional clustering. Following the taxonomy set by HCFdC09 a first classification of these algorithms is carried out according to the use of fixed or variable number initial of clusters, as well as to the representation of the clusters of a data set. Concretely, 20 state-of-art EA proposals are included, of which 23 programs are implemented see Table 1.1.

LEAC is based on the current standards of the C++ language, as well as on Standard Template Library (STL) and also OpenBLAS to have a better performance. Taking advantage of the characteristics of the C++ language as hybrid language, generic programming, multi-paradigms and lambda function and the C++11 versions and C++14. It allowed the implementation of different evolutionary algorithms. The approach of LEAC to implement the particular characteristics of each algorithm is to encode the diversity of the proposed genetic operators and to use the containers and interpliers of STL to evolve the population according to the flowchart of the algorithms.

2 Get and Install LEAC software

For Windows® systems, perform steps 1 through 7 and 12. For GNU/Linux systems and Mac OS X®, perform steps 1, 2 and 8 through 12.

1. Download the leac project from https://github.com/kdis-lab/leac.

2. Unzip the file `leac.zip`, we recommend you in the directory `c:\leac` for Windows® and `/home/user/leac` 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 EAC binary or executable programs, which result from the compilation of using LEAC.

   `data`　　Directory used to store the data sets to be processed.

   `doc`　　　In the 'doc' directory you will find all the necessary 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`　Contains LEAC library header files and source code.

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

   `openblas`　Contains only the header files needed to compile a program with some functionality of the OpenBlas library.

   `sse_kernel`
   　　　　　`sse_kernel` is a module based on OpenBlas and GotoBLAS2, own of LEAC. The functionality of this module together with that of OpenBlas is 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 8], page 7.

3. Download and install one of the two IDE with the `MinGW` option Dev-C++ or Code::Blocks

4. Check the `PATH` where MinGW is installed, it can be `C:\Program Files (x86)\Dev-Cpp\MinGW64\bin` or `C:\Program Files (x86)\CodeBlocks\MinGW\bin` and add it 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 2.1).

      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 want 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:\Program Files (x86)\Dev-Cpp\MinGW64\bin'

   e. press `OK -> OK -> OK` and you are done.

5. Download and install gnuplot. The recommendation for the installation is to use the file gp530-20170911-win64-mingw.zip. Unzip in the `c:\gnuplot` directory and add `c:\gnuplot\bin` in the environment variable `PATH` in the same way as in [Step 4], page 5.

6. Optionally install the epsviewer file viewer, to visualize the data sets and the clusters created by the different programs

7. With the compiler installed See [Step 4], page 5, you can now compile the EAC applications. Open a `cmd`, you must change the directory to the `leac` directory, For example: 'cd c:\leac\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 12], page 8.

8. 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. Running 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`', '`sudo port install gcc5`'.

For Mac OS X go to .

9. If you want to use compile your applications with high-performance modules `OpenBLAS` and `sse_kernel`, for now this option only works on the `x86-64` architecture with GNU/Linux. If you do not want this option, go to and compile with the option `WITH_OPEN_BLAS = no`.

First 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, 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 the static libraries of each of the components.

`OpenBLAS`

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

   b. Unzip the file with the '`tar zxvf OpenBLAS-0.2.20.tar.gz`' command.
     '`cd OpenBLAS-0.2.20`'

   c. After editing `Makefile.rule` '`NO_CBLAS=1, NO_LAPACK=1, NO_LAPACKE=1`' and run '`make FC=gfortran`'

   d. Copy `libopenblas.a` static library from the `OpenBLAS-0.2.20` directory to the `openblas` directory of `leac`, e.g. '`cp libopenblas.a leac/openblas`'

`CBLAS, LAPACK and LAPACKE`

   a. Download lapack-3.8.0.tar.gz from http://www.netlib.org/lapack/

   b. '`tar zxvf lapack-3.8.0.tar.gz`', '`cd lapack-3.8.0`'

   c. '`cp make.inc.example make.inc`'

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

e. Then you must execute the 'make cblaslib', 'make lapacklib' and 'make lapackelib'.

f. Copy static libraries 'cp libcblas.a leac/openblas/', 'cp liblapack.a leac/openblas/' and 'cp liblapacke.a leac/openblas/'

sse_kernel

a. Change to sse_kernel directory, within leac

b. Just type make to compile the library and get libssekernel.a

10. Install gnuplot, as a system administrator (root), for GNU/Linux run 'apt-get install gnuplot-x1'. For Mac OS X 'sudo port install gnuplot'.

11. You can now compile the EAC applications, change to the eac inside the leac home directory 'cd leac/eac'.

First edit the Makefile file and change the name of the compiler you are using 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 evolutionary behavior of the 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 must complete See [Step 9], page 7,

12. The API documentation of LEAC was written for Doxygen. For generate the LEAC library API documentation, 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 must also 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, type 'doxygen Doxyfile' in the leac 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'.

If you do not want to install Doxygen and generate the documentation, we recommend that you use the integrated documentation contained in the html.zip file of the doc directory.
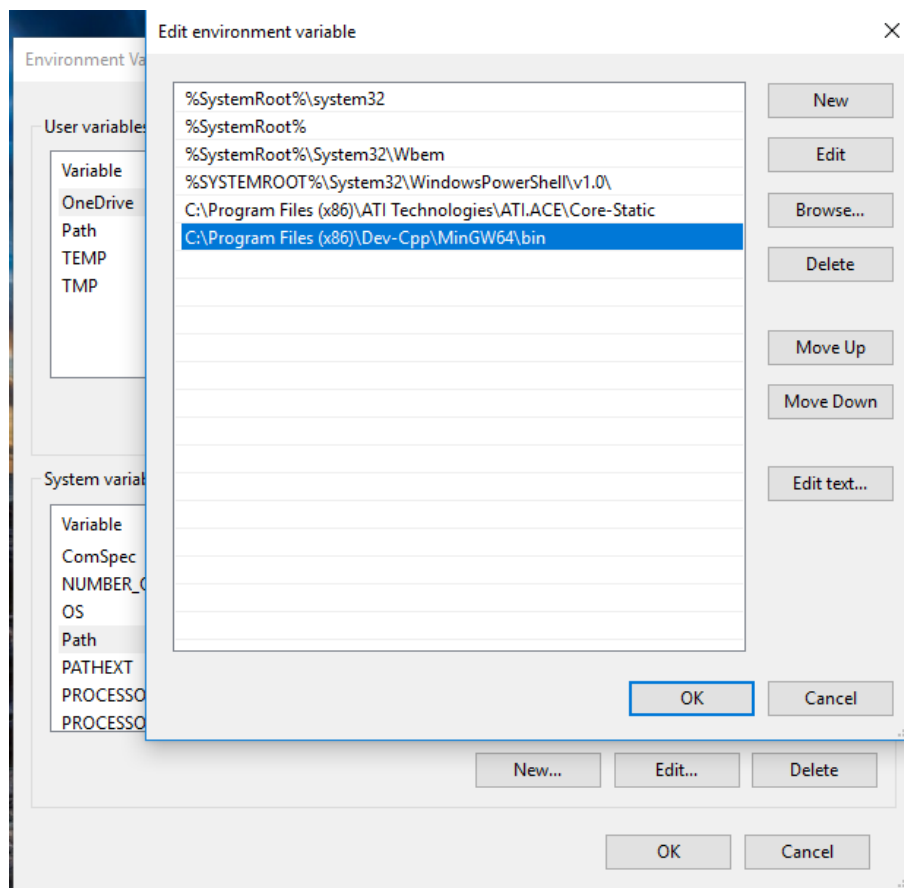
Figure 2.1: Dialog to add the `MinGW` compiler to the `PATH` environment variable

3 LEAC Software

In this chapter it 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 71. The complete documentation of the LEAC components can be found in the doc/html folder.

If you want to build a new algorithm, you must select the components and put them together in a source file and in the next Section 3.2 [Make an executable for a new algorithm], page 36, we describe how to create the executable file. The third section (Section 3.3 [Using implemented algorithms], page 42) describes how to use the algorithms implemented with LEAC as the end user. If you want to use the implementations of the algorithms listed in Table 1.1, you can omit the first two sections.

3.1 Implementation of an algorithm

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

There are different coding schemes proposed, for the case of the clustering problem traditional encoding string as *binary*, *integer* or *real*, You can also use others based on a partition of the objects in the dataset as pair of *partitioning table and cluster centroids*. The output of an evolutionary algorithms depends on the type of coding used by each for the chromosomes and its associated phenotype: *centroid*, *medoid*, *label*, *tree*, or *graph-based* representations. The terms genotype, chromosome, and individual usually have the same meaning in the literature on evolutionary algorithms.

The different encodings are implemented in the LEAC chromosome class hierarchy shown in Figure 3.1.
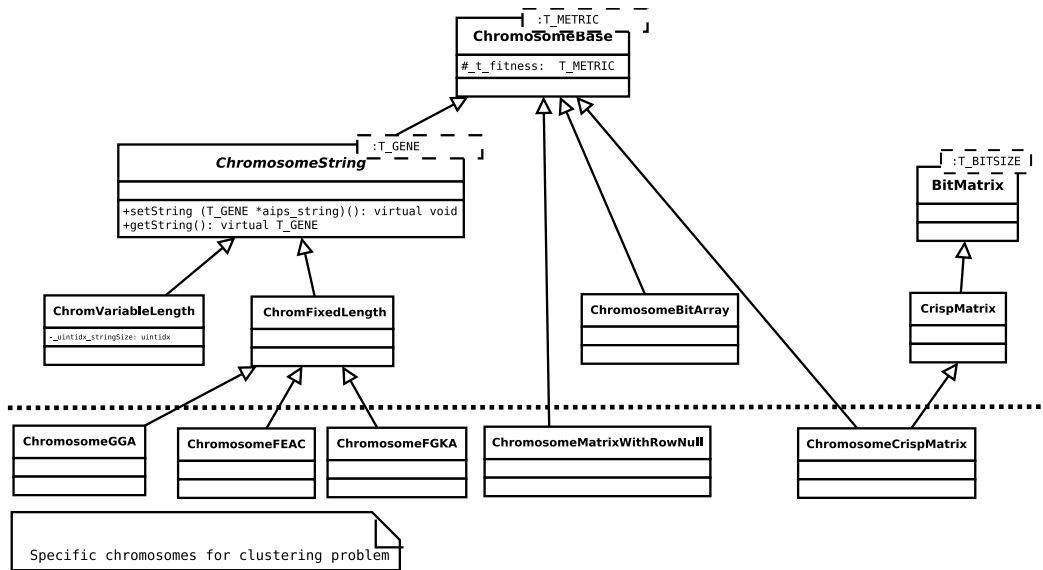
Figure 3.1: Class diagrams of the Chromosomes used for encoding

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 evolution. The constructor method is:

   ChromFixedLength   [Method on `gaencode::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:

   static void setStringSize   [Method on `gaencode::ChromFixedLength`]
            (uintidx aiuintidx_stringSize)
         See [Example], page 73

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

   ChromVariableLength   [Method on `gaencode::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 above chromosomes could be used with the `T_GENE` parameter equal to `bool`, but to have a better efficiency in storage and performance in the application of genetic operators, bit-level management is performed.

ChromosomeBitArray   [Method on `gaencode::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 and the ith element establishes a relation of belonging from the ith instance to a cluster.

To instantiate the *string-of-group-numbers* chromosomes, you can use the class of use [gaencode::ChromFixedLength], page 12, where `T_GENE` is 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. Formally defined by BEF84 called *crisp partition* or *hard partition*:

$$M_c = \{U_{k \times n} | u_{ji} \in \{0,1\}; \sum_{i=1}^{n} u_{ji} > 0, \text{for all } j, \ \sum_{i=1}^{n} u_{ji} = 1, \text{for all } i\} \qquad (4.1)$$

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

ChromosomeCrispMatrix   [Method on `gaencode::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 it es the type of data for fitness function
See [Example ChromosomeCrispMatrix], page 89.

3.1.1.2 Centroid-based

a. **Real encoding** A chromosome in this encoding is a vector of real numbers that contains the coordinates of each centroid consecutively of the clusters. For an $d-$dimensional 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 centre, the next d positions represent those of the second cluster centre, and so on:

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

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 73.

When a *centroid-based* partition is used, it can be derived by the *nearest object rule* into account the proximities between objects and centroids such a way that the ith object is assigned to the cluster represented by the closer (i.e., the most similar). With the centroids of the groups μ_j, so the object x_i belongs to the cluster C_j if:

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

b. **Binary encoding**

Another algorithm based centroids, and with a binary coding is proposed by 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 every V_i is used as a seed to generate a higher level cluster.

The length of each chromosomes is m, where the ith position of the string will be '1' therefore, centroid V_i is used as a seed to group those who have a '0' gene and are closer to it.

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 representation of the dataset. In this case, each array element represents the index of the object x_i, where $i = 1, 2, ..., n$.

For implementation you can use `gaencode::ChromFixedLength` with T_GENE as index data type. See [gaencode::ChromFixedLength], page 12.

b. **Binary encoding**

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

For implementation you can use `gaencode::ChromosomeBitArray`. See [gaencode::ChromosomeBitArray], page 13.

3.1.1.4 Graph-based

a. **Binary encoding**

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 data set objects. As the MST have $n-1$ edges. This is the length of the chromosomes. 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 $k-1$.

3.1.2 Initialization of population

Before initializing the population, you must create a container from the `STL` library, such as `std::vector` or `std::list`. See [Example a vector of chromosomes], page 73, to represent the population or pool mating.

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.

In the case studies of this document see Section A.2 [GA algorithm], page 87, and Section A.1 [KGA algorithm], page 71. They use an initialization of seed centroids, selected randomly from the instances and all instances are distributed in groups around these centroids by *nearest object rule*.

