copulaedas: An R Package for Estimation of Distribution Algorithms Based on Copulas

Yasser González-Fernández
Institute of Cybernetics,
Mathematics and Physics

Marta Soto
Institute of Cybernetics,
Mathematics and Physics

Abstract

The use of probabilistic models based on copulas in EDAs (Estimation of Distribution Algorithms) is currently an active area of research. In this context, the **copulaedas** R package intends to provide a platform where EDAs based on copulas can be implemented and studied. The package offers complete implementations of various EDAs based on copulas and vines, a group of well-known benchmark problems, utility functions to study the behavior of EDAs and the possibility of implementing new algorithms that can be integrated into the package. EDAs are implemented using S4 classes with generic functions for its main parts: seeding, selection, learning, sampling, replacement, local optimization, termination, and reporting. This paper provides an overview of EDAs based on copulas, describes the implementation of **copulaedas** and illustrates its use with examples. The examples include running the EDAs implemented in the package, implementing new algorithms and performing an empirical study to compare the behavior of a group of EDAs.

Keywords: optimization, estimation of distribution algorithms, copula, vine, R.

1. Introduction

EDAs (Estimation of Distribution Algorithms) (Mühlenbein and Paaß 1996; Baluja 1994; Larrañaga and Lozano 2002; Pelikan *et al.* 2002) are evolutionary optimization methods characterized by the explicit use of probabilistic models. These algorithms explore the search space by iteratively estimating and sampling a probability distribution built from promising solutions.

Due to its tractable properties, the normal distribution has been commonly used to model the search distributions of EDAs for real-valued optimization problems (Bosman and Thierens 2006; Kern *et al.* 2003). Nevertheless, its use is often inconsistent with the empirical evidence and leads to the construction of incorrect models. Copula functions (Joe 1997; Nelsen 2006) offer an alternative to tackle these problems. By means of Sklar's Theorem (Sklar 1959), any multivariate distribution can be decomposed into marginal distributions and a copula that determines the dependence structure between the variables. EDAs based on copulas inherit these properties and consequently can build more realistic search distributions.

Although several EDAs based on copulas have been proposed in the literature, there are no publicly available implementations of such algorithms. Aiming to fill this gap, the **copulaedas** package (González-Fernández and Soto 2011a) for the R language and environment for statis-

$i \leftarrow 1$
repeat
  if $i == 1$ **then**
    Generate an initial population P_1 using a *seeding method*.
    Evaluate the solutions in the population P_1.
    If required, apply a *local optimization method* to the population P_1.
  else
    Select a population $P_i^{Selected}$ from P_{i-1} according to a *selection method*.
    Learn a probabilistic model M_i from $P_i^{Selected}$ using a *learning method*.
    Sample a new population $P_i^{Sampled}$ from M_i using a *sampling method*.
    Evaluate the solutions in the population $P_i^{Sampled}$.
    If required, apply a *local optimization method* to the population $P_i^{Sampled}$.
    Create the population P_i from P_{i-1} and $P_i^{Sampled}$ using a *replacement method*.
  end if
  If required, report progress information using a *reporting method*.
  $i \leftarrow i + 1$
until A criterion of the *termination method* is met.

Algorithm 1: General procedure of an EDA.

tical computing (R Development Core Team 2011) has been published on the Comprehensive R Archive Network at `http://CRAN.R-project.org/package=copulaedas`.

The **copulaedas** package intends to provide a platform where EDAs based on copulas can be implemented and studied. It contains implementations of various EDAs based on copulas, a group of well-known benchmark problems and utility functions to study EDAs.

The rest of this paper is organized as follows. Section 2 presents the necessary background on EDAs based on copulas. Section 3 describes the details of the implementation of **copulaedas** while Section 4 illustrates its use with examples. Finally, concluding remarks are given in Section 5.

2. Estimation of distribution algorithms based on copulas

This section begins by describing the general procedure of an EDA, according to the implementation included in **copulaedas**. Then, a general overview of the EDAs based on copulas presented in the literature with emphasis on the algorithms implemented in the package is given.

2.1. General procedure of an EDA

The general procedure of an EDA is outlined in Algorithm 1. Each iteration of this procedure is referred to as one generation of the EDA. The main steps of the algorithm are highlighted in italics.

The first step of an EDA is the generation of an initial population of solutions. The initial population is usually generated randomly but it can be generated using a particular heuristic

when a priori information about the characteristics of the optimal solutions is available. In both cases, we call the method used to generate the initial population a *seeding method*.

The results of global optimization algorithms such as EDAs can often be improved if combined with *local optimization methods* that look for better solutions in the neighborhood of each solution. Local optimization methods can also be used to implement repairing methods for constrained problems where the simulated solutions may be unfeasible and some strategy to repair these solutions is available.

A *selection method* is used to determine the solutions to be modeled by the search distribution. These solutions are usually the most promising solutions of the population. An example selection method is truncation selection, which creates the selected population with a percentage of the best solutions of the current population.

The estimation and simulation of the search distribution are essential steps of an EDA. These steps are implemented by *learning and sampling methods*, respectively. Both methods are closely related. Learning methods estimate structure and parameters of the probabilistic model used by the algorithm from the selected population, while sampling methods are used to generate a new population of solutions from the learned probabilistic model.

A *replacement method* is used to incorporate a new population of solutions into the current population. An example replacement strategy is to replace completely the current population with the new population. Other replacement strategies retain the best solutions found so far or are used to maintain the diversity of solutions.

Reporting methods provide progress information during the execution of the EDA. Relevant progress information can be the number of evaluations of the objective function and the best solution found so far.

Finally, a *termination method* determines when the algorithm stops according to certain criteria; for example, a fixed number of function evaluations are realized or a certain value of the objective function is reached.

We are particularly interested in EDAs whose learning and sampling steps involve probabilistic models based on copulas. The next section provides an overview of such algorithms.

2.2. Overview of EDAs based on copulas

To the best of our knowledge, the technical report (Soto *et al.* 2007) and the theses (Arderí 2007; Barba-Moreno 2007) were the first attempts to incorporate copulas into EDAs. Since then, a considerable number of EDAs based on copula theory have been proposed in the literature (e.g., Wang *et al.* 2009b,a; Salinas-Gutiérrez *et al.* 2009; Gao 2009; Soto and González-Fernández 2010; Salinas-Gutiérrez *et al.* 2010; Cuesta-Infante *et al.* 2010; Ye *et al.* 2010; González-Fernández 2011). As evidence of its increasing popularity, the use of copulas in EDAs has been identified as an emerging approach for the solution of real-valued optimization problems (Hauschild and Pelikan 2011).