For the particular case of population initialization in the `GA algorithm` (Section A.2 [GA algorithm], page 87), the following two functions are used:

With non-repeated instance indices, the centroids of the clusters can be constructed:

void `clusteringop::randomInitialize`   [Function]
  (*mat::MatrixBase<T_FEATURE>* &*aomatrixt_centroids*,
  const INPUT_ITERATOR `aiiterator_instfirst`,
  const INPUT_ITERATOR `aiiterator_instlast`)
  See [Example clusteringop::randomInitialize], page 92

And finally with the centroids is created an initial partition:

void `clusteringop::getPartition`   [Function]
  (*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 92

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 GAs algorithms are based on the optimization of some objective function that guides the evolutionary search, In the clustering problem we use different measures used for the optimization function used to evaluate the so-called *fitness function*. For the metrics available by LEAC See Section 3.1.3.2 [Unsupervised measures], page 18.

3.1.3.1 Distances

Distance measures is the key in clustering to find the similarity between two objects x_i and x_i'. To calculate the different clustering metrics a *distance* is used. 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
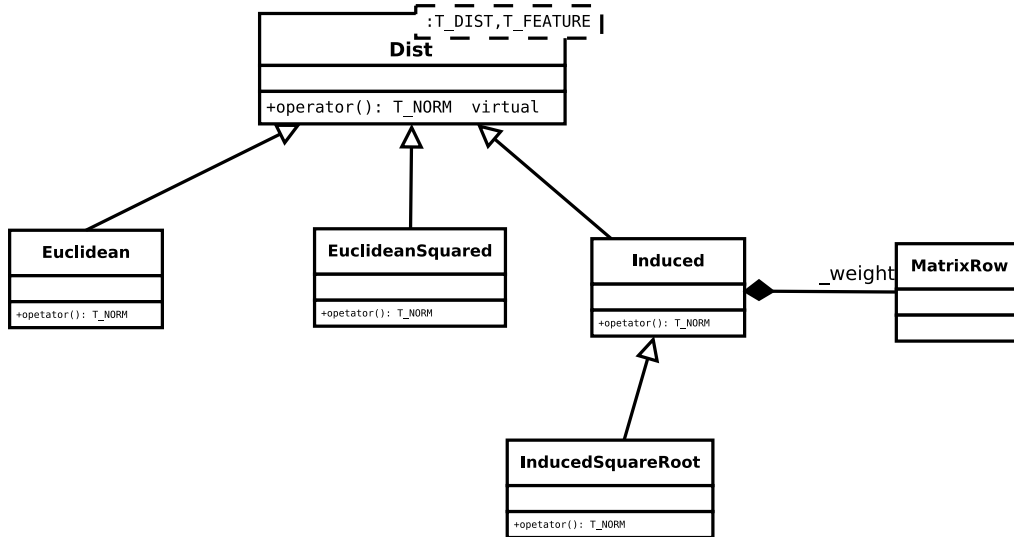
Figure 3.2: Class diagrams of the Distances

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

T_DIST *operator*()   [Method on `dist::Dist`]
        (*const T_FEATURE*, const T_FEATURE*, const uintidx*)

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

Euclidean <*T_DIST,T_FEATURE*> ()   [Method on `dist::Euclidean`]

Example

```
dist::Dist<DATATYPE_REAL,DATATYPE_FEATURE>
  *pfunct2p_distAlg = NULL;

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;
}
```

Induced<T_DIST,T_FEATURE>   [Method on `dist::Induced`]

     (*const mat::MatrixRow<T_DIST>&* `aimatrix_weight`)

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 (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

mat::MatrixRow<T_FEATURE> mat::getIdentity   [Function]
        (*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

mat::MatrixRow<T_FEATURE> dist::getMatrixMahalonobis   [Function]
        (*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 used as an matrix of weights at the *induced distance* is equivalent
> to *Mahalanobis distance* ($A = C_x^{-1}$).
> See [Example dist::getMatrixMahalonobis], page 17

mat::MatrixRow<T_FEATURE> dist::getMatrixDiagonal   [Function]
        (*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

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. This is why this unsupervised measure are sometimes called as internal measures ABSSJF+12. All *unsupervised measures* function of the library are defined in the header file `unsupervised_measures.hpp`, to do calculations of metrics you can 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 in CZZ09 as

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

   Where x_i represents the instance ith of the dataset. 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 in KM99, using [Crisp Partition], page 13, and calling it *total within-cluster variation* (TWCV)

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

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

Or with some slight variation *Sum of Euclidean Distance* SED:

$$\text{SED} = \sum_{C_j} \sum_{x_i \in C_j} \|x_i - \mu_j\| \qquad (3.6)$$

This is probably 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 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 16), to obtain the variations of the metric:

std::pair<T_METRIC,bool> `um::SSE`   [Function]
       (*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 14.
     See [Example um::SSE], page 78

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:

T_METRIC `um::SSE`   [Function]
       (*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`)

std::pair<T_METRIC,bool> `um::SSE`   [Function]
       (*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, you have a set of partition clusters classes (`partition::Partition`) for calculating metrics generically. See Figure 3.3. For example, a partition based on (3.2), the constructor you can use is

[Method 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 for one based on a crisp matrix (4.1):

[Method on partition::PartitionCrispMatrix]

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

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

T_METRIC `partition::makePartition`   [Function]
(*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*)
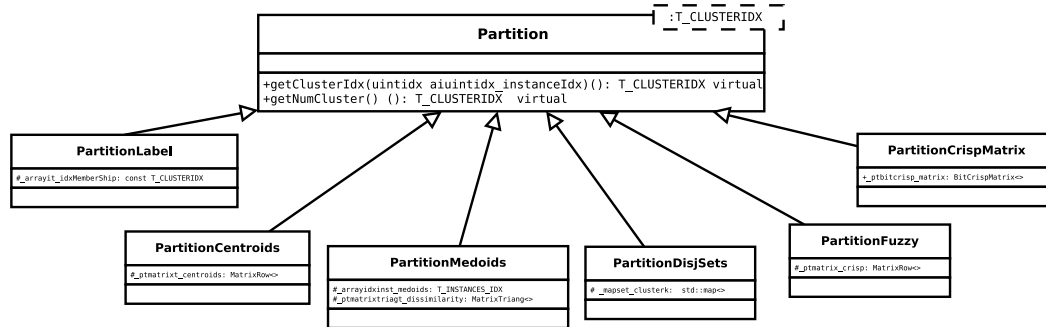
Figure 3.3: Class diagram of the partitions used to calculate the metrics

2. **Distortion**

The distortion of the clusters is a measure define by FKKN97. Similar to SSE but
considers the number of instances and attributes:

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

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

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

std::pair<T_METRIC,bool> um::distortion   [Function]
   (*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), we obtain the cost function sum of Euclidean distances to the most representative instance:

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

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

T_METRIC um::SSEMedoid   [Function]
   (*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.

mat::MatrixTriang<T_DIST> medoids::getMatrixDissimilarity   [Function]
   (*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 (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*, described in BEF84

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

Where

$U \in M_{fc}$ (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 17,

T_METRIC `um::jm`   [Function]
          (*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 will be based on $J_m(U, \mu)$ from (3.10), we will rewrite J_1 as:

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

T_METRIC `um::j1`   [Function]
          (*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 92

5. **Davis-Bouldin Index**

Davies–Bouldin index (DB) 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 as

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

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

$$R_{C_j, C_{1 \le j' \le k}} = \max_{j',\, j' \ne j} R_{C_j, C_{j'}}$$

where $R_{C_j, C_{j'}}$ is a measure between a pair of cluster 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 j^{th} 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 qth root of the qth moment of the points in cluster j with respect to their mean, and is a measure of the dispersion of the points in cluster j. $d_{jj', t}$ is the Minkowski distance of order t between the centroids that characterize clusters j and j'.

DB use in BM02b.

T_METRIC   um::DBindex   [Function]
        (*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 KR90. Consider an object x_i belonging to cluster C_j. So, 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 $C_j \ne Cj'$, 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 $s(x_i)$ given by (ACH06):

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

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

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

   Use in HE03 and ABSSJF+12.

T_METRIC   um::silhouette   [Function]
        (*mat::MatrixTriang<T_METRIC> &aimatrixtriagrt_dissimilarity*,
        ds::PartitionLinkedNumInst<T_CLUSTERIDX,T_INSTANCES_CLUSTER_K>
        &aipartlinknuminst_memberShip)

7. **Simplified Silhouette**

The silhouette proposed in KR90 depends on the computation of all distances between objects, leading to a computational cost of $O(n^2)$, which is often not sufficiently efficient for real-world clustering applications (e.g. data mining, text mining, gene-expression data analysis). To circumvent this limitation, a simplified silhouette can be employed. The simplified silhouette is 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) becomes 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. While these modifications reduce the computational cost from $O(n^2)$ to $O(n)$ ACH06.

std::vector<T_METRIC> um::simplifiedSilhouette   [Function]
        (*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 CSL04 DAK08 is defined as

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

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.

CSL04 Establish that this measure is a function of the ratio of the sum of within-cluster scatter to between-cluster separation. The smallest $CS(C)$ indicates a valid optimal partition. The CS measure has the same rationale as the DI (See [Dunn's index], page 25) and the DB (See [Davis-Bouldin Index], page 22).

T_METRIC   um::CSmeasure   [Function]
    (*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**

   A well-established hard cluster validity measure is the Dunn's index (DI) that identifies
   sets of clusters that are well separated. Dunn's index is defined as (CSL04)

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

   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 as k and n
   increase. The largest $DI(C)$ indicates a valid optimal partition CSL04.

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

   To avoid calculating distance between instances again and improve performance in the
   DI evaluation To avoid calculating the distance between the instances and improving
   performance in the evaluation, use the following function:

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

10. **Simplified Dunn's index**

    Just as the [silhouette], page 23, can also simplify [Dunn's measure], page 25, to reduce
    the computational cost of $O(n^2)$ to $O(n)$ using the centroids. This measure will be
    called *Simplified Dunn's index* (SDI).

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

Where

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

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

And the function to calculate *Simplified Dunn's index*

T_METRIC `um::simplifiedDunnIndex`   [Function]
      (*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) sometimes called *Calinski–Harabasz index* initially proposed by CH74 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 as:

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

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.

T_METRIC **um::VRC** [Function]
> (*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- and inter-cluster distance**

The definition of *intra- and inter-cluster distance* (DIIC) (TY01) is given by the equation:

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

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

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

And w is a weight. If the value of w is small, we emphasize 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, we emphasize the importance of $D_{inter}(C_j)$. This tends to produce fewer clusters and each cluster tends to be loose. TY01.

T_METRIC **um::Dintra** [Function]
> (*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`)

T_METRIC **um::Dinter** [Function]
> (*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. For a clustering $C_1, C_2, ..., C_k$ 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* described 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 as follows:

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

Where k is the number of clusters

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

and

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

n is the total number of objects x_i. $U(X) = [u_{ji}]_{k \times n}$ is a partition matrix of the objects and μ_j is the centroid es el centro j^{th}. The value of k that maximizes $I(k)$ is considered the correct number of clusters.

T_METRIC `um::indexI`   [Function]
      (*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) XB91 is defined for *fuzzy c-partitions*. See [Definition fuzzy c-partitions], page 21. This index can be extended to a crisp partition. See [crisp partition], page 13. 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}.

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

In detail

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

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

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

T_METRIC **um::xb**   [Function]
(*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).

T_METRIC **um::xb**   [Function]
(*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* Ran71 is defined for two partitions of the same data set X, C in k cluster and R in k' known clases. 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 it as follows:

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

   Where:

   - a: Number of pairs of data objects belonging to the same class in R and to the same cluster in C.

   - b: Number of pairs of data objects belonging to the same class in R yet to different clusters in C.

   - c: Number of pairs of data objects belonging to different classes in R yet to the same cluster in C.

   - d: 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

T_METRIC `sm::randIndex`   [Function]
        (*const*
        sm::ConfusionMatchingMatrix<T_INSTANCES_CLUSTER_K>
        &`aimatchmatrix_confusion`)

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

sm::ConfusionMatchingMatrix**<T_INSTANCES_CLUSTER_K>**   [Function]
        `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 95

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 MRS08.

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

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

T_METRIC `sm::purity` (*const*   [Function]
        sm::ConfusionMatchingMatrix<T_INSTANCES_CLUSTER_K>
        &`aimatchmatrix_confusion`)

3. **Precision**

To calculate the accuracy, we use the pairs of the R and C partitions, and based on Faw06.

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

T_METRIC `sm::precision` (*const*   [Function]
        ConfusionMatchingMatrix<T_INSTANCES_CLUSTER_K>
        &`aimatchmatrix_confusion`)

4. **Recall**

Based on Faw06.

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

T_METRIC **sm::recall** (*const*   [Function]
     ConfusionMatchingMatrix<T_INSTANCES_CLUSTER_K>
     &`aimatchmatrix_confusion`)

3.1.4 Stop Criterion

There exists no 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 string 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 string is observed for a fixed number of iterations, and the best string obtained is taken to be the optimal one MC96.

3.1.5 Select individuals

In this step, the individuals of the population are selected in a mating group to apply the crossing and mutation operators. In LEAC has implemented three 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:

    std::vector**<T_REAL> prob::makeDistRouletteWheel**   [Function]
         (*INPUT_ITERATOR* `aiiterator_instfirst`,
         INPUT_ITERATOR `aiiterator_instlast`,
         const FITNESSOPERATION `fitness_func`)
         See [Example prob::makeDistRouletteWheel], page 82

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

    T_INTIDX **gaselect::getIdxRouletteWheel**   [Function]
         (*const std::vector<T_PROBABILITY>* &`aivectorrt_probDist`,
         const T_INTIDX `aiuintidx_begin`)
         See [Example gaselect::getIdxRouletteWheel], page 82

 2. Tournament. Involves running several "tournaments" between a small number of individuals specified by the variable *aiuintidx_orderTournament* chosen at random from the population, the individual with the best fitness of each tournament is selected:

    INPUT_ITERATOR **gaselect::tournament**   [Function]
         (*const INPUT_ITERATOR* `aiiterator_instfirst`,
         const INPUT_ITERATOR `aiiterator_instlast`,
         const uintidx `aiuintidx_orderTournament`,
         const FITNESSOPERATION `fitness_func`)

 3. Elitism. Some algorithms select the best individuals to be used in the crossing, as

in BEF84 (See Section A.2 [GA algorithm], page 87). In BM02a elitism has been implemented in each generation by replacing the worst chromosome (select the worst and replace it with the best chromosome See [Example elitism replace the worst], page 79) of the population with the best one seen up to the previous generation (See [Example elitism select the best], page 80).