In general, the learning step of copula-based EDAs consist of two parts: the estimation of the marginal distributions and the estimation of the probabilistic dependence structure. Usually, a particular distribution (e.g., normal or beta) is assumed for each margin and its parameters are estimated by maximum likelihood (Soto *et al.* 2007; Arderí 2007; Wang *et al.* 2009b,a; Salinas-Gutiérrez *et al.* 2009; Soto and González-Fernández 2010; Salinas-Gutiérrez *et al.* 2010; Ye *et al.* 2010; González-Fernández 2011; Salinas-Gutiérrez *et al.* 2011). In other cases, ker-

nel density estimation (Soto *et al.* 2007; Arderí 2007; Gao 2009; Salinas-Gutiérrez *et al.* 2011) or empirical marginal distributions (Cuesta-Infante *et al.* 2010) have been used. Once the marginal distributions are estimated, the selected population is transformed into uniform variables in $(0, 1)$ by the evaluation of each marginal cumulative distribution function. This transformed population is then used to estimate a copula-based model of the dependence structure among variables.

The simulation step usually starts with the generation of a population of uniform variables in $(0, 1)$ with the dependence structure described by the copula-based model estimated in the learning step. Finally, this uniform population is transformed to the domain of the variables through the evaluation of the inverse of each marginal cumulative distribution function.

According to the copula model used, EDAs based on copulas can be classified as EDAs based on either multivariate or factorized copulas. In the rest of this section we describe algorithms belonging to each group.

EDAs based on multivariate copulas

The research on EDAs based on multivariate copulas has focused on the use of the normal copula (Soto *et al.* 2007; Arderí 2007; Barba-Moreno 2007; Wang *et al.* 2009b) and Archimedean copulas (Wang *et al.* 2009a; Gao 2009).

The algorithms described in (Soto *et al.* 2007; Arderí 2007; Barba-Moreno 2007) are theoretically similar but they present differences in the estimation of the marginal distributions and the use of techniques such as variance scaling. Wang *et al.* (2009b) present the bivariate case and, since only normal marginal distributions are used, the proposed algorithm is equivalent to EMNA (Estimation of Multivariate Normal Algorithm) (Larrañaga *et al.* 2001).

The algorithms presented in (Wang *et al.* 2009a; Gao 2009) use exchangeable Archimedean copulas. Wang *et al.* (2009a) propose two algorithms that use Clayton and Ali-Mikhail-Haq copulas, respectively. In this work, the parameters of the copulas are not estimated from the selected population. Gao (2009) does not state which members of the family of Archimedean copulas are used in the algorithm.

Two EDAs based on multivariate copulas are implemented in **copulaedas**, one is based on the product or independence copula and the other on the normal copula.

The first algorithm is UMDA (Univariate Marginal Distribution Algorithm) for continuous variables (Larrañaga *et al.* 1999, 2000). UMDA can be integrated into the framework of EDAs based on copulas, although originally it was not defined in terms of copulas. A consequence of Sklar's Theorem is that random variables are independent if and only if the underlying copula is the product copula. Thus, UMDA can be described as an EDA based on copulas that models the dependence structure between the variables using a multivariate product copula.

The second EDA based on a multivariate copula implemented in **copulaedas** is GCEDA (Gaussian Copula Estimation of Distribution Algorithm) (Soto *et al.* 2007; Arderí 2007). This algorithm is based on the multivariate normal copula, which allows the construction of multivariate distributions with normal dependence structure and non-normal margins. The dependence structure of the multivariate normal copula is determined by a positive-definite correlation matrix. If the marginal distributions are not normal, the correlation matrix is estimated by the inversion of the non-parametric estimator of Kendall's tau for each pair of variables (see e.g., Nelsen 2006). If the resulting matrix is not positive-definite, the correction proposed by

Rousseeuw and Molenberghs (1993) can be applied. GCEDA is equivalent to EMNA when all marginal distributions are normal.

The implementation of UMDA and GCEDA provided by **copulaedas** has been used for the solution of a real-world problem known as the molecular docking problem (Soto *et al.* 2012).

EDAs based on copula factorizations

The use of multivariate copulas to model the dependence structure between variables offers several advantages over the use of a multivariate normal distribution; nevertheless, it presents limitations. The number of tractable copulas when more than two variables are involved is limited. In fact, most of the available parametric copulas are bivariate. Moreover, the multivariate copulas are not appropriate when all pairs of variables do not have the same dependence structure. Another limitation is that multivariate extensions, such as exchangeable Archimedean copulas or the multivariate t copula, have only one parameter to describe certain aspects of the overall dependence. This can be a serious issue when there are pairs of variables with different patterns of dependence.

One alternative is to use copula factorizations that build high-dimensional probabilistic models by using lower-dimensional copulas as building blocks. Several EDAs based on copula factorizations have been proposed in the literature (Salinas-Gutiérrez *et al.* 2009; Soto and González-Fernández 2010; Salinas-Gutiérrez *et al.* 2010; Cuesta-Infante *et al.* 2010; Ye *et al.* 2010; González-Fernández 2011), although the authors are not always aware of the limitations of the multivariate copula approach and present the algorithms without comments about these issues.

The EDA introduced in (Salinas-Gutiérrez *et al.* 2009) is an extension of MIMIC (Mutual Information Maximization for Input Clustering) for continuous domains (Larrañaga *et al.* 1999, 2000) that uses bivariate copulas in a chain structure instead of bivariate normal distributions. Two instances of this algorithm were presented, one uses normal copulas and the other Frank copulas. This algorithm is described in more detail in Section 4.2, where we illustrate the implementation of a copula-based EDA by using **copulaedas**.

The exchangeable Archimedean copulas employed in (Wang *et al.* 2009a; Gao 2009) represent highly specialized dependence structures (Berg and Aas 2007; McNeil 2008). Nested Archimedean copulas provide a more flexible way to build multivariate Archimedean copulas. Among the different nesting structures that have been proposed in the literature (see e.g., Berg and Aas 2007 for a review), hierarchically nested Archimedean copulas present one of the most flexible structures. Ye *et al.* (2010) propose an EDA that uses a representation of hierarchically nested Archimedean copulas based on Lévy subordinators (Hering *et al.* 2010).

Cuesta-Infante *et al.* (2010) investigate the use of bivariate empirical copulas and a multivariate extension of Archimedean copulas. The EDA based on bivariate empirical copulas is completely nonparametric: it employs empirical marginal distributions and a construction based on bivariate empirical copulas to represent the dependence among variables. The marginal distributions and the bivariate empirical copulas are defined through the linear interpolation of the sample in the selected population. The EDA based on Archimedean copulas uses a construction similar to a fully nested Archimedean copula. This algorithm uses copulas from one of the families Frank, Clayton or HRT (i.e., heavy right tail copula or Clayton survival copula). The parameters of the copulas are not estimated from the selected population but fixed to a constant value. The marginal distributions are modeled as in the EDA based on bivariate empirical copulas.

The class of VEDAs (Vine EDAs) was introduced in (Soto and González-Fernández 2010; González-Fernández 2011). Algorithms of this class model the search distributions using vines (Joe 1996; Bedford and Cooke 2001; Aas *et al.* 2009), which are graphical models that represent high-dimensional distributions by decomposing the multivariate density into bivariate copulas and one-dimensional densities. A vine on n variables is a set of nested trees $T_1, \ldots, T_{n-1}$, where the edges of tree T_j are the nodes of the tree T_{j+1} with $j = 1, \ldots, n-2$. The edges of the trees represent the bivariate copulas in the decomposition. Since all bivariate copulas do not have to belong to the same family, vines model a rich variety of dependences by combining bivariate copulas from different families.

C-vines (canonical vines) and D-vines (drawable vines) are two types of vines, each of which determine a specific decomposition of the multivariate density. In a C-vine, each tree T_j has a unique root node that is connected to $n-j$ edges. In a D-vine, no node is connected to more than two edges. Two EDAs based on these models were presented in (Soto and González-Fernández 2010; González-Fernández 2011): CVEDA (C-Vine EDA) and DVEDA (D-Vine EDA) based on C-vines and D-vines, respectively. Since both algorithms are implemented in **copulaedas**, we describe them in more detail in the rest of this section.

The general idea of inference and simulation methods for C-vines and D-vines was developed by Aas *et al.* (2009). The inference algorithm should consider two main aspects: the selection of the structure of the vines and the choice of the bivariate copulas in the factorization. The simulation algorithm is based on the conditional distribution method (see e.g., Devroye 1986).

At each generation of CVEDA and DVEDA, the selection of the structure of the vine involves selecting the bivariate dependences that will be explicitly modeled in the first tree. This is accomplished by using greedy heuristics based on the empirical Kendall's tau between each pair of variables in the selected population assigned to the edges of the tree. In a C-vine, the node that maximizes the sum of the weights of its edges to the other nodes is chosen as the root node of the first tree. In a D-vine, the problem of constructing the first tree consists of finding the maximum weighted sequence of the variables. Brechmann (2010) transforms this problem into a TSP (Traveling Salesman Problem) instance. For efficiency reasons, in **copulaedas** we find an approximate solution of the TSP by using the cheapest insertion heuristic (Rosenkrantz *et al.* 1977).

The selection of each bivariate copula in both decompositions starts with an independence test (Genest and Rémillard 2004; Genest *et al.* 2007). The product copula is selected if there is not enough evidence against the null hypothesis of independence at a given significance level. In the other case, the parameters of a group of candidate copulas are estimated and the copula that minimizes a Cramér-von Mises statistic based on the empirical copula is selected (Genest and Rémillard 2008).

The cost of the construction of C-vines and D-vines increases with the number of variables. To simplify the construction we apply the truncation strategy presented in (Brechmann 2010). If a vine is truncated at a given tree, all the copulas in the subsequent trees are assumed to be product copulas. A model selection procedure based on either AIC (Akaike Information Criterion) (Akaike 1974) or BIC (Bayesian Information Criterion) (Schwarz 1978) is applied to detect the required number of trees. This procedure expands the tree T_{j+1} if the value of the information criterion calculated up to the tree T_{j+1} is smaller than the value obtained up to the previous tree; otherwise, the vine is truncated at the tree T_j.

At this point, it is important to note that the algorithm presented in (Salinas-Gutiérrez *et al.*

2010) also uses a D-vine. In this algorithm only normal copulas are used in the first two trees and conditional independence is assumed for the rest of the trees, i.e., the D-vine is always truncated at the second tree.

The implementation of CVEDA and DVEDA included in **copulaedas** uses the truncation procedure based on AIC and the candidate copulas normal, t, Clayton, Frank and Gumbel. The parameters of all copulas but the t copula are estimated using the inversion of Kendall's tau. For the t copula, the correlation coefficient is computed as in the normal copula and the degrees of freedom are estimated by maximum likelihood with the correlation parameter fixed (Demarta and McNeil 2005).

González-Fernández (2011) presents a study about intrinsic characteristics of CVEDA and DVEDA, such as the impact of the truncation procedure and the effect of the selection of the structure of C-vines and D-vines. The implementation of these algorithms provided by **copulaedas** also has been used in the solution of the molecular docking problem with satisfactory results (Soto *et al.* 2012).

3. Implementation in R

The implementation of **copulaedas** follows an object-oriented design inspired by the **Mateda-2.0** (Santana *et al.* 2010) toolbox for MATLAB. Each EDA implemented in the package is represented by an S4 class (Chambers 2008) with generic functions for its main steps.

The main class of the package is `EDA`. This class is the base class of all classes implementing EDAs in the package. The `EDA` class has two slots: `name` and `parameters`. The `name` slot stores the name of the EDA and it is used by the `show` generic function to print the name of the algorithm when invoked with an `EDA` instance as argument. The `parameters` slot has greater importance, since it keeps all the parameters of the EDA in a list.

Each step of the general procedure of an EDA outlined in Algorithm 1 is represented in R by a generic function that expects an `EDA` instance as its first argument. Table 1 shows a description of these functions and its default methods. The help page of each generic function in the documentation of **copulaedas** contains information about its arguments, the return value, and the methods for each generic function already implemented in the package.

Generic functions that implement the steps of an EDA look at the `parameters` slot of the `EDA` instance received as first argument for the values of the parameters that affect its behavior. Only named members of the list should be used and reasonable default values should be assumed when a certain component is missing. For example, the `edaSeedUniform` method for the `edaSeed` generic function consults the `popSize` member of the list to know the number of solutions to be generated for the initial population. If the `popSize` component is not defined, an initial population of 100 solutions is generated. The help page of each generic function describes the members of the list in the `parameters` slot interpreted by each function and its default values.