The `<algorithm>` header of the library `STL Algorithms` defines a collection of functions specially designed to be used in ranges of elements, such as `std::max` and `std::sort` that are used to implement elitism.

3.1.6 Crossover operator

To apply the crossover operator LEAC has two functions to iterate over the population and mating pool:

void `gaiterator::crossover`   [Function]
        (*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 82

void `gaiterator::crossoverRandSelect`   [Function]
        (*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 97

Within the iterator function, the crossover operator is applied. In 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* encodings. For a classification of operators see 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.

```
gagenericop::
```
+ onePointCrossover (ChromFixedLength)
+ onePointCrossover (ChromVariableLength)
+ pathCrossover (ChromFixedLength)

```
garealop::
```
+ heuristicCrossover (ChromosomeString)
+ averageCrossover (ChromosomeString)
+ randomMutation (ChromFixedLength)

```
gabinaryop::
```
+ onePointCrossover (ChromosomeBitArray)
+ onePointDistCrossover (ChromosomeBitArray)
+ onePointDistCrossover (BitMatrix)
+ uniformCrossover (ChromosomeBitArray)
+ bitMutation (CrispMatrix)
+ bitMutation (ChromosomeBitArray)
+ eachBitArrayMutation (ChromosomeBitArray)

```
gaclusteringop::
```
+ crossPNNnew (ChromosomeCBGA)
+ onePointCrossover (ChromosomeMatrixWithRowNull)
+ crossoverCGA (ChromFixedLength)
+ mergeCrossover (ChromosomeGGA)
+ MO1 (ChromFixedLength)
+ MO1 (ChromosomeFEAC)
+ MO2 (ChromosomeFEAC)
+ MO2 (ChromFixedLength)
+ splittingMutation (ChromosomeGGA)
+ mergeMutation (ChromosomeGGA)
+ randomMutation (ChromosomeMatrixWithRowNull)
+ splittingMutation (ChromosomeGGA)
+ biDirectionHMutation (ChromosomeString)
+ biDirectionMutation (ChromosomeString)

```
gaintegerop::
```
+ recombinationD_MX (ChromosomeString)
+ mutation (ChromFixedLength)
+ mutationgka (ChromFixedLength)

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

The crossover operators used by the algorithms implemented in section Appendix A [Example source code], page 71, they use `Single-point` and `Two-point` Crossover described below:

void **gagenericop::onePointCrossover**   [Function]
        (*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 gagenericop::onePointCrossover], page 83

void **gabinaryop::onePointDistCrossover**   [Function]
        (*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 97

3.1.7 Mutation operator

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 71, are described below.

BBHB94 use a mutation operator to change the one bit from one row to another in an aletory manner in a *crisp matrix*:

void **gabinaryop::bitMutation**   [Function]
    (mat::CrispMatrix<T_BITSIZE,T_CLUSTERIDX>
    &*aiobitcrispmatrix_chrom*)
    See [Example gabinaryop::bitMutation], page 97.

In BM02a they propose a mutation operator for (4.2) chromosomes (See [centroid-based], page 14). 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} be 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.

void **gaclusteringop::biDirectionHMutation**   [Function]
    (*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 85

3.1.8 Other parameters

It is common for GAs and EAs for clustering to use local search. The `k-means algorithm` is more popular, this is a procedure of fine-tuning of maximum descent, thus speeding up its convergence. The way they apply it varies. LEAC includes an extensive list of functions for local search, some of which are discussed below:

void clusteringop::updateCentroids   [Function]
        (*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`)

With rule (3.2) each point is assigned x_i a the clusters C_j See [Equation (3.2)], page 14. Update 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. Returns the new centroids, the sum of instances and their number per cluster.
See [Example clusteringop::updateCentroids], page 77

Other algorithms propose to use the `k-means algorithms` as an operator (KM99)

T_CLUSTERIDX clusteringop::kmeansoperator   [Function]
        (*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 tags, centroids, sum of instances and number of instances in each cluster.

For *k-medoids* SL04 proposes a heuristic search:

For each cluster C_j finds the most representative object

1. Assign each object in x_i to the cluster C_j with the closest medoid

2. For each cluster C_j, repeat until the medoid does not change

   - Choose a subset C_{subset} in Cj the corresponds to m_j and its p nearest neighbors of m_j.

   - Calulate the new medoid

$$m_j^* = \begin{array}{c} \arg\min \\ x_i \in C_{subset} \end{array} \sum_{x_i' \in C_j} \|x_i - x_i'\|$$

   - if m_j is different from m_j^* replace with the new medoid

3. Repat 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:

void clusteringop::updateMedoids   [Function]
        (*uintidx *aoarrayuiidx_medoids*,
        T_CLUSTERIDX aicidx_numClusterK,
        uintidx aiuiidx_nearestNeighborsP,
        mat::MatrixTriang<T_DIST> &aimatrixtriagt_dissimilarity)
    Update k-medoids, based on SL04
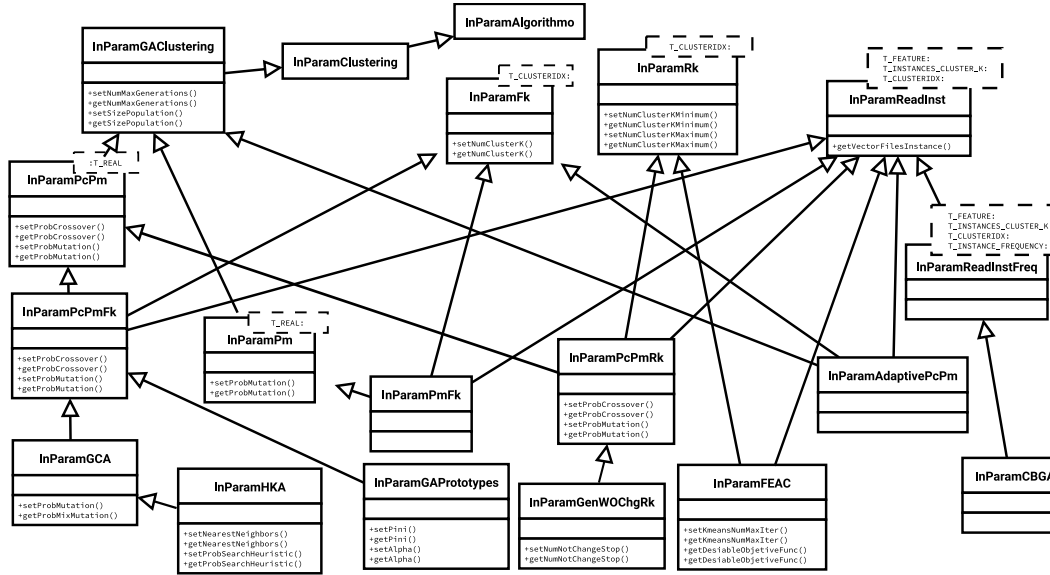
Figure 3.5: Classes used for the input of parameters for the execution of an algorithm

3.2 Make an executable for a new algorithm

There are two options to make an implementation of a new algorithm. The first is simply to include all the necessary operations in the main file. The second option 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 71). In both cases, the configuration scheme of an evolutionary algorithm must be followed see Section 3.1 [Implementation of an algorithm], page 11. The steps you need 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 type of data with which you will work. The datatype_instance_real.hpp and datatype_instance_integer.hpp files suggest the types of data you can use for the selection of variable types, include in source file one for the real '#include <datatype_instance_real.hpp>' or integer '#include <datatype_instance_integer.hpp>' domain respectively 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 one. For example `InParamPcPmFk` include the file '`#include <inparam_pcpmfk.hpp>`'.

`InParamPcPmFk`   [Method on `inout::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. Instance the 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_ClusteringEA
   ("Acronym of the algorithm",
    "Algorithm Authors",
    inout::CENTROIDS,
    INPARAMCLUSTERING_DISTANCE_EUCLIDEAN
    );

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

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

If you are using a class of the class diagram (Figure 3.5), go to [Step 7], page 40. Otherwise do the following. First, you must define the two directives to the preprocessor in the file of your new parameter class, for example:

```
#define __ALG_CLUSTERING__
#define __INPARAM_MY_PCPMFK__
```

The first must be exactly the same name, the second must be a label that refers to the parameters of the algorithm different from the existing ones.

Define similar code blocks that reference the parameters of the new algorithm in the
inparamclustering_getparameter.hpp file.

a. Find the `inparamclustering_usage` function that receives an object with the
parameters of your algorithm and add the directive that was previously defined,
as shown in the following example:

```
#ifdef __INPARAM_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,
 InParamPcPmFk
 <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_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 appropriate `inparamclustering_getParameter` function and add the
directive or definition a similar new one:

```
#ifdef __INPARAM_PCPMFK__
template<typename T_CLUSTERIDX,
         typename T_REAL,
         typename T_FEATURE,
```

```
                    typename T_FEATURE_SUM,
                    typename T_INSTANCES_CLUSTER_K
                    >
          void
          inparamclustering_getParameter
          (InParamPcPmFk
           <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 matrix where the parameter labels are defined and add the directive or define a new matrix with the labels with the parameters for the new algorithm, as shown in the following example:

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

e. Add the directive in the `long_options` parameters, or define for your algorithm

```
#ifdef __INPARAM_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_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 step, you can now invoke the `inparamclustering_` `getParameter` function, to modify or complete the parameters online:

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

Otherwise just read the parameters as in .

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

std::vector<data::Instance<T_FEATURE>* > inout::instancesRead [Function]
   (*inout::InParamReadInst<T_FEATURE,*
   T_INSTANCES_CLUSTER_K, T_CLUSTERIDX>
   &aiipri_inParamReadInst `&aiipri_inParamReadInst`,
   const bool `&aib_fileTest = false`)

std::vector<data::Instance<T_FEATURE>* > [Function]
   inout::instancesReadWithClass
   (*inout::InParamReadInst<T_FEATURE,*
   T_INSTANCES_CLUSTER_K, T_CLUSTERIDX>
   &aiipri_inParamReadInst `&aiipri_inParamReadInst`,
   const bool `&aib_fileTest = false`)

std::vector<data::Instance<T_FEATURE>* > [Function]
   inout::instancesReadWithFreq
   (*inout::InParamReadInstFreq<T_FEATURE,*
   T_INSTANCES_CLUSTER_K, T_CLUSTERIDX,
   T_INSTANCE_FREQUENCY> &aiipri_inParamReadInst
   `&aiipri_inParamReadInst`,
   const bool `&aib_fileTest = false`)

std::vector<data::Instance<T_FEATURE>* > [Function]
   inout::instancesReadWithFreqClass
   (*inout::InParamReadInstFreq<T_FEATURE,*
   T_INSTANCES_CLUSTER_K, T_CLUSTERIDX,
   T_INSTANCE_FREQUENCY> &aiipri_inParamReadInst
   `&aiipri_inParamReadInst`,
   const bool `&aib_fileTest = false`)

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

```
std::vector<data::Instance<DATATYPE_FEATURE>* > lvectorptinst_instances;
std::vector<data::Instance<DATATYPE_FEATURE>* > lvectorptinst_instancesTest;

if ( linparam_ClusteringEA.getClassInstanceColumn() ) {
  lvectorptinst_instances =
    inout::instancesReadWithClass
    (linparam_ClusteringEA,
     false
     );
  if ( linparam_ClusteringEA.getNumFilesInstanceTest() > 0) {
    lvectorptinst_instancesTest =
      inout::instancesReadWithClass
      (linparam_ClusteringEA,
       true
       );
  }
}
else { /*Instances*/
```

```
lvectorptinst_instances =
  inout::instancesRead
  (linparam_ClusteringEA,
   false
   );
if ( linparam_ClusteringEA.getNumFilesInstanceTest() > 0) {
  lvectorptinst_instancesTest =
    inout::instancesRead
    (linparam_ClusteringEA,
     true
    );
}
}
```

9. Include the genetic operators in the main function or invoke the function that has the implementation of the new algorithm in the main function, for example:

```
auto lchrom_best =
eac::kga_fkcentroid
(loop_outParamEAC,
 linparam_ClusteringEA,
 lvectorptinst_instances.begin(),
 lvectorptinst_instances.end(),
 *pfunct2p_distAlg
);
```

10. With the source files completed, compile your new algorithm, with the following options.

```
g++ -std=c++11 -I ../../include -I ../../include_inout/ new_alg_ea.cpp
 -o new_alg_ea
```

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.

3.3 Using implemented algorithms

This section shows how to use the programs located in the `eac` directory to find a solution to the problem of clustering. For the use and obtain better results, the algorithms on which the programs are based, we categorize them into three aspects: if the number the clusters 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 directory `bin` directory with the command 'cd c:\leac\bin' for Windows® or 'cd leac/bin' for GNU/Linux from a `cmd` or `terminal` respectively.

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, fixed or variable k and the coding used.

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

All EAC programs 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: [Name]], page 44,

For example, here are some realistic execution '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
```

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


```
--generations
--population-size
```

they only vary in the number of generations and in the number of chromosome proposed by the different authors.

The following sections describe the evolutionary algorithm currently implemented with the LEAC library, based on taxonomy proposed by HCFdC09, *k-fixed* vs. *k-variable* and the coding they use to represent the chromosomes, see Table 1.1. We also include practical examples of clustering applications with real data sets provided by UC Irvine Machine Learning Repository.