The `edaRun` function implements the Algorithm 1 by linking together the generic functions for each step. This function expects four arguments: the `EDA` instance, the objective function and two vectors specifying the lower and upper bounds of the variables of the objective function. The length of the vectors with the lower and upper bounds should be the same, since it determines the number of variables of the objective function. When `edaRun` is called, it runs the main loop of the EDA until the call to the `edaTerminate` generic function returns `TRUE`.

Generic function	Description
`edaSeed`	*Seeding method.* The default method `edaSeedUniform` generates the values of each variable in the initial population from a continuous uniform distribution.
`edaOptimize`	*Local optimization method.* The use of a local optimization method is disabled by default.
`edaSelect`	*Selection method.* The default method `edaSelectTruncation` implements truncation selection.
`edaLearn`	*Learning method.* No default method.
`edaSample`	*Sampling method.* No default method.
`edaReplace`	*Replacement method.* The default method `edaReplaceComplete` completely replaces the current population with the new population.
`edaReport`	*Reporting method.* Reporting progress information is disabled by default.
`edaTerminate`	*Termination method.* The default method `edaTerminateMaxGen` ends the execution of the algorithm after a maximum number of generations.

Table 1: Description of the generic functions that implement the steps of the general procedure of an EDA outlined in Algorithm 1 and its default methods.

Then, the function returns an instance of the `EDAResult` class that encapsulates the results of the algorithm. A description of the slots of this class is shown in Table 2.

Two subclasses of `EDA` are defined in the package: `CEDA`, that represents EDAs based on multivariate copulas; and `VEDA`, that represents EDAs based on vines. The implementation of UMDA, GCEDA, CVEDA and DVEDA strongly relies on the **copula** (Kojadinovic and Yan 2010) and **vines** (González-Fernández and Soto 2011b) R packages. These packages implement the algorithms for the estimation and simulation of the probabilistic models used by these EDAs.

Slot	Description
`eda`	`EDA` instance.
`f`	Objective function.
`lower`	Lower bounds of the variables of the objective function.
`upper`	Upper bounds of the variables of the objective function.
`numGens`	Total number of generations.
`fEvals`	Total number of evaluations of the objective function.
`bestSol`	Best solution.
`bestEval`	Evaluation of the best solution.
`cpuTime`	Run time of the algorithm in seconds.

Table 2: Description of the slots of the `EDAResult` class.

4. Using copulaedas

In this section, we illustrate how to use **copulaedas**. The first group of examples show how to run the EDAs implemented in the package. Next, we explain how to implement a new EDA based on copulas by using the functionalities provided by the package. Finally, we show how to perform an empirical study to compare a group of EDAs.

Six well-known test functions are used in the examples. The objective functions are Sphere, Griewank, Ackley, Summation Cancellation, Rastrigin and Rosenbrock. The corresponding R functions are `fSphere`, `fGriewank`, `fAckley`, `fSummationCancellation`, `fRastrigin` and `fRosenbrock`. The definition of each function for a vector $\boldsymbol{x} = (x_1, \ldots, x_n)$ is given below.

$$f_{\text{Sphere}}(\boldsymbol{x}) = \sum_{i=1}^{n} x_i^2$$

$$f_{\text{Griewank}}(\boldsymbol{x}) = 1 + \sum_{i=1}^{n} \frac{x_i^2}{4000} - \prod_{i=1}^{n} \cos\left(\frac{x_i}{\sqrt{i}}\right)$$

$$f_{\text{Ackley}}(\boldsymbol{x}) = -20 \exp\left(-0.2\sqrt{\frac{1}{n}\sum_{i=1}^{n} x^2}\right) - \exp\left(\frac{1}{n}\sum_{i=1}^{n} \cos\left(2\pi x_i\right)\right) + 20 + \exp\left(1\right)$$

$$f_{\text{Summation Cancellation}}(\boldsymbol{x}) = \frac{1}{10^{-5} + \sum_{i=1}^{n} |y_i|},\ y_1 = x_1,\ y_i = y_{i-1} + x_i$$

$$f_{\text{Rastrigin}}(\boldsymbol{x}) = \sum_{i=1}^{n} \left(x_i^2 - 10\cos\left(2\pi x_i\right) + 10\right)$$

$$f_{\text{Rosenbrock}}(\boldsymbol{x}) = \sum_{i=1}^{n-1} \left(100\left(x_{i+1} - x_i^2\right)^2 + \left(1 - x_i\right)^2\right)$$

Sphere, Griewank, Ackley, Rastrigin and Rosenbrock are minimization problems. Summation Cancellation is originally a maximization problem but it is implemented in the package as a minimization problem. Sphere, Griewank, Ackley and Rastrigin have their global optimum at $\boldsymbol{x} = (0, \ldots, 0)$ with evaluation zero, Summation Cancellation has its global optimum at $\boldsymbol{x} = (0, \ldots, 0)$ with evaluation -10^5 and Rosenbrock has its global optimum at $\boldsymbol{x} = (1, \ldots, 1)$ with evaluation zero. For a description of the characteristics of these functions see (Bengoetxea *et al.* 2002; Bosman and Thierens 2006; Chen and Lim 2008).

The results presented in this section were obtained using R version 2.13.0 with **copulaedas** version 1.1.0, **copula** version 0.9-7 and **vines** version 1.0.3. Computations were performed on an Intel(R) Pentium(R) D CPU 3.00 GHz processor.

In the rest of this section, we assume **copulaedas** and the packages it depends on have been loaded. This can be attained by running the following command:

```
R> library("copulaedas")
```

4.1. Running the EDAs implemented in the package

We begin by illustrating how to run the EDAs based on copulas implemented in **copulaedas**. As an example, we execute GCEDA to optimize Sphere in five dimensions.

GCEDA is represented in the package by the `CEDA` class for EDAs based on multivariate copulas. Before creating a new instance of the class, we set up the generic functions for the steps of the EDA according to the expected behavior of the algorithm.

The termination criterion is either to find the optimum of the objective function or to reach a maximum number of generations. That is why we set the method for the `edaTerminate` generic function to a combination of the functions `edaTerminateEval` and `edaTerminateMaxGen` through the auxiliary function `edaTerminateCombined`.

```
R> setMethod("edaTerminate", "EDA",
+      edaTerminateCombined(edaTerminateEval, edaTerminateMaxGen))
```

The method for the `edaReport` generic function is set to `edaReportSimple` to make the algorithm print progress information at each generation. This function prints one line at each generation of the EDA with the minimum, mean and standard deviation of the evaluation of the solutions in the current population.

```
R> setMethod("edaReport", "EDA", edaReportSimple)
```

Note that these methods were set for the base class `EDA` and therefore they will be inherited by all subclasses. Generally, we find convenient to define methods of the generic functions that implement the steps of the EDA for the base class, except when different subclasses should use different methods.