3.3.1 Genetic algorithms for fixed k-clusters

3.3.1.1 Based on cluster label

The genetic algorithms in this section use an [string-of-group-numbers encoding], page 13. The algorithms included in LEAC are the following:

- `gaclustering_fklabel`

  Based on MC96, optimize to [SED], page 19, the operators that use are `gagenericop::onePointCrossover` and `gaintegerop::mutation` (change a random gene). The classification of these operators can be considered *object-oriented*, that randomly moves 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:

  `--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]

- `gka_fklabel`

  Based on KM99, Optimize to [TWCV], page 18. The authors of this document propose not to use the crossover operator, instead they use the `k-means algorithm`. HCFdC09 state that this algorithm must be an evolutionary algorithm rather than a genetic algorithm. LEAC implements several variants of the `k-means algorithm`, including the algorithm used by this algorithm ([clusteringop::kmeansoperator], page 35). Mutation change 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:

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

- `igka_fklabel` based on LLF+04b, and `fgka_fklabel` based on LLF+04a.

  optimize to [SSE], page 18,

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

  `fgka_fklabel`

  Based on LLF+04a, optimize to [SSE], page 18,

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

3.3.1.2 Based on the centroids

The algorithms in this section seek to find the centroids of the cluster for a user-defined k. If you are looking for precision to locate the centroid of the clusters, these algorithms are a good option. The way they encode the solutions as a string with the coordinates

of the centroids consecutively, see See [real encoding], page 14. The genetic algorithms implemented in this class are listed below:

- `gas_fkcentroid`

  Based on MB00, optimize to [SED], page 19,

  `--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]`

- `kga_fkcentroid`

  Based on BM02a, optimize to [SED], page 19,

  `--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]`

- `gagr_fkcentroid`

  Based on CZZ09, optimize to [SSE], page 18,

- `cbga_fkcentroid_int` and `cbga_fkcentroid`

  Based on FKKN97, optimize to [Distortion], page 20,

  `--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]`

Next, we describe the steps to execute KGA algorithm base on BM02a and discuss the parameters that can be used to carry out an experimental study. Something similar would be included for all the algorithms.

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 the program `stdvar_milligan_cooper1988` Based on (MC88) is available as support for the normalization of the data set.

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

The Wine data set includes 13 variables from column 2 to column 14 and the column from class 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 KGA BM02a will be run, for the normalized data

'`kga_fkcentroid -i ../data/wine_std.data -a "1-13" -c 14 --number-clusters 3 -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 terminal and 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 KGA algorithm is

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

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

            Random seed: 605281295 2141350197 2332488985 1350226326 4001754309
            1842645844 2127210415 1490264447

    OUT:

    CROMOSOME:BEST:objetive,449.524,fitness,0.00222458:0.875627,-0.30372,0.318045,
    -0.662654,0.563299,0.87404,0.940985,-0.583943,0.580146,0.166718,0.482367,
    0.764896,1.15509,0.164444,0.869095,0.186373,0.522892,-0.0752605,-0.976575,
    -1.21183,0.724021,-0.777513,0.93889,-1.16151,-1.28878,-0.405943,-0.936362,
    -0.390863,-0.437966,0.2084,-0.462469,-0.0531982,0.0667156,-0.0197664,0.0646097,
    -0.879594,0.451708,0.288923,-0.753899


            Cluster number (K): 3
                           SSE: 449.524
                      DB-index: 1.39179
                    Silhouette: 0.285942
                           VRC: 70.8369
                    CS measure: 0.437609
                  Dunn's index: 0.176897
           Execution time (seg): 2.03319
    Generations find the best: 7


    Centroids:

      Col:    0             1             2             3             4
      Row

       0: 0.875627      -0.30372      0.318045      -0.662654     0.563299
       1: 0.164444      0.869095      0.186373      0.522892      -0.0752605
       2: -0.936362     -0.390863     -0.437966     0.2084        -0.462469

      Col:    5             6             7             8             9
```

```
    Row

       0: 0.87404        0.940985       -0.583943       0.580146       0.166718
       1: -0.976575      -1.21183        0.724021       -0.777513      0.93889
       2: -0.0531982      0.0667156      -0.0197664      0.0646097     -0.879594

    Col:    10              11             12
    Row

       0: 0.482367        0.764896        1.15509
       1: -1.16151        -1.28878       -0.405943
       2: 0.451708         0.288923      -0.753899
```

<MEMBERCLUSTERTRAINING,_algorithmo,KGA,_author,Bandyopadhyay and Maulik
2002,_runnig date,20171205:021341,_number run,1,_runnig date,20171205:
021341,_number run,1,_times run,1,_dataset_training,../data/wine_std.data,
_outK,3,PartitionCentroids[0x7ffe314e40f0],length,178>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,
0,0,0,0,0,0,0,0,0,0,0,0,0,2,2,1,2,2,2,2,2,2,2,2,2,2,2,2,0,2,2,2,2,2,2,2,2,
2,2,1,2,2,2,2,2,2,2,2,2,2,2,0,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,
2,1,2,2,2,2,2,2,2,2,2,2,2,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,
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

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 output the standard. 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 shown below.

In addition to the measure of similarity used by the algorithm, the program calculates others that can be used to evaluate the goodness of the grouping. (See [unsupervised measures], page 47).

To repeat the same result of the program, you can use the '`-z`' option and as a 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:

'`kga_fkcentroid -i ../data/wine_std.data -a "1-13" -c 14 --number-clusters 3 -C wine_centroids.data -M wine_membership.data -z "605281295 2141350197 2332488985 1350226326 4001754309 1842645844 2127210415 1490264447"`'

The program `plot_clustering` is another EAC utility, which allows to visualize a data set, with the results obtained from the different programs. This uses Gnuplot, as an example you can run the `plot_clustering` program with the following parameters:

'`plot_clustering -i ../data/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`, try the following command:

'`plot_clustering -i ../data/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`'
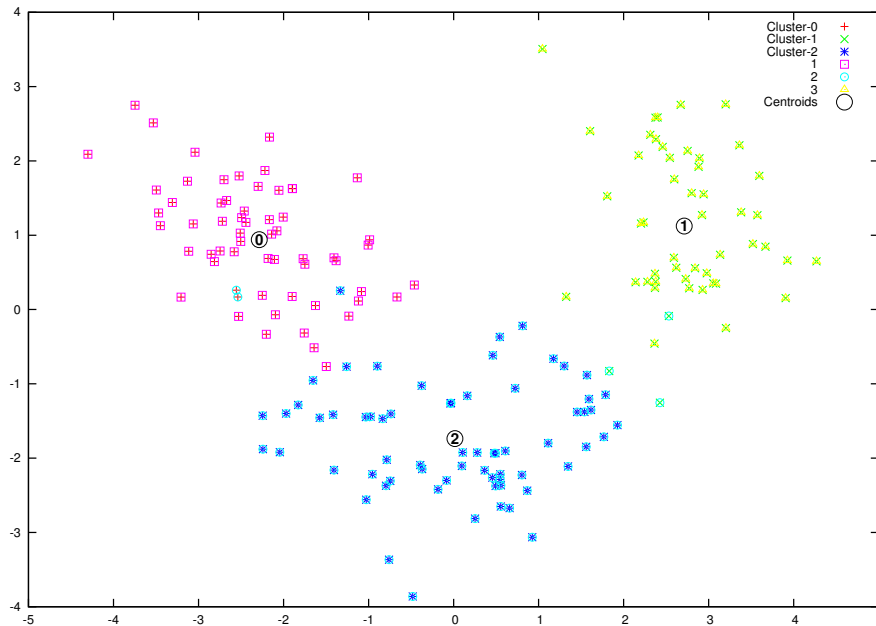
Figure 3.6: Clusters of Wine data set, obtained with `kga_fkcentroid`

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 (3.2).

To demonstrate how to process a data set with training and test data, you can use the Libras Movement Data Set, with 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 rango to be betweeen -1 and 1. To have better accuracy, we center on $(0.5, 0, 5)$ each of the curves 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. To run the script, type:

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

With the transformed dataset we apply the KGA algorithm:

'kga_fkcentroid -i ../data/movement_libras_trasn.data -t ../data/movement_libras_1.data -a "1-90" -c 91 -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: SSE

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

          Data set test: ../data/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
                           SSE: 209.665
                      DB-index: 1.15626
                    Silhouette: 0.284789
                           VRC: 87.1936
                    CS measure: 1.36284
                  Dunn's index: 0.0855026

                 Test data SSE: 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 testing, as well as 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, 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.
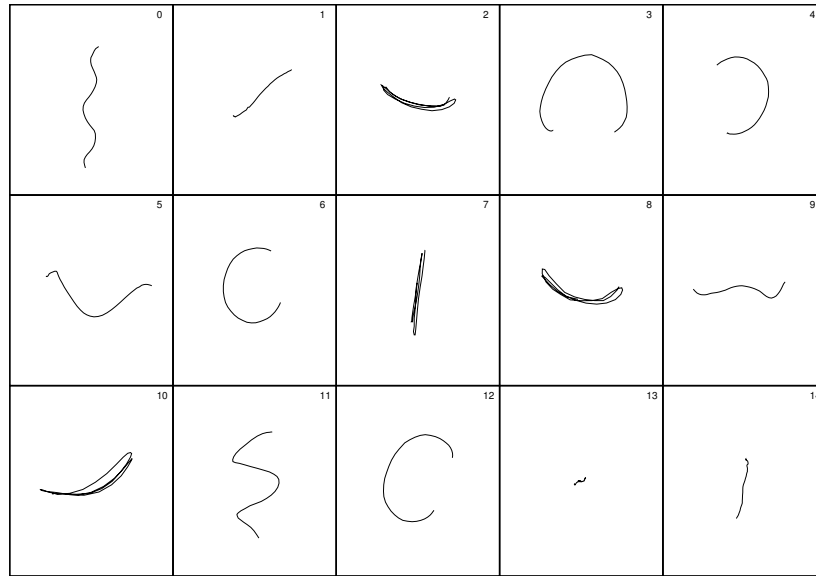

Figure 3.7: Average of the movements of the libras data set obtained with the program `kga_fkcentroid`

3.3.1.3 Based on the most representative

K-medoid 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).

- `gaprototypes_fkmedoid`

  Based on KB97, optimize to $[J_1]$, page 22,

  `--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]`

- `gca_fkmedoid`

  Based on LDK93, optimize to [SEDmedoid], page 21,

  `--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]

- `hka_fkmedoid`

  Based on SL04, optimize to [SEDmedoid], page 21,

  `--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]

As an illustrative example of algorithms that finds the most representative instances for each cluster, we describe the `hka_fkmedoid` program based on the HKA algorithm (SL04)

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

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

A possible exit from the program would be:

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

          Data set: ../data/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
                      SSE: 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 ../data/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'

And graphically show the prototypes and groups in Figure 3.8.
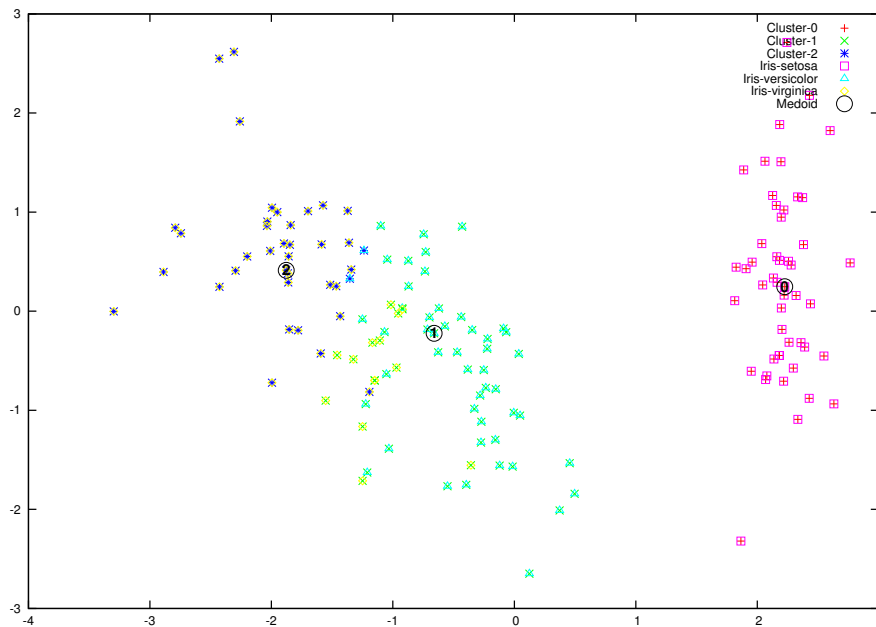
Figure 3.8: The most representative instances of the Iris data set, obtained with the program 'hka_fkmedoid'

3.3.2 Genetic algorithms for variable k-clusters

The genetic algorithms described in the following sections direct the search both to find the best cluster number (k^*) and cluster formation, in which the objects belonging to the same

clusters are similar and with the objects of the other different clusters. In this case, there is no information about the most appropriate value in the data set.

The clustering is an exploratory technique, which can be used to make the automatic classification. To do this, you can use an algorithm that finds the appropriate number of clusters, when an expert is not available, or also compare the clusters obtained against the predefined classes.

The parameters that are common 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.

3.3.2.1 Based on the centroids

The genetic algorithms in this section use an See [real encoding], page 14, with some variant to allow the search for the optimum k. The algorithms included in LEAC are the following:

- `gcuk_vkcentroid`

  Based on BM02b, optimize to [DB], page 22. Encodes the chromosomes as strings of real numbers that represent the coordinates of the centroids, combined with `#` symbols, allow the diversity of chromosomes with different k, through the application of genetic operators `onePointCrossover` and `randomMutation`.

  Parameters:

  `--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]`

- `tgca_vkcentroid`

  Based on HT12, optimize to [VRC], page 26. It is a novel genetic algorithm, called by its authors as a *two-stage genetic clustering algorithm*. First, the 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:

  `--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]
```

With the `gcuk_vkcentroid` program, you will find an automatic classification of the Zoo data set. The data set zoo.data has 7 classes with 17 attributes. All attributes are binary, with the exception of number 14, which can be seen as nominal.

To process it 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
}
```

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

'gcuk_vkcentroid -i ../data/zoo_bin.csv -h yes -a "2-22" -c 23 --k-minimum=2 --k-maximum=20 -C c_zoo_gcuk.data -M m_zoo_gcuk.data -T stdout --table-format yes'
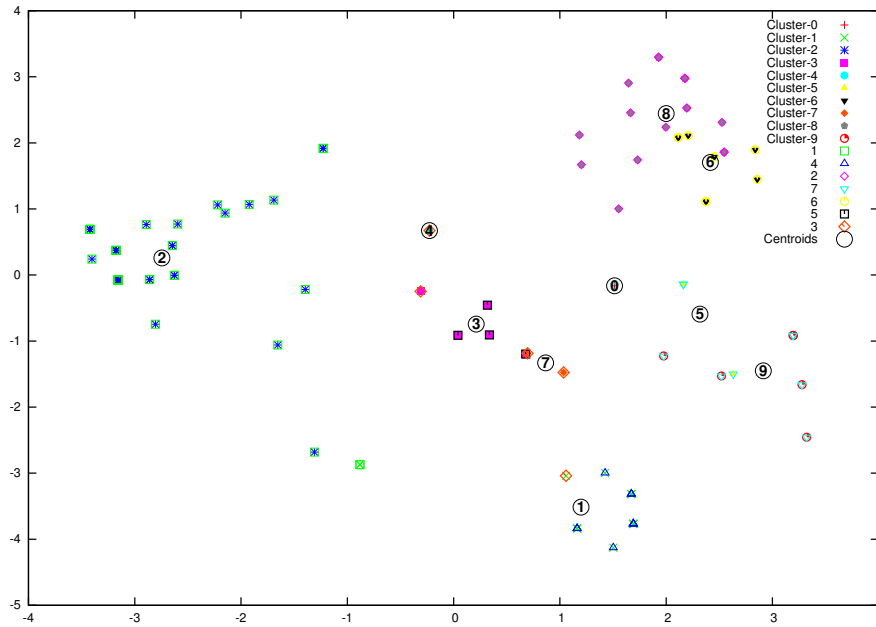
Figure 3.9: Clusters obtained in the data set Zoo with `gcuk_vkcentroid`

```
IN:
     Algorithmo name: GCUK
           Based on: Bandyopadhyay and Maulik 2002
        Metric used: DB-index

           Data set: ../data/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
                       SSE: 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 program, 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 shown in the Figure 3.10 And the summary in the Table 3.1.

```
`plot_clustering -i ../data/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 4}
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

3.3.2.2 Based on cluster label

The genetic algorithms in this section use an See [string-of-group-numbers encoding], page 13, with some variant to allow the search for the optimum k. The algorithms included in LEAC are the following:

- `gga_vklabeldbindex` and `gga_vklabelsilhouette`

  Based on ABSSJF+12, optimize to [DB], page 22, and [Silhouette], page 23. Chromosome is formed by two section [*element* | *group*]. The element section each position (gene) corresponds to the belongings of the object to a cluster. The group section corresponds to the alphabet of possible values of the genes $\{1, 2, 3, ..., k\}$. An island model, where operators `mergeCrossover`, `mergeMutation` and `splittingMutation` are applied

  `--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]`

- `cga_vklabel`

  Based on HE03 optimize to [Silhouette], page 23,

  String of label of $(n + 1)$ positions. Each position corresponds to an instance, i.e., the i-th position (gene) represents the i-th object, whereas the last gene represents the number of clusters (k).

  `--crossover-probability[=NUMBER]`

  > real number in the interval `[0.25, 1]` `[NUMBER=0.5]`

  `--mutation-probability[=NUMBER]`

  > for operator 1 and 2 real number in the interval `[0, 0.5]` `[NUMBER=0.25]`

- `eac_vklabel`

  Based on HCdC06 optimize to

  `--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]`

- `feac_vklabel`, and its variants `eaci_vklabel`, `eacii_vklabel` and `eaciii_vklabel`

  Based on ACH06

  `--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 itera-
            tions is less than or equal to [NUMBER=0.001]
```

As an illustrative example, the Ionosphere, data set is processed with the program `gga_vklabelsilhouette`, this data set has the complexity that the instances of different classes overlap. For this case, the See [silhouette], page 23, metric was the most appropriate.

'`gga_vklabelsilhouette -i ../data/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: ../data/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,
    3,3,0,3,0,3,4,3,0,3,0,3,3,3,0,3,1,3,3,3,3,3,3,3,4,3,3,3,4,2,4,3,3,4,3,0,3,0,3,
    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,
    2,0,2,0,3,0,3,0,3,0,3,0,3,0,3,0,3,0,3,3,2,0,2,1,3,0,0,0,3,0,3,3,3,0,3,3,3,0,
    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,
    3,0,3,3,3,0,3,0,2,0,2,0,2,2,2,3,3,3,3,3,4,4,4,4,4,3,3,3,3,3,3,3,3,3,3,3,4,
    4,4,4,2,0,3,3,3,3,3,3,3,3,3,3,3,3,4,2,2,2,2,2,3,3,3,3,3,4,4,2,2,2,3,3,2,2,2,
    3,3,3,3,3,3,3,2,2,2,2,2,3,3,3,3,3,3,3,2,2,2,2,0,3,3,3,3,3,3,3,3,3,3,3|0,1,2,3,4

            Cluster number (K): 5
                    Silhouette: 0.320094
                           SSE: 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 ../data/ionosphere.data -a "1-34" -c 35 --member-infile
m_gga_ionosphere.data --graphics-outfile gga_ionosphere'
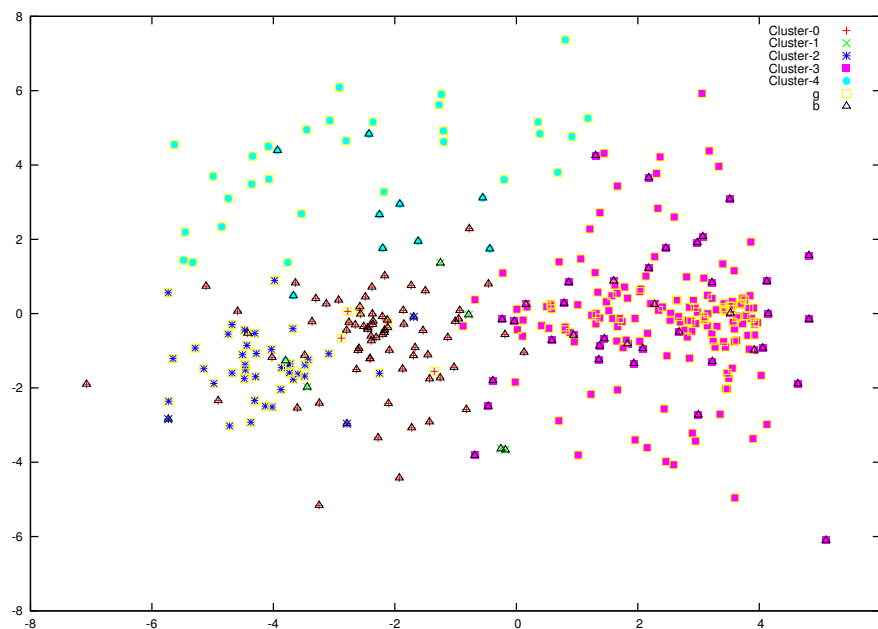
Figure 3.11: Clusters obtained with `gga_vklabelsilhouette`

3.3.2.3 Based on other encoding schemes

- `gaclustering_vktreebinary`

  Based on CdLM03 optimize to [VRC], page 26, 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 $(k-1)$, where k is the number of clusters.

  Parameters:

  `--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]
```

- clustering_vksubclusterbinary

  Based on TY01 optimize [Intra- and inter-cluster distance], page 27,

  Parameters:

```
--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]
```

As an illustrative example, the Ecoli, data set was processed, in order to obtain a cluster number automatically and compare it with the classification proposed in the data set

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

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

               Data set: ../data/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,215.739,000000000000000000000000000000
    00000000000000000000000000000000000000000000000000000000000000000000000000000000
    00000000000000000000000000000000000000000000000000000000000000000000000000000000
    00000000000010000000000000000000000000000000000000000000000000000000000000000000
    00000000000000000000000000000000000000000000000000000000000000000000000000000010

            Cluster number (K): 3
     Variance Ratio Criterion: 215.739
                          SSE: 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 ../data/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'
```
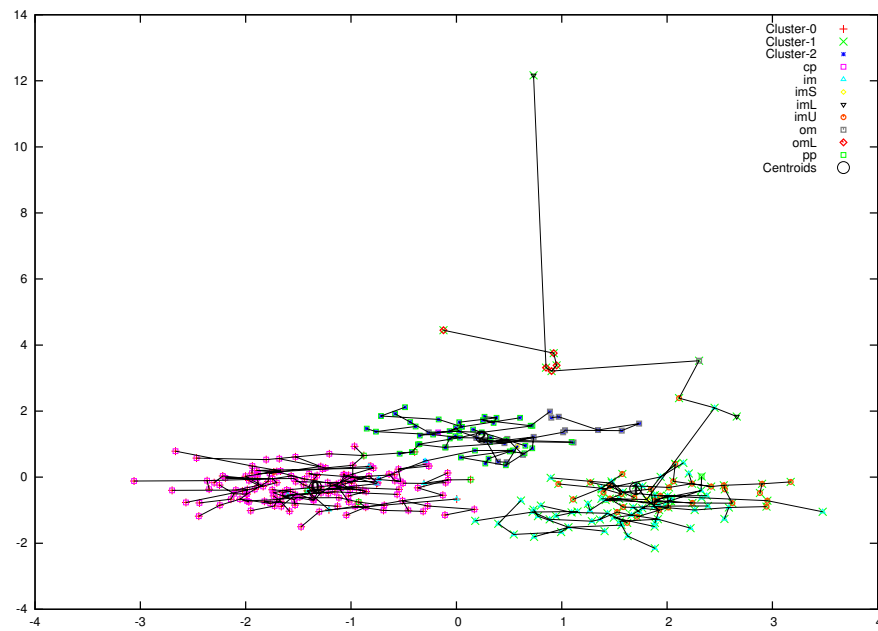
Figure 3.12: Minimum spanning tree (MST) and clusters obtained with `gaclustering_` `vktreebinary` program for the ecoli data set

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
 * This file is part of the LEAC.
 *
 * Implementation of the KGA algorithm based on the paper:
 *
 * S. Bandyopadhyay and U. Maulik. An evolutionary technique based
 * on k-means algorithm for optimal clustering in rn. Inf. Sci. Appl.,
 * 146(1-4):221--237, 2002. URL: http://www.sciencedirect.com/science/
 * article/pii/S0020025502002086, doi:http://dx.doi.org/10.1016/S0020-
 * 0255(02)00208-6.
 *
 * Library Evolutionary Algorithms for Clustering (LEAC) is a library
 * for the implementation of evolutionary and genetic algorithms
 * focused on the partition type clustering problem. Based on the
 * current standards of the C++ language, as well as on Standard
 * Template Library STL and also OpenBLAS to have a better performance.
 *
 * (c)  Hermes Robles-Berumen <hermes@uaz.edu.mx>
 *
 * For the full copyright and license information, please view the LICENSE
 * file that was distributed with this source code.
 */

#ifndef __KGA_FKCENTROID_HPP__
#define __KGA_FKCENTROID_HPP__

#include <vector>
#include <algorithm>

#include <leac.hpp>
#include "inparam_gaclustering_pcpm_fixedk.hpp"
#include "outparam_gaclustering.hpp"

#include "plot_runtime_function.hpp"

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

  \author Hermes Robles-Berumen
  \date    2015-2017
  \copyright GPLv3 license
*/

namespace eac {

/*! \fn gaencode::ChromFixedLength<T_FEATURE,T_REAL> kga_fkcentroid
  (inout::OutParamGAClustering<T_REAL,T_CLUSTERIDX> &aoopcga_outParamClusteringGA,
```

```
    inout::InParamGAClusteringProbCProbMFixedK<T_CLUSTERIDX,T_REAL,T_FEATURE,
    T_FEATURE_SUM,T_INSTANCES_CLUSTER_K> &aiinpcgaprobfixedk_inParamKGA,
    const INPUT_ITERATOR aiiterator_instfirst,
    const INPUT_ITERATOR aiiterator_instlast,
    const dist::Dist<T_REAL,T_FEATURE> &aifunc2p_dist)
   \brief GAS, KGA
   \details Implementation of KGA algorithm based on BM02a. 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$m_j\f$, represents the medoid of cluster \f$C_j\f$
   \param aoopcga_outParamClusteringGA a outparam::OutParamGAClustering with
   the output parameters of the algorithm
   \param aiinpcgaprobfixedk_inParamKGA a
   inout::InParamGAClusteringProbCProbMFixedK 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::OutParamGAClustering
 <T_REAL,
 T_CLUSTERIDX>                        &aoopcga_outParamClusteringGA,
 inout::InParamGAClusteringProbCProbMFixedK
 <T_CLUSTERIDX,
 T_REAL,
 T_FEATURE,
 T_FEATURE_SUM,
 T_INSTANCES_CLUSTER_K>               &aiinpcgaprobfixedk_inParamKGA,
 const INPUT_ITERATOR                 aiiterator_instfirst,
 const INPUT_ITERATOR                 aiiterator_instlast,
 const dist::Dist<T_REAL,T_FEATURE>   &aifunc2p_dist
 )
{
  const uintidx lconstui_numClusterFixedK =
     (uintidx) aiinpcgaprobfixedk_inParamKGA.getNumClusterK();


/*Defines the size of the chromosome

   Specifically, each chromosome is described by a sequence of
   length(Ch) = l × k real-valued numbers where
   l is the dimension of the instances, and k
   is the number of clusters. That is to say, the chromosome of
   the algorithm is written as (4.2) (See [centroid-based], page 14)
```

```
*/
        /*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
          (aiinpcgaprobfixedk_inParamKGA.getSizePopulation());

        /*CREATE SPACE FOR STORE MATINGPOOL---------------------------------------------
         */
        std::vector<gaencode::ChromFixedLength<T_FEATURE,T_REAL> >
          lvectorchromfixleng_matingPool
          (aiinpcgaprobfixedk_inParamKGA.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::OutParamGAClustering&: "
          << "aoopcga_outParamClusteringGA["
          << &aoopcga_outParamClusteringGA << "]\n"
          << "\t input  InParamGAClusteringProbCProbMFixedK&: "
          <<"aiinpcgaprobfixedk_inParamKGA["
          << &aiinpcgaprobfixedk_inParamKGA << "]\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 = "
          << aiinpcgaprobfixedk_inParamKGA.getSizePopulation()
          << "\n\t\tProbCrossover = "
          << aiinpcgaprobfixedk_inParamKGA.getProbCrossover()
          << "\n\t\tProbMutation  = "
          << aiinpcgaprobfixedk_inParamKGA.getProbMutation()
```