The auxiliary function `CEDA` can be used to create instances of the class with the same name. Arguments of this function are interpreted as parameters of the EDA to be added as members of the list in the `parameters` slot of the new instance. An instance of `CEDA` corresponding to GCEDA using empirical marginal distributions smoothed with normal kernels can be created as follows:

```
R> gceda <- CEDA(copula = "normal", margin = "kernel",
+      popSize = 200, fEval = 0, fEvalTol = 1e-6, maxGen = 50)
R> gceda@name <- "Gaussian Copula Estimation of Distribution Algorithm"
```

The methods that implement the generic functions `edaLearn` and `edaSample` for `CEDA` instances expect three parameters. The `copula` parameter specifies the multivariate copula, it should be set to `"normal"` for GCEDA. The marginal distributions are determined by the value of `margin`. All EDAs implemented in the package use this parameter for the same purpose. As `margin` is set to `"kernel"`, the algorithm will look for three functions named `fkernel`, `pkernel` and `qkernel` already defined in the package to fit the parameters of the margins and to evaluate the distribution and quantile functions, respectively. The `fkernel` function computes the bandwidth parameter of the normal kernel according to the rule-of-thumb of Silverman (1986) and `pkernel` implements the empirical cumulative distribution function. The quantile function is evaluated following the procedure described in (Azzalini 1981). The `popSize` parameter determines the population size while the rest of the arguments of `CEDA` are parameters of the functions that implement the termination criterion.

Now, we can run GCEDA by calling `edaRun`. The lower and upper bounds of the variables are set so that the values of the variables in the optimum of the function are located at 25%

of the interval. It was shown in (Arderí 2007) that the use of empirical marginal distributions smoothed with normal kernels improves the behavior of GCEDA when the initial population is generated asymmetrically with respect to the optimum of the function.

```
R> result <- edaRun(gceda, fSphere, rep(-300, 5), rep(900, 5))
```

```
  Generation      Minimum         Mean    Std. Dev.
           1 9.482661e+04 1.007874e+06 5.271801e+05
           2 2.505026e+04 4.479002e+05 2.681643e+05
           3 2.937460e+04 2.091392e+05 1.264960e+05
           4 5.581990e+03 1.017533e+05 5.642366e+04
           5 3.718832e+03 4.862920e+04 2.923179e+04
           6 7.132640e+02 2.283238e+04 1.306885e+04
           7 1.381820e+03 1.046310e+04 5.386455e+03
           8 3.068758e+02 4.943787e+03 2.744929e+03
           9 1.910194e+02 2.188175e+03 1.324063e+03
          10 5.062607e+01 9.492492e+02 5.924008e+02
          11 1.812797e+01 3.922013e+02 2.294571e+02
          12 8.197173e+00 1.755258e+02 1.023085e+02
          13 6.354410e+00 8.173253e+01 4.020714e+01
          14 3.244178e+00 4.448070e+01 2.528163e+01
          15 8.257841e-01 1.949224e+01 1.085053e+01
          16 7.161607e-01 9.814025e+00 5.889123e+00
          17 4.792109e-01 4.450473e+00 2.243748e+00
          18 2.711282e-01 2.365315e+00 1.299843e+00
          19 1.060200e-01 1.121201e+00 6.513729e-01
          20 3.438796e-02 5.884943e-01 3.215504e-01
          21 3.353496e-02 2.756226e-01 1.773181e-01
          22 1.524750e-03 1.117457e-01 5.788006e-02
          23 6.755015e-03 6.367963e-02 3.382219e-02
          24 2.900885e-03 3.517951e-02 1.744429e-02
          25 2.286571e-04 1.906427e-02 1.041386e-02
          26 8.635889e-04 9.387225e-03 4.927262e-03
          27 5.090779e-04 4.185834e-03 2.275273e-03
          28 7.411229e-05 1.810591e-03 1.063558e-03
          29 6.164902e-05 8.022974e-04 4.755964e-04
          30 2.663512e-05 3.368331e-04 1.955830e-04
          31 2.466309e-05 1.657867e-04 9.601912e-05
          32 4.888452e-06 7.180790e-05 3.945560e-05
          33 3.626218e-06 3.662413e-05 2.063811e-05
          34 1.424262e-06 1.737351e-05 9.561411e-06
          35 8.645225e-07 8.936281e-06 5.409103e-06
```

The `result` variable contains an instance of the `EDAResult` class. A method for the `show` generic function prints the results of the execution of the algorithm.

```
R> show(result)
```

```
Results for Gaussian Copula Estimation of Distribution Algorithm
Best function evaluation    8.645225e-07
No. of generations          35
No. of function evaluations 7000
CPU time                    10.55 seconds
```

Due to the stochastic nature of EDAs, it is often useful to analyze a sequence of independent runs of these algorithms to ensure reliable results. The `edaIndepRuns` function supports executing independent runs of an EDA. To avoid generating lot of unnecessary output, we first disable reporting progress information on each generation by setting `edaReport` to `edaReportDisabled`.

```
R> setMethod("edaReport", "EDA", edaReportDisabled)
```

Now we can invoke the `edaIndepRuns` function to perform 30 independent runs of GCEDA.

```
R> results <- edaIndepRuns(gceda, fSphere, rep(-300, 5), rep(900, 5), 30)
```