```
          << "\n\t)"
          << std::endl;
  }
#endif /*__VERBOSE_YES*/

  runtime::ListRuntimeFunction<COMMON_IDOMAIN>
    llfh_listFuntionHist
    (aiinpcgaprobfixedk_inParamKGA.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 ( aiinpcgaprobfixedk_inParamKGA.getWithPlotStatObjetiveFunc() ) {

    lvectorT_statfuncObjetiveFunc.reserve
      ( aiinpcgaprobfixedk_inParamKGA.getSizePopulation());
    //DEFINE FUNCTION
    lofh_SSE  = new runtime::RuntimeFunctionValue<T_REAL>
      ("SSE",
       aiinpcgaprobfixedk_inParamKGA.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,
          aiinpcgaprobfixedk_inParamKGA.getAlgorithmoName(),
          RUNTIMEFUNCTION_NOT_STORAGE
        );
      llfh_listFuntionHist.addFuntion(lofhs_statObjectiveFunc[li_i]);
    }

    //OPEN FILE STRORE FUNCTION
    aoopcga_outParamClusteringGA.setFileNameOutPlotStatObjetiveFunc
      (aiinpcgaprobfixedk_inParamKGA.getFileNamePlotStatObjetiveFunc(),
       aiinpcgaprobfixedk_inParamKGA.getTimesRunAlgorithm()
       );

    lfileout_plotStatObjetiveFunc.open
      (aoopcga_outParamClusteringGA.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
   */
  aoopcga_outParamClusteringGA.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
     );

    /*INITIALIZE POPULATION-------------------------------------------------------
    3.1.1 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 od the centers
    in K-Means algorithm. This process es repeat 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();
```

```
/*3.1.2 CLUSTERING

In this step, the cluster 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
```

$$\| x_i - \mu_j \| \ \leq \ \| x_i - \mu_j' \| , \quad j' = 1, 2, ..., k, \quad and \quad j \ \neq \ j'$$

```
.
All ties are resolved arbitrarily. As like the K-Means algorithm, for each cluster
$C_i$, its new center $\mu^*$ 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 $\mu^*$ now replace the preious $\mu_i$ 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-------------------------------------------------------
```

```
/* 3.1.3 Fitness computation
   For each chromosome, the clusters formed in the previous step are utilized
   computing the clustering metric,   SSE, as follows:
```

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

```
   For finding the appropriate clusters SSE has to be minimized. 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.
*/
        { /*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*/

      }

      aoopcga_outParamClusteringGA.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---------------------------------------------------------------
      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;

          aoopcga_outParamClusteringGA.setIterationGetsBest
            (llfh_listFuntionHist.getDomainUpperBound());
          aoopcga_outParamClusteringGA.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 ( aiinpcgaprobfixedk_inParamKGA.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()
          < aiinpcgaprobfixedk_inParamKGA.getNumMaxGenerations() )
        )
      break;

    /*3.1.4 GENETIC OPERATIONS
      BM02a      */

    /*SELECTION----------------------------------------------------------
      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 pop-
      ulation.
      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-----------------------------------------------------------------
     Crossover 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 × 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.
*/
            { /*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) <
                   aiinpcgaprobfixedk_inParamKGA.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;
                      }
                   }
                   );

         aoopcga_outParamClusteringGA.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
        probabiity 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 34
       */
       { /*BEGIN MUTATION*/
#ifdef __VERBOSE_YES
         geverbosepc_labelstep = "MUTATION";
         ++geiinparam_verbose;
         if ( geiinparam_verbose <= geiinparam_verboseMax ) {
```

```cpp
        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)
             < aiinpcgaprobfixedk_inParamKGA.getProbMutation() )
          { //IF BEGIN  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 BEGIN  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);
  aoopcga_outParamClusteringGA.setNumClusterK
    (aiinpcgaprobfixedk_inParamKGA.getNumClusterK());
  aoopcga_outParamClusteringGA.setMetricFuncRun
    (lochromfixleng_best.getObjetiveFunc());
  aoopcga_outParamClusteringGA.setAlgorithmRunTime
    (runtime::getTime(let_executionTime));
  aoopcga_outParamClusteringGA.setFitness
    (lochromfixleng_best.getFitness());
  aoopcga_outParamClusteringGA.setNumTotalGenerations
    (llfh_listFuntionHist.getDomainUpperBound());

#ifndef __WITHOUT_PLOT_STAT
  if ( aiinpcgaprobfixedk_inParamKGA.getWithPlotStatObjetiveFunc() ) {
    runtime::plot_funtionHist
      (llfh_listFuntionHist,
       aiinpcgaprobfixedk_inParamKGA,
       aoopcga_outParamClusteringGA
       );
  }

#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
 * This file is part of the LEAC.
 *
 * Implementation of the GA algorithm based on the paper:
 *
 * J.C. Bezdek, S. Boggavarapu, L.O. Hall, and A. Bensaid.
 * Genetic algorithm guided clustering. In Evolutionary Computation,
 * 1994. IEEE World Congress on Computational Intelligence., Proceed-
 * ings of the First IEEE Conference on, pages 34--39 vol.1, Jun 1994.
 * doi:10.1109/ICEC.1994.350046.
 *
 * Library Evolutionary Algorithms for Clustering (LEAC) is a library
 * for the implementation of evolutionary and genetic algorithms
 * focused on the partition type clustering problem. Based on the
 * current standards of the C++ language, as well as on Standard
 * Template Library STL and also OpenBLAS to have a better performance.
 *
 * (c)  Hermes Robles-Berumen <hermes@uaz.edu.mx>
 *
 * For the full copyright and license information, please view the LICENSE
 * file that was distributed with this source code.
 */

#ifndef __GACLUSTERING_FKCRISPMATRIX_HPP__
#define __GACLUSTERING_FKCRISPMATRIX_HPP__

#include <iostream>
#include <iomanip>
#include <vector>

#include <leac.hpp>

#include "plot_runtime_function.hpp"
#include "inparam_gaclustering_withoutpcpm.hpp"
#include "outparam_gaclustering.hpp"

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

  \author Hermes Robles-Berumen
  \date   2015-2017
  \copyright GPLv3 license
*/

namespace eac {

/*! \fn gaencode::ChromosomeCrispMatrix<T_BITSIZE,T_CLUSTERIDX,T_REAL>
gaclustering_fkcrispmatrix
(inout::OutParamGAClustering<T_REAL,T_CLUSTERIDX> &aoopcga_outParamClusteringGA,
inout::InParamGAClusteringWithoutProbCProbM<T_CLUSTERIDX,T_BITSIZE,T_FEATURE,
T_FEATURE_SUM,T_INSTANCES_CLUSTER_K> &aiinpkbezdekga_inParam,
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 par-
tition of a data set, for a defined k.
  \param aoopcga_outParamClusteringGA a inout::OutParamGAClustering that contains
  information relevant to program execution
  \param aiinpkbezdekga_inParam a inout::InParamGAClusteringWithoutProbCProbM 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::OutParamGAClustering
 <T_REAL,
 T_CLUSTERIDX>                    &aoopcga_outParamClusteringGA,
 inout::InParamGAClusteringWithoutProbCProbM
 <T_CLUSTERIDX,
 T_BITSIZE,
 T_FEATURE,
 T_FEATURE_SUM,
 T_INSTANCES_CLUSTER_K>           &aiinpkbezdekga_inParam,
 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::OutParamGAClustering&: aoopcga_outParamClusteringGA["
      << &aoopcga_outParamClusteringGA << "]\n"
      << "\t input  InParamClusteringBezdekGA1994&: aiinpkbezdekga_inParam["
      << &aiinpkbezdekga_inParam << "]\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 = "
```

```
      << aiinpkbezdekga_inParam.getSizePopulation()
      << "\n\t\tMatingPool size = "
      << aiinpkbezdekga_inParam.getSizeMatingPool()
      << "\n\t\t Generations  = "
      << aiinpkbezdekga_inParam.getNumMaxGenerations()
      << "\n\t\trandom-seed = "
      << aiinpkbezdekga_inParam.getRandomSeed()
      << "\n\t)"
      << std::endl;
  }
#endif /*__VERBOSE_YES*/

  const uintidx  luintidx_numClusterK =
    (uintidx) aiinpkbezdekga_inParam.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_mmcidxOK
    (0,aiinpkbezdekga_inParam.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 ( aiinpkbezdekga_inParam.getSizePopulation()
       <= aiinpkbezdekga_inParam.getSizeMatingPool() )
    throw std::invalid_argument
      ("gaclustering_fkcrispmatrix: "
       "size population should be greater than size matingpool"
       );

  runtime::ListRuntimeFunction<COMMON_IDOMAIN>
    llfh_listFuntionHist
    (aiinpkbezdekga_inParam.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 ( aiinpkbezdekga_inParam.getWithPlotStatObjetiveFunc() ) {

     lvectorT_statfuncObjetiveFunc.reserve
       ( aiinpkbezdekga_inParam.getSizePopulation());
     //Variable to monitor in the execution of the program
     lofh_J1  = new runtime::RuntimeFunctionValue<T_REAL>
       ("J1",
         aiinpkbezdekga_inParam.getAlgorithmoName(),
         RUNTIMEFUNCTION_NOT_STORAGE
         );

     llfh_listFuntionHist.addFuntion(lofh_J1);

     if ( aiinpkbezdekga_inParam.getClassInstanceColumn()  ) {
       lofh_misclassified =
         new runtime::RuntimeFunctionValue<T_INSTANCES_CLUSTER_K>
         ("Misclassified",
          aiinpkbezdekga_inParam.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,
           aiinpkbezdekga_inParam.getAlgorithmoName(),
           RUNTIMEFUNCTION_NOT_STORAGE
           );
       llfh_listFuntionHist.addFuntion(lofhs_statObjectiveFunc[li_i]);
     }

     //OPEN FILE STRORE FUNCTION
     aoopcga_outParamClusteringGA.setFileNameOutPlotStatObjetiveFunc
       (aiinpkbezdekga_inParam.getFileNamePlotStatObjetiveFunc(),
        aiinpkbezdekga_inParam.getTimesRunAlgorithm()
        );

     lfileout_plotStatObjetiveFunc.open
       (aoopcga_outParamClusteringGA.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
      (aiinpkbezdekga_inParam.getSizePopulation() + 1);
    for (uintidx lui_i = 0;
         lui_i < aiinpkbezdekga_inParam.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
      (aiinpkbezdekga_inParam.getSizeMatingPool());

    /*Space for chromosomes R
     */
    lvectorchromfixleng_childR.reserve
      (aiinpkbezdekga_inParam.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, we choose the kth element of the cluster center to be the kth 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, population P (the population size) U matrices are generated in this manner.

```
*/
     {/*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*/


/*Population sort by $J_1$
```

The U matrices are sorted by J_1 value. and the R with the lowest J_1,
values are choses to reproduce.
```
*/
      {/*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
          */
        aoopcga_outParamClusteringGA.setIterationGetsBest
          (llfh_listFuntionHist.getDomainUpperBound());
        aoopcga_outParamClusteringGA.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 ( aiinpkbezdekga_inParam.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()
              >= aiinpkbezdekga_inParam.getNumMaxGenerations()) ||
              (runtime::elapsedTime(let_executionTime) >
               aiinpkbezdekga_inParam.getMaxExecutiontime())
              )
          break;

        /*Selection
          R matrices with the lowest J_1, values are choses to reproduce.
         */

       /*Selection
          R matrices with the lowest J_1, values are choses to reproduce.
         */

       {/*BEGIN SELECTION
          */
          auto ichrom_population = lvectorchrombitcrispmatrix_population.begin();

          for (uintidx lui_i = 0;
               lui_i < aiinpkbezdekga_inParam.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.
*/

          {/*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 < aiinpkbezdekga_inParam.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 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.
*/
      {/*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*/

    {/*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*/

      } /*EVALUATE J1 FOR CHILDR*/

      /*The R chuild U matrices are added to the population
        with the P-R U matrices with the greatest J1 values
        dropped from the population.
      */
      { /*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
          (aiinpkbezdekga_inParam.getSizePopulation() + 1);

        uintidx luintidx_l = 0;
        uintidx luintidx_r = 0;

        for (uintidx lui_i = 0;
             lui_i < aiinpkbezdekga_inParam.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);
    aoopcga_outParamClusteringGA.setNumClusterK
      (aiinpkbezdekga_inParam.getNumClusterK());
    aoopcga_outParamClusteringGA.setMetricFuncRun
      (lochrombitcrispmatrix_best.getObjetiveFunc());
    aoopcga_outParamClusteringGA.setAlgorithmRunTime
      (runtime::getTime(let_executionTime));

    aoopcga_outParamClusteringGA.setFitness
      (lochrombitcrispmatrix_best.getObjetiveFunc());
    aoopcga_outParamClusteringGA.setNumTotalGenerations
      (llfh_listFuntionHist.getDomainUpperBound());

    /*FREE: COMPUTING STATISTICAL AND METRIC OF THE ALGORITHM
     */
#ifndef __WITHOUT_PLOT_STAT

    if ( aiinpkbezdekga_inParam.getWithPlotStatObjetiveFunc() ) {
      plot_funtionHist
        (llfh_listFuntionHist,
         aiinpkbezdekga_inParam,
         aoopcga_outParamClusteringGA
         );
    }

#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__*/
```

Bibliography

[**ABSSJF+12**]   L. E. Agustín-Blas, S. Salcedo-Sanz, S. Jiménez-Fernández, L. Carro-Calvo, J. Del Ser, and J. A. Portilla-Figueras. *A new grouping genetic algorithm for clustering problems.* Expert Syst. Appl., 39(10):9695–9703, August 2012. doi:http://dx.doi.org/10.1016/j.eswa.2012.02.149.