The return value of the `edaIndepRuns` function is an instance of the `EDAResults` class. This class is simply a wrapper for a list with instances of `EDAResult` as members. Each member stores the results of an execution of the EDA. A `show` method for `EDAResults` instances prints a table with the results of the runs of the EDA.

```
R> show(results)
```

```
       Generations Evaluations Best Evaluation CPU Time
Run 1           37        7400    7.829213e-07    11.02
Run 2           37        7400    1.927911e-07    10.99
Run 3           38        7600    4.835526e-07    11.35
Run 4           35        7000    8.577429e-07    10.43
Run 5           35        7000    9.451111e-07    10.40
Run 6           35        7000    9.302367e-07    10.40
Run 7           36        7200    9.909941e-07    10.74
Run 8           37        7400    4.724555e-07    11.02
Run 9           35        7000    5.222054e-07    10.32
Run 10          36        7200    4.951474e-07    10.69
Run 11          37        7400    8.988045e-07    11.03
Run 12          34        6800    9.875791e-07    10.07
Run 13          36        7200    9.133316e-07    10.69
Run 14          38        7600    5.486231e-07    11.34
Run 15          34        6800    2.389598e-07    10.18
Run 16          35        7000    9.484775e-07    10.35
Run 17          31        6200    6.356923e-07     9.22
Run 18          36        7200    7.726292e-07    10.80
Run 19          35        7000    8.990815e-07    10.31
Run 20          34        6800    7.237225e-07    10.13
```

```
Run 21          36        7200    6.837205e-07    10.74
Run 22          35        7000    6.937608e-07    10.38
Run 23          34        6800    8.049177e-07    10.13
Run 24          34        6800    9.615774e-07    10.14
Run 25          39        7800    2.666713e-07    11.56
Run 26          35        7000    6.968256e-07    10.43
Run 27          36        7200    5.148476e-07    10.74
Run 28          36        7200    6.639083e-07    10.69
Run 29          35        7000    7.000933e-07    10.39
Run 30          37        7400    1.578787e-07    11.04
```

Also, the `summary` function can be used to generate a table with a statistical summary of the results of the 30 runs of the algorithm.

```
R> summary(results)

           Generations Evaluations Best Evaluation CPU Time
Minimum     31.000000   6200.0000    1.578787e-07  9.22000
Median      35.500000   7100.0000    6.984595e-07 10.56000
Maximum     39.000000   7800.0000    9.909941e-07 11.56000
Mean        35.600000   7120.0000    6.794754e-07 10.59067
Std. Dev.    1.566899    313.3798    2.462059e-07  0.47365
```

4.2. Implementation of a new EDA based on copulas

Now, we illustrate how to implement a new EDA based on copulas by using **copulaedas**. Since the algorithm in question matches the general procedure of an EDA presented in Algorithm 1, only the functions corresponding to the learning and simulation steps have to be implemented. The main loop and the rest of the steps of the EDA are already implemented in the package.

As an example, we implement the extension of MIMIC for continuous domains proposed in (Salinas-Gutiérrez *et al.* 2009). Similar to MIMIC, this extension learns a chain dependence structure but it uses bivariate copulas instead of bivariate normal distributions to model dependences.

Two instances of the extension of MIMIC based on copulas were presented in (Salinas-Gutiérrez *et al.* 2009), one uses bivariate normal copulas while the other uses bivariate Frank copulas. In this article, the algorithm will be denoted as Copula MIMIC.

The first step in the implementation of a new EDA using **copulaedas** is to define an S4 class to represent the algorithm. The new class should inherit from `EDA`. For convenience, we also define an auxiliary function `CopulaMIMIC` that can be used to create new instances of the class with the same name.

```
R> setClass("CopulaMIMIC", contains = "EDA",
+          prototype = prototype(name = "Copula MIMIC"))
R> CopulaMIMIC <- function (...) {
+      new("CopulaMIMIC", parameters = list(...))
+  }
```

Copula MIMIC models the marginal distributions with the beta distribution. A linear transformation is used to map the sample of the variables in the selected population into the $(0, 1)$ interval to match the domain of definition of the beta distribution. Note that this transformation does not affect the dependence between the variables because the copula is scale-invariant.

To be consistent with the marginal distributions already implemented in **copulaedas**, we define three functions with the common suffix `betamargin` and the prefixes `f`, `p` and `q` to fit the parameters of the margins and for the evaluation of the distribution and quantile functions, respectively. By following this convention, the algorithms already implemented in the package can use beta marginal distributions by setting the `margin` parameter to `"betamargin"`. The `betamargin` suffix was selected to avoid the redefinition of the `pbeta` and `qbeta` functions of the **stats** package.

```
R> fbetamargin <- function (x, lower, upper) {
+      x <- (x - lower) / (upper - lower)
+      loglik <- function (s) sum(dbeta(x, s[1], s[2], log = TRUE))
+      s <- optim(c(1, 1), loglik, control = list(fnscale = -1))$par
+      list(lower = lower, upper = upper, a = s[1], b = s[2])
+  }
R> pbetamargin <- function (q, lower, upper, a, b) {
+      q <- (q - lower) / (upper - lower)
+      pbeta(q, a, b)
+  }
R> qbetamargin <- function (p, lower, upper, a, b) {
+      q <- qbeta(p, a, b)
+      lower + q * (upper - lower)
+  }
```

The `CopulaMIMIC` class inherits methods for the generic functions that implement all the steps of the EDA except learning and sampling. To complete the implementation of the algorithm, we implement the estimation and simulation of the probabilistic model as methods for the generic functions `edaLearn` and `edaSample`, respectively.

The method for `edaLearn` starts with the estimation of the parameters of the marginal distributions and the transformation of the selected population to uniform variables in $(0, 1)$ by the evaluation of the marginal cumulative distribution functions. Then, the mutual information between all pairs of variables is calculated through the copula entropy (Davy and Doucet 2003). To accomplish this, the parameters of each possible bivariate copula should be estimated. The parameters of the copulas are estimated by the method of maximum likelihood. The value of the parameter obtained by the inversion of Kendall's tau is used as an initial approximation.

To determine the chain dependence structure learned by the algorithm, a permutation of the variables that maximizes the pairwise mutual information is selected. Because this is a computationally intensive task, a greedy algorithm is used to compute an approximate solution (De Bonet *et al.* 1997; Larrañaga *et al.* 1999).

Finally, the method for `edaLearn` returns a list with three components that represents the probabilistic model learned in the generation: the parameters of the marginal distributions,

the permutation of the variables and the copulas in the chain dependence structure.

```
R> edaLearnCopulaMIMIC <- function (eda, gen, previousModel,
+          selectedPop, selectedEval, lower, upper) {
+      margin <- eda@parameters$margin
+      copula <- eda@parameters$copula
+
+      if (is.null(margin)) margin <- "betamargin"
+      if (is.null(copula)) copula <- "normal"
+
+      fmargin <- get(paste("f", margin, sep = ""))
+      pmargin <- get(paste("p", margin, sep = ""))
+      copula <- switch(copula,
+          normal = normalCopula(0), frank = frankCopula(0))
+
+      n <- ncol(selectedPop)
+
+      # Estimate the parameters of the marginal distributions.
+      margins <- lapply(seq(length = n),
+          function (i) fmargin(selectedPop[ , i], lower[i], upper[i]))
+      uniformPop <- sapply(seq(length = n),
+          function (i) do.call(pmargin,
+              c(list(selectedPop[ , i]), margins[[i]])))
+
+      # Calculate pairwise mutual information by using copula entropy.
+      C <- matrix(list(NULL), nrow = n, ncol = n)
+      I <- matrix(0, nrow = n, ncol = n)
+      for (i in seq(from = 2, to = n)) {
+          for (j in seq(from = 1, to = i - 1)) {
+              # Estimate the parameters of the copula.
+              data <- cbind(uniformPop[ , i], uniformPop[ , j])
+              startCopula <- fitCopula(copula, data, method = "itau",
+                  estimate.variance = FALSE)@copula
+              C[[i, j]] <- tryCatch(
+                  fitCopula(startCopula, data, method = "ml",
+                      start = startCopula@parameters,
+                      estimate.variance = FALSE)@copula,
+                  error = function (error) startCopula)
+              # Calculate mutual information.
+              if (is(C[[i, j]], "normalCopula")) {
+                  I[i, j] <- -0.5 * log(1 - C[[i, j]]@parameters^2)
+              } else {
+                  u <- rcopula(C[[i, j]], 100)
+                  I[i, j] <- sum(log(dcopula(C[[i, j]], u))) / 100
+              }
+              C[[j, i]] <- C[[i, j]]; I[j, i] <- I[i, j]
+          }
```

```
+      }
+
+      # Pick a permutation of the variables.
+      perm <- as.vector(arrayInd(which.max(I), dim(I)))
+      copulas <- C[perm[1], perm[2]]
+      I[perm, ] <- -Inf
+      for (k in seq(length = n - 2)) {
+          ik <- which.max(I[ , perm[1]])
+          perm <- c(ik, perm)
+          copulas <- c(C[perm[1], perm[2]], copulas)
+          I[ik, ] <- -Inf
+      }
+
+      list(margins = margins, perm = perm, copulas = copulas)
+  }
R> setMethod("edaLearn", "CopulaMIMIC", edaLearnCopulaMIMIC)
```

The method for the `edaSample` generic function receives the representation of the probabilistic model returned by `edaLearn` as the `model` argument. The generation of a new solution with n variables starts with the simulation of an n-dimensional vector U having uniform marginal distributions in $(0, 1)$ and the dependence described by the copulas in the chain dependence structure.

The first step is to simulate an independent uniform variable U_{π_n} in $(0, 1)$, where π_n denotes the variable in the position n of the permutation π selected by the `edaLearn` method. The rest of the uniform variables are simulated conditionally on the previously simulated variable by using the conditional copula $C(U_{\pi_k}|U_{\pi_{k+1}})$, with $k = n-1, n-2, \ldots, 1$.

Finally, the new solution is determined through the evaluation of the beta quantile functions and the application of the inverse of the linear transformation. This procedure is repeated for each solution to be generated.

```
R> edaSampleCopulaMIMIC <- function (eda, gen, model, lower, upper) {
+      popSize <- eda@parameters$popSize
+      margin <- eda@parameters$margin
+
+      if (is.null(popSize)) popSize <- 100
+      if (is.null(margin)) margin <- "betamargin"
+
+      qmargin <- get(paste("q", margin, sep = ""))
+
+      n <- length(model$margins)
+      perm <- model$perm
+      copulas <- model$copulas
+
+      # Simulate the chain structure with the copulas.
+      uniformPop <- matrix(0, nrow = popSize, ncol = n)
+      uniformPop[ , perm[n]] <- runif(popSize)
```

```
+      for (k in seq(from = n - 1, to = 1)) {
+          u <- runif(popSize)
+          v <- uniformPop[ , perm[k + 1]]
+          uniformPop[ , perm[k]] <- hinverse(copulas[[k]], u, v)
+      }
+
+      # Evaluate the inverse of the marginal distributions.
+      pop <- sapply(seq(length = n),
+          function (i) do.call(qmargin,
+              c(list(uniformPop[ , i]), model$margins[[i]])))
+
+      pop
+ }
R> setMethod("edaSample", "CopulaMIMIC", edaSampleCopulaMIMIC)
```

The implementation of Copula MIMIC is now complete. As it was illustrated with GCEDA in the previous section, the algorithm can be executed by creating an instance of the `CopulaMIMIC` class and calling the `edaRun` function.

4.3. Performing an empirical study

Finally, we show how to use **copulaedas** to perform an empirical study of the behavior of a group of EDAs based on copulas on benchmark problems. The algorithms to be compared are UMDA, GCEDA, CVEDA, DVEDA and Copula MIMIC. The first three algorithms are included in **copulaedas** and the fourth algorithm was implemented in Section 4.2. All functions described at the beginning of Section 4 are considered as benchmark problems in 10 dimensions.

The aim of this empirical study is to assess the behavior of these algorithms when only linear and independence relationships are considered. Thus, only normal and product copulas are used in these EDAs. UMDA and GCEDA use multivariate product and normal copulas, respectively. CVEDA and DVEDA are configured to combine bivariate product and normal copulas in the vines. Copula MIMIC learns a chain dependence structure with normal copulas. All algorithms use normal marginal distributions. Note that in this case, GCEDA corresponds to EMNA and Copula MIMIC is similar to MIMIC for continuous domains.

In the following code fragment, we create class instances corresponding to the algorithms described in the previous paragraph.

```
R> umda <- CEDA(copula = "indep", margin = "norm")
R> umda@name <- "UMDA"
R> gceda <- CEDA(copula = "normal", margin = "norm")
R> gceda@name <- "GCEDA"
R> cveda <- VEDA(vine = "CVine", indepTestSigLevel = 0.01,
+      copulas = c("normal"), margin = "norm")
R> cveda@name <- "CVEDA"
R> dveda <- VEDA(vine = "DVine", indepTestSigLevel = 0.01,
+      copulas = c("normal"), margin = "norm")
R> dveda@name <- "DVEDA"
```

```
R> copulamimic <- CopulaMIMIC(copula = "normal", margin = "norm")
R> copulamimic@name <- "CopulaMIMIC"
```

The initial population is generated using the default method of the `edaSeed` generic function, therefore, it is sampled uniformly in the real interval of each variable. The lower and upper bounds of the variables are set so that the values of the variables in the optimum of the function are located in the middle of the interval. We use the intervals $[-600, 600]$ in Sphere and Griewank, $[-30, 30]$ in Ackley, $[-0.16, 0.16]$ in Summation Cancellation, $[-5.12, 5.12]$ in Rastrigin, and $[-9, 11]$ in Rosenbrock.