[**ACH06**]   V. S. Alves, R. J. G. B. Campello, and E. R. Hruschka. *Towards a fast evolutionary algorithm for clustering.* In IEEE International Conference on Evolutionary Computation, CEC 2006, part of WCCI 2006, Vancouver, BC, Canada, 16-21 July 2006, pages 1776–1783. IEEE, 2006. doi:http://dx.doi.org/10.1109/CEC.2006.1688522.

[**AIS93**]   Rakesh Agrawal, Tomasz Imieliński, and Arun Swami. Mining association rules between sets of items in large databases. SIGMOD Rec., 22(2):207–216, June 1993. doi:http://doi.acm.org/10.1145/170036.170072, doi:10.1145/170036.170072.

[**BBHB94**]   J. C. Bezdek, S. Boggavarapu, L. O. Hall, and A. Bensaid. Genetic algorithm guided clustering. In Evolutionary Computation, 1994. IEEE World Congress on Computational Intelligence., Proceedings of the First IEEE Conference on, pages 34–39 vol.1, Jun 1994. doi:http://dx.doi:10.1109/ICEC.1994.350046.

[**BEF84**]   J. C. Bezdek, R. Ehrlich, and W. Full. Fcm: *The fuzzy c-means clustering algorithm.* Computers & Geosciences, 10(2):191–203, 1984. http://www.sciencedirect.com/science/article/pii/0098300484900207, doi:http://dx.doi.org/10.1016/0098-3004(84)90020-7.

[**DB79**]   David L. Davies and Donald W. Bouldin. A cluster separation measure. Pattern Analysis and Machine Intelligence, IEEE Transactions on, PAMI-1(2):224–227, April 1979. doi:http://dx.doi.org/10.1109/TPAMI.1979.4766909.

[**BM02a**]   S. Bandyopadhyay and U. Maulik. *An evolutionary technique based on k-means algorithm for optimal clustering in rn.* Inf. Sci. Appl., 146(1-4):221–237, 2002. ttp://www.sciencedirect.com/science/article/pii/S0020025502002086, doi:http://dx.doi.org/10.1016/S0020-0255(02)00208-6.

[**BM02b**]   S. Bandyopadhyay and U. Maulik. *Genetic clustering for automatic evolution of clusters and application to image classification.* Pattern Recognition, 35(6):1197 – 1208, 2002. http://www.sciencedirect.com/science/article/pii/S003132030100108X, doi:http://dx.doi.org/10.1016/S0031-3203(01)00108-X.

[**BM07**]   S. Bandyopadhuay and U. Maulik. *Multiobjective genetic clustering for pixel classification in remote sensing imagery.* IEEE Trans. Geosci. Remote Sensing, 45:1506–1511, May 2007

[**CdLM03**]   A. Casillas, M.T. González de Lena, and R. Martínez. *Document clustering into an unknown number of clusters using a genetic algorithm.* In Václav Matoušek and Pavel Mautner, editors, Text, Speech and Dialogue, volume 2807 of Lecture Notes in Computer Science, pages 43–49. Springer Berlin Heidelberg, 2003. doi:http://dx.doi.org/10.1007/978-3-540-39398-6_7.

[**CH74**]   T. Caliński and J. Harabasz. *A dendrite method for cluster analysis.* Communications in Statistics, 3(1):1–27, January 1974. doi:http://dx.doi.org/10.1080/03610927408827101.

[**CSL04**]   C.-H. Chou, M.-C. Su, and E. Lai. *A new cluster validity measure and its application to image compression*. Pattern Analysis and Applications, 7(2):205–220, 2004. doi:http://dx.doi.org/10.1007/s10044-004-0218-1.

[**CZZ09**]   Dong-Xia Chang, Xian-Da Zhang, and Chang-Wen Zheng. *A genetic algorithm with gene rearrangement for k-means clustering*. Pattern Recogn., 42(7):1210–1222, 2009. doi:http://dx.doi.org/10.1016/j.patcog.2008.11.006.

[**DAK08**]   S. Das, A. Abraham, and A. Konar. *Automatic clustering using an improved differential evolution algorithm*. Systems, Man and Cybernetics, Part A: Systems and Humans, IEEE Transactions on, 38(1):218–237, Jan 2008. doi:http://dx.doi.org/10.1109/TSMCA.2007.909595.

[**Faw06**]   Tom Fawcett. *An introduction to roc analysis*. Pattern Recogn. Lett., 27(8):861–874, June 2006. doi:http://dx.doi.org/10.1016/j.patrec.2005.10.010.

[**FKKN97**]   Pasi Fränti, Juha Kivijärvi, Timo Kaukoranta, and Olli Nevalainen. *Genetic algorithms for large-scale clustering problems*. The Computer Journal, 40(9):547–554, Jan 1997. URL: https://academic.oup.com/comjnl/article-abstract/40/9/547/343025?redirectedFrom=fulltext, doi:http://dx.doi.org/:10.1093/comjnl/40.9.547.

[**Gol89**]   David E. Goldberg. *Genetic Algorithms in Search, Optimization and Machine Learning*. Addison-Wesley Longman Publishing Co., Inc., Boston, MA, USA, 1st edition, 1989.

[**HCdC06**]   E. R. Hruschka, R. J. G. B. Campello, and L. N. de Castro. *Evolving clusters in gene-expression data*. Inf. Sci., 176(13):1898–1927, July 2006. doi:http://dx.doi.org/10.1016/j.ins.2005.07.015.

[**HCFdC09**]   E.R. Hruschka, R.J.G.B. Campello, A.A. Freitas, and A.C.P.L.F. de Carvalho. *A survey of evolutionary algorithms for clustering*. IEEE Transactions on Systems, Man and Cybernetics, Part C: Applications and Reviews, 39(2):133–155, March 2009. http://www.cs.kent.ac.uk/pubs/2009/2884.

[**HE03**]   E. R. Hruschka and N. F. F. Ebecken. *A genetic algorithm for cluster analysis*. Intell. Data Anal., 7(1):15–25, January 2003. http://dl.acm.org/citation.cfm?id=1293920.1293922.

[**HK17**]   Emrah Hancer and Dervis Karaboga. *A comprehensive survey of traditional, merge-split and evolutionary approaches proposed for determination of cluster number*. Swarm and Evolutionary Computation, 32:49 – 67, 2017. http://www.sciencedirect.com/science/article/pii/S2210650216300475, https://dx.doi.org/10.1016/j.swevo.2016.06.004.

[**HPY00**]   Jiawei Han, Jian Pei, and Yiwen Yin. Mining frequent patterns without candidate generation. SIGMOD Rec., 29(2):1–12, May 2000. URL: http://doi.acm.org/10.1145/335191.335372, doi:doi:10.1145/335191.335372.

[**HT12**]   Hong He and Yonghong Tan. *A two-stage genetic algorithm for automatic clustering*. Neurocomput., 81:49–59, April 2012. doi:http://dx.doi.org/10.1016/j.neucom.2011.11.001.

[**Int10**]   Intel, Santa Clara, CA, USA. *Intel®64 and IA-32 Architectures Software Developer's Manual Volume 3A: System Programming Guide*, Part 1, jun 2010.

[**JMF99**]   A. K. Jain, M. N. Murty, and P. J. Flynn. *Data clustering: A review*. ACM Comput. Surv., 31(3):264–323, September 1999. doi:http://doi.acm.org/10.1145/331499.331504.

[**KB97**]   L. I. Kuncheva and J. C. Bezdek. *Selection of cluster prototypes from data by a genetic algorithm*. In inProc. 5th Eur. Congr. Intell. Tech. Soft Comput., pages 1683–1688, 1997.

[**KM99**]   K. Krishna and M. Narasimha Murty. *Genetic k-means algorithm*. IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics), 29(3):433–439, Jun 1999. http://ieeexplore.ieee.org/document/764879/, doi:http://dx.doi.org/10.1109/3477.764879.

[**KR90**]   L. Kaufman and P. J. Rousseeuw. *Finding groups in data: an introduction to cluster analysis*. John Wiley and Sons, New York, 1990.

[**LDK93**]   C.B. Lucasius, A.D. Dane, and G. Kateman. *On k-medoid clustering of large data sets with the aid of a genetic algorithm: background, feasibility and comparison*. Analytica Chimica Acta, 282:647–669, 1993. http://www.sciencedirect.com/science/article/pii/000326709380130D, doi:https://doi.org/10.1016/0003-2670(93)80130-D.

[**LLF+04a**]   Yi Lu, Shiyong Lu, Farshad Fotouhi, Youping Deng, and Susan J. Brown. *Fgka: a fast genetic k-means clustering algorithm*. In Proceedings of the 2004 ACM symposium on Applied computing, SAC '04, pages 622–623, New York, NY, USA, 2004. ACM. doi:http://doi.acm.org/10.1145/967900.968029.

[**LLF+04b**]   Yi Lu, Shiyong Lu, Farshad Fotouhi, Youping Deng, and Susan J. Brown.*Incremental genetic k-means algorithm and its application in gene expression data analysis*. BMC Bioinformatics, 5:172, 2004.

[**MB00**]   U. Maulik and S. Bandyopadhyay. *Genetic algorithm-based clustering technique*. Pattern Recognition, 33(9):1455–1465, 2000.

[**MB02**]   U. Maulik and S. Bandyopadhyay. *Performance evaluation of some clustering algorithms and validity indices*. IEEE Trans. Pattern Anal. Mach. Intell., 24:1650–1654, December 2002. doi:http://dx.doi.org/10.1109/TPAMI.2002.1114856.

[**MC88**]   G.W. Milligan and M.C. Cooper. *A study of standardization of variables in cluster analysis*. J. Classification, 5:181–204, 1988. doi:http://www.springerlink.com/content/t588424722r23031.

[**MC96**]   C. A. Murthy and Nirmalya Chowdhury. *In search of optimal clusters using genetic algorithms*. Pattern Recogn. Lett., 17(8):825–832, 1996. doi:http://dx.doi.org/10.1016/0167-8655(96)00043-8.

[**Mic92**]   Zbigniew Michalewicz. *Genetic Algorithms + Data Structures = Evolution Programs*. Springer, Berlin,1992.

[**MRS08**]   Christopher D. Manning, Prabhakar Raghavan, and Hinrich Schütze. *Introduction to Information Retrieval*. Cambridge University Press, Cambridge, UK, 2008. http://nlp.stanford.edu/IR-book/information-retrieval-book.html.

[**NP14**]   Satyasai Jagannath Nanda and Ganapati Panda. *A survey on nature inspired metaheuristic algorithms for partitional clustering*. Swarm and Evolutionary Computation, 16:1–18, 2014. http://www.sciencedirect.com/science/article/pii/S221065021300076X, doi:http://dx.doi.org/10.1016/j.swevo.2013.11.003.

[**Ran71**]   William M. Rand. *Objective criteria for the evaluation of clustering methods*. Journal of the American Statistical Association, 66(336):846–850, 1971. doi:http://dx.doi.org/10.2307/2284239.

[**SL04**] Weiguo Sheng and Xiaohui Liu. *A hybrid algorithm for k-medoid clustering of large data sets.* In Evolutionary Computation, 2004. CEC2004. Congress on, volume 1, pages 77–82 Vol.1, June 2004. doi:http://dx.doi.org/10.1109/CEC.2004.1330840.

[**XB91**] Xuanli Lisa Xie and Gerardo Beni. *A validity measure for fuzzy clustering.* IEEE Trans. Pattern Anal. Mach. Intell., 13(8):841–847, August 1991. doi:http://dx.doi.org/10.1109/34.85677.

[**TY01**] Lin Yu Tseng and Shiueng Bien Yang. *A genetic approach to the automatic clustering problem.* Pattern Recognition, 34(2):415 – 424, 2001. doi:http://dx.doi.org/10.1016/S0031-3203(00)00005-4.

Appendix B GNU Free Documentation License

Version 1.3, 3 November 2008

Copyright © 2000, 2001, 2002, 2007, 2008 Free Software Foundation, Inc.
http://fsf.org/

Everyone is permitted to copy and distribute verbatim copies
of this license document, but changing it is not allowed.

0. PREAMBLE

The purpose of this License is to make a manual, textbook, or other functional and useful document *free* in the sense of freedom: to assure everyone the effective freedom to copy and redistribute it, with or without modifying it, either commercially or non-commercially. Secondarily, this License preserves for the author and publisher a way to get credit for their work, while not being considered responsible for modifications made by others.

This License is a kind of "copyleft", which means that derivative works of the document must themselves be free in the same sense. It complements the GNU General Public License, which is a copyleft license designed for free software.

We have designed this License in order to use it for manuals for free software, because free software needs free documentation: a free program should come with manuals providing the same freedoms that the software does. But this License is not limited to software manuals; it can be used for any textual work, regardless of subject matter or whether it is published as a printed book. We recommend this License principally for works whose purpose is instruction or reference.

1. APPLICABILITY AND DEFINITIONS

This License applies to any manual or other work, in any medium, that contains a notice placed by the copyright holder saying it can be distributed under the terms of this License. Such a notice grants a world-wide, royalty-free license, unlimited in duration, to use that work under the conditions stated herein. The "Document", below, refers to any such manual or work. Any member of the public is a licensee, and is addressed as "you". You accept the license if you copy, modify or distribute the work in a way requiring permission under copyright law.

A "Modified Version" of the Document means any work containing the Document or a portion of it, either copied verbatim, or with modifications and/or translated into another language.

A "Secondary Section" is a named appendix or a front-matter section of the Document that deals exclusively with the relationship of the publishers or authors of the Document to the Document's overall subject (or to related matters) and contains nothing that could fall directly within that overall subject. (Thus, if the Document is in part a textbook of mathematics, a Secondary Section may not explain any mathematics.) The relationship could be a matter of historical connection with the subject or with related matters, or of legal, commercial, philosophical, ethical or political position regarding them.

The "Invariant Sections" are certain Secondary Sections whose titles are designated, as being those of Invariant Sections, in the notice that says that the Document is released

under this License. If a section does not fit the above definition of Secondary then it is not allowed to be designated as Invariant. The Document may contain zero Invariant Sections. If the Document does not identify any Invariant Sections then there are none.