All algorithms use the default truncation selection method with a truncation factor of 0.3. Three termination criteria are combined using the `edaTerminateCombined` function: to find the global optimum of the function with a precision greater than 10^{-6}, to reach 300000 function evaluations or to loose diversity in the population, i.e., the standard deviation of the evaluation of the solutions in the population is less than 10^{-8}. These criteria are implemented in the functions `edaTerminateEval`, `edaTerminateMaxEvals` and `edaTerminateEvalStdDev`, respectively.

The population size of EDAs along with the truncation method determine the sample available for the estimation of the search distribution. An arbitrary selection of the population size could lead to misleading conclusions of the results of the experiments. When the population size is too small, the search distributions might not be accurately estimated. On the other hand, the use of an excessively large population size usually does not result in a better behavior of the algorithms but certainly in a greater number of function evaluations.

We advocate the use of the critical population size when comparing the performance of EDAs. The critical population size is the minimum population size required by the algorithm to find the global optimum of the function with a high success rate. To find the optimum of the function in 30 of 30 sequential independent runs can be generally considered a high success rate.

An approximate value of the critical population size can be determined empirically using a bisection method (see e.g., Pelikan 2005 for a pseudocode of the algorithm). The bisection method begins with an initial interval where the critical population size should be located and discards one half of the interval at each step. This procedure is implemented in the `edaCriticalPopSize` function. In the experimental study carried out in this section, the initial interval is $[50, 2000]$. If the critical population size is not found at this interval, the results of the algorithm with the population size determined by the upper bound are presented.

The complete empirical study consists of performing 30 independent runs of every algorithm on every function using the critical population size. We proceed with the definition of a list containing all algorithm-function pairs.

```
R> edas <- list(umda, gceda, cveda, dveda, copulamimic)
R> fNames <- c("Sphere", "Griewank", "Ackley", "SummationCancellation",
+     "Rastrigin", "Rosenbrock")
R> experiments <- list()
R> for (eda in edas) {
+     for (fName in fNames) {
+         experiment <- list(eda = eda, fName = fName)
+         experiments <- c(experiments, list(experiment))
```

```
+     }
+ }
```

Now we define a function to process the elements of the `experiments` list. This function implements all the experimental setup described before. The output of `edaCriticalPopSize` and `edaIndepRuns` is redirected to a different plain-text file for each algorithm-function pair.

```
R> runExperiment <- function (experiment) {
+     eda <- experiment$eda
+     fName <- experiment$fName
+
+     # Information of the objective function.
+     fInfo <- list(
+         Sphere = list(lower = -600, upper = 600, fEval = 0),
+         Griewank = list(lower = -600, upper = 600, fEval = 0),
+         Ackley = list(lower = -30, upper = 30, fEval = 0),
+         SummationCancellation = list(lower = -0.16, upper = 0.16,
+             fEval = -1e5),
+         Rastrigin = list(lower = -5.12, upper = 5.12, fEval = 0),
+         Rosenbrock = list(lower = -9, upper = 11, fEval = 0)
+     )
+     lower <- rep(fInfo[[fName]]$lower, 10)
+     upper <- rep(fInfo[[fName]]$upper, 10)
+     f <- get(paste("f", fName, sep = ""))
+
+     # Configure termination criteria.
+     eda@parameters$fEval <- fInfo[[fName]]$fEval
+     eda@parameters$fEvalTol <- 1e-6
+     eda@parameters$fEvalStdDev <- 1e-8
+     eda@parameters$maxEvals <- 300000
+     setMethod("edaTerminate", "EDA",
+         edaTerminateCombined(edaTerminateEval, edaTerminateMaxEvals,
+             edaTerminateEvalStdDev))
+
+     sink(paste(eda@name, "_", fName, ".txt", sep = ""))
+     # Determine the critical population size.
+     results <- edaCriticalPopSize(eda, f, lower, upper,
+         eda@parameters$fEval, eda@parameters$fEvalTol, lowerPop = 50,
+         upperPop = 2000, totalRuns = 30, successRuns = 30,
+         stopPercent = 10, verbose = TRUE)
+     if (is.null(results)) {
+         # Run the experiment with the largest population size, if the
+         # critical population size was not determined.
+         eda@parameters$popSize <- 2000
+         edaIndepRuns(eda, f, lower, upper, runs = 30, verbose = TRUE)
+     }
```

```
+      sink(NULL)
+  }
```

We can run all the experiments by calling `runExperiment` for each element of the list.

```
R> for (experiment in experiments) {
+      runExperiment(experiment)
+  }
```

Running the complete empirical study is a computationally demanding operation. If various processing units are available, it can be speeded up significantly by running the experiments in parallel. The **snow** package (Tierney *et al.* 2011) offers a great platform to achieve this purpose, since it provides a high-level interface for using a cluster of workstations for parallel computations in R. The functions `clusterApply` or `clusterApplyLB` can be used to call `runExperiment` for each element of the `experiments` list in parallel, with minor modifications to the code presented here.

A summary of the results of the algorithms in Sphere, Griewank, Ackley, Summation Cancellation, Rastrigin and Rosenbrock with the critical population size is shown in Tables 3, 4, 5, 6, 7 and 8, respectively. We conclude this section with an overview of the results, since a detailed analysis of the behavior of each algorithm is out of the scope of this paper.

All algorithms are able to find the global optimum of Sphere, Griewank, Ackley and Rastrigin and in the 30 independent runs with similar function values. Only GCEDA, CVEDA and DVEDA optimize Summation Cancellation and no algorithm is capable of optimizing Rosenbrock.

UMDA exhibits the best behavior in terms of the number of function evaluations in Sphere Griewank and Ackley. There are no strong dependences between the variables of these functions and it seems that the marginal information is enough to find the global optimum efficiently. The other algorithms require the calculation of a greater number of parameters to represent the relationships between the variables, hence larger populations are needed to compute them reliably. The requirement of larger population sizes results in a greater number of function evaluations. CVEDA and DVEDA do not assume a normal dependence structure between the variables and for this reason are less affected by this issue. The estimation procedure used by the vine-based algorithms selects the product copula if there is no enough evidence of dependence. This technique allows CVEDA and DVEDA to perform similarly to UMDA in these problems.

Both UMDA and Copula MIMIC fail to optimize Summation Cancellation. A correct representation of the strong linear interactions between the variables of this function appears to be essential to find the global optimum. UMDA completely ignores this information by assuming independence between the variables and it exhibits the worst behavior. Copula MIMIC reaches better fitness