The "Cover Texts" are certain short passages of text that are listed, as Front-Cover Texts or Back-Cover Texts, in the notice that says that the Document is released under this License. A Front-Cover Text may be at most 5 words, and a Back-Cover Text may be at most 25 words.

A "Transparent" copy of the Document means a machine-readable copy, represented in a format whose specification is available to the general public, that is suitable for revising the document straightforwardly with generic text editors or (for images composed of pixels) generic paint programs or (for drawings) some widely available drawing editor, and that is suitable for input to text formatters or for automatic translation to a variety of formats suitable for input to text formatters. A copy made in an otherwise Transparent file format whose markup, or absence of markup, has been arranged to thwart or discourage subsequent modification by readers is not Transparent. An image format is not Transparent if used for any substantial amount of text. A copy that is not "Transparent" is called "Opaque".

Examples of suitable formats for Transparent copies include plain ASCII without markup, Texinfo input format, LaTeX input format, SGML or XML using a publicly available DTD, and standard-conforming simple HTML, PostScript or PDF designed for human modification. Examples of transparent image formats include PNG, XCF and JPG. Opaque formats include proprietary formats that can be read and edited only by proprietary word processors, SGML or XML for which the DTD and/or processing tools are not generally available, and the machine-generated HTML, PostScript or PDF produced by some word processors for output purposes only.

The "Title Page" means, for a printed book, the title page itself, plus such following pages as are needed to hold, legibly, the material this License requires to appear in the title page. For works in formats which do not have any title page as such, "Title Page" means the text near the most prominent appearance of the work's title, preceding the beginning of the body of the text.

The "publisher" means any person or entity that distributes copies of the Document to the public.

A section "Entitled XYZ" means a named subunit of the Document whose title either is precisely XYZ or contains XYZ in parentheses following text that translates XYZ in another language. (Here XYZ stands for a specific section name mentioned below, such as "Acknowledgements", "Dedications", "Endorsements", or "History".) To "Preserve the Title" of such a section when you modify the Document means that it remains a section "Entitled XYZ" according to this definition.

The Document may include Warranty Disclaimers next to the notice which states that this License applies to the Document. These Warranty Disclaimers are considered to be included by reference in this License, but only as regards disclaiming warranties: any other implication that these Warranty Disclaimers may have is void and has no effect on the meaning of this License.

2. VERBATIM COPYING

You may copy and distribute the Document in any medium, either commercially or noncommercially, provided that this License, the copyright notices, and the license notice saying this License applies to the Document are reproduced in all copies, and that you add no other conditions whatsoever to those of this License. You may not use technical measures to obstruct or control the reading or further copying of the copies you make or distribute. However, you may accept compensation in exchange for copies. If you distribute a large enough number of copies you must also follow the conditions in section 3.

You may also lend copies, under the same conditions stated above, and you may publicly display copies.

3. COPYING IN QUANTITY

If you publish printed copies (or copies in media that commonly have printed covers) of the Document, numbering more than 100, and the Document's license notice requires Cover Texts, you must enclose the copies in covers that carry, clearly and legibly, all these Cover Texts: Front-Cover Texts on the front cover, and Back-Cover Texts on the back cover. Both covers must also clearly and legibly identify you as the publisher of these copies. The front cover must present the full title with all words of the title equally prominent and visible. You may add other material on the covers in addition. Copying with changes limited to the covers, as long as they preserve the title of the Document and satisfy these conditions, can be treated as verbatim copying in other respects.

If the required texts for either cover are too voluminous to fit legibly, you should put the first ones listed (as many as fit reasonably) on the actual cover, and continue the rest onto adjacent pages.

If you publish or distribute Opaque copies of the Document numbering more than 100, you must either include a machine-readable Transparent copy along with each Opaque copy, or state in or with each Opaque copy a computer-network location from which the general network-using public has access to download using public-standard network protocols a complete Transparent copy of the Document, free of added material. If you use the latter option, you must take reasonably prudent steps, when you begin distribution of Opaque copies in quantity, to ensure that this Transparent copy will remain thus accessible at the stated location until at least one year after the last time you distribute an Opaque copy (directly or through your agents or retailers) of that edition to the public.

It is requested, but not required, that you contact the authors of the Document well before redistributing any large number of copies, to give them a chance to provide you with an updated version of the Document.

4. MODIFICATIONS

You may copy and distribute a Modified Version of the Document under the conditions of sections 2 and 3 above, provided that you release the Modified Version under precisely this License, with the Modified Version filling the role of the Document, thus licensing distribution and modification of the Modified Version to whoever possesses a copy of it. In addition, you must do these things in the Modified Version:

A. Use in the Title Page (and on the covers, if any) a title distinct from that of the Document, and from those of previous versions (which should, if there were any,

be listed in the History section of the Document). You may use the same title as
a previous version if the original publisher of that version gives permission.

B. List on the Title Page, as authors, one or more persons or entities responsible for
authorship of the modifications in the Modified Version, together with at least five
of the principal authors of the Document (all of its principal authors, if it has fewer
than five), unless they release you from this requirement.

C. State on the Title page the name of the publisher of the Modified Version, as the
publisher.

D. Preserve all the copyright notices of the Document.

E. Add an appropriate copyright notice for your modifications adjacent to the other
copyright notices.

F. Include, immediately after the copyright notices, a license notice giving the public
permission to use the Modified Version under the terms of this License, in the form
shown in the Addendum below.

G. Preserve in that license notice the full lists of Invariant Sections and required Cover
Texts given in the Document's license notice.

H. Include an unaltered copy of this License.

I. Preserve the section Entitled "History", Preserve its Title, and add to it an item
stating at least the title, year, new authors, and publisher of the Modified Version
as given on the Title Page. If there is no section Entitled "History" in the Docu-
ment, create one stating the title, year, authors, and publisher of the Document
as given on its Title Page, then add an item describing the Modified Version as
stated in the previous sentence.

J. Preserve the network location, if any, given in the Document for public access to
a Transparent copy of the Document, and likewise the network locations given in
the Document for previous versions it was based on. These may be placed in the
"History" section. You may omit a network location for a work that was published
at least four years before the Document itself, or if the original publisher of the
version it refers to gives permission.

K. For any section Entitled "Acknowledgements" or "Dedications", Preserve the Title
of the section, and preserve in the section all the substance and tone of each of the
contributor acknowledgements and/or dedications given therein.

L. Preserve all the Invariant Sections of the Document, unaltered in their text and
in their titles. Section numbers or the equivalent are not considered part of the
section titles.

M. Delete any section Entitled "Endorsements". Such a section may not be included
in the Modified Version.

N. Do not retitle any existing section to be Entitled "Endorsements" or to conflict in
title with any Invariant Section.

O. Preserve any Warranty Disclaimers.

If the Modified Version includes new front-matter sections or appendices that qualify
as Secondary Sections and contain no material copied from the Document, you may at
your option designate some or all of these sections as invariant. To do this, add their

titles to the list of Invariant Sections in the Modified Version's license notice. These titles must be distinct from any other section titles.

You may add a section Entitled "Endorsements", provided it contains nothing but endorsements of your Modified Version by various parties—for example, statements of peer review or that the text has been approved by an organization as the authoritative definition of a standard.

You may add a passage of up to five words as a Front-Cover Text, and a passage of up to 25 words as a Back-Cover Text, to the end of the list of Cover Texts in the Modified Version. Only one passage of Front-Cover Text and one of Back-Cover Text may be added by (or through arrangements made by) any one entity. If the Document already includes a cover text for the same cover, previously added by you or by arrangement made by the same entity you are acting on behalf of, you may not add another; but you may replace the old one, on explicit permission from the previous publisher that added the old one.

The author(s) and publisher(s) of the Document do not by this License give permission to use their names for publicity for or to assert or imply endorsement of any Modified Version.

5. COMBINING DOCUMENTS

   You may combine the Document with other documents released under this License, under the terms defined in section 4 above for modified versions, provided that you include in the combination all of the Invariant Sections of all of the original documents, unmodified, and list them all as Invariant Sections of your combined work in its license notice, and that you preserve all their Warranty Disclaimers.

   The combined work need only contain one copy of this License, and multiple identical Invariant Sections may be replaced with a single copy. If there are multiple Invariant Sections with the same name but different contents, make the title of each such section unique by adding at the end of it, in parentheses, the name of the original author or publisher of that section if known, or else a unique number. Make the same adjustment to the section titles in the list of Invariant Sections in the license notice of the combined work.

   In the combination, you must combine any sections Entitled "History" in the various original documents, forming one section Entitled "History"; likewise combine any sections Entitled "Acknowledgements", and any sections Entitled "Dedications". You must delete all sections Entitled "Endorsements."

6. COLLECTIONS OF DOCUMENTS

   You may make a collection consisting of the Document and other documents released under this License, and replace the individual copies of this License in the various documents with a single copy that is included in the collection, provided that you follow the rules of this License for verbatim copying of each of the documents in all other respects.

   You may extract a single document from such a collection, and distribute it individually under this License, provided you insert a copy of this License into the extracted document, and follow this License in all other respects regarding verbatim copying of that document.

7. AGGREGATION WITH INDEPENDENT WORKS

A compilation of the Document or its derivatives with other separate and independent documents or works, in or on a volume of a storage or distribution medium, is called an "aggregate" if the copyright resulting from the compilation is not used to limit the legal rights of the compilation's users beyond what the individual works permit. When the Document is included in an aggregate, this License does not apply to the other works in the aggregate which are not themselves derivative works of the Document.

If the Cover Text requirement of section 3 is applicable to these copies of the Document, then if the Document is less than one half of the entire aggregate, the Document's Cover Texts may be placed on covers that bracket the Document within the aggregate, or the electronic equivalent of covers if the Document is in electronic form. Otherwise they must appear on printed covers that bracket the whole aggregate.

8. TRANSLATION

Translation is considered a kind of modification, so you may distribute translations of the Document under the terms of section 4. Replacing Invariant Sections with translations requires special permission from their copyright holders, but you may include translations of some or all Invariant Sections in addition to the original versions of these Invariant Sections. You may include a translation of this License, and all the license notices in the Document, and any Warranty Disclaimers, provided that you also include the original English version of this License and the original versions of those notices and disclaimers. In case of a disagreement between the translation and the original version of this License or a notice or disclaimer, the original version will prevail.

If a section in the Document is Entitled "Acknowledgements", "Dedications", or "History", the requirement (section 4) to Preserve its Title (section 1) will typically require changing the actual title.

9. TERMINATION

You may not copy, modify, sublicense, or distribute the Document except as expressly provided under this License. Any attempt otherwise to copy, modify, sublicense, or distribute it is void, and will automatically terminate your rights under this License.

However, if you cease all violation of this License, then your license from a particular copyright holder is reinstated (a) provisionally, unless and until the copyright holder explicitly and finally terminates your license, and (b) permanently, if the copyright holder fails to notify you of the violation by some reasonable means prior to 60 days after the cessation.

Moreover, your license from a particular copyright holder is reinstated permanently if the copyright holder notifies you of the violation by some reasonable means, this is the first time you have received notice of violation of this License (for any work) from that copyright holder, and you cure the violation prior to 30 days after your receipt of the notice.

Termination of your rights under this section does not terminate the licenses of parties who have received copies or rights from you under this License. If your rights have been terminated and not permanently reinstated, receipt of a copy of some or all of the same material does not give you any rights to use it.

10. FUTURE REVISIONS OF THIS LICENSE

The Free Software Foundation may publish new, revised versions of the GNU Free Documentation License from time to time. Such new versions will be similar in spirit to the present version, but may differ in detail to address new problems or concerns. See http://www.gnu.org/copyleft/.

Each version of the License is given a distinguishing version number. If the Document specifies that a particular numbered version of this License "or any later version" applies to it, you have the option of following the terms and conditions either of that specified version or of any later version that has been published (not as a draft) by the Free Software Foundation. If the Document does not specify a version number of this License, you may choose any version ever published (not as a draft) by the Free Software Foundation. If the Document specifies that a proxy can decide which future versions of this License can be used, that proxy's public statement of acceptance of a version permanently authorizes you to choose that version for the Document.

11. RELICENSING

"Massive Multiauthor Collaboration Site" (or "MMC Site") means any World Wide Web server that publishes copyrightable works and also provides prominent facilities for anybody to edit those works. A public wiki that anybody can edit is an example of such a server. A "Massive Multiauthor Collaboration" (or "MMC") contained in the site means any set of copyrightable works thus published on the MMC site.

"CC-BY-SA" means the Creative Commons Attribution-Share Alike 3.0 license published by Creative Commons Corporation, a not-for-profit corporation with a principal place of business in San Francisco, California, as well as future copyleft versions of that license published by that same organization.

"Incorporate" means to publish or republish a Document, in whole or in part, as part of another Document.

An MMC is "eligible for relicensing" if it is licensed under this License, and if all works that were first published under this License somewhere other than this MMC, and subsequently incorporated in whole or in part into the MMC, (1) had no cover texts or invariant sections, and (2) were thus incorporated prior to November 1, 2008.

The operator of an MMC Site may republish an MMC contained in the site under CC-BY-SA on the same site at any time before August 1, 2009, provided the MMC is eligible for relicensing.

ADDENDUM: How to use this License for your documents

To use this License in a document you have written, include a copy of the License in the document and put the following copyright and license notices just after the title page:

```
Copyright (C)  year  your name.
Permission is granted to copy, distribute and/or modify this document
under the terms of the GNU Free Documentation License, Version 1.3
or any later version published by the Free Software Foundation;
with no Invariant Sections, no Front-Cover Texts, and no Back-Cover
Texts.  A copy of the license is included in the section entitled ``GNU
Free Documentation License''.
```

If you have Invariant Sections, Front-Cover Texts and Back-Cover Texts, replace the "with...Texts." line with this:

```
with the Invariant Sections being list their titles, with
the Front-Cover Texts being list, and with the Back-Cover Texts
being list.
```

If you have Invariant Sections without Cover Texts, or some other combination of the three, merge those two alternatives to suit the situation.

If your document contains nontrivial examples of program code, we recommend releasing these examples in parallel under your choice of free software license, such as the GNU General Public License, to permit their use in free software.

Appendix C Concept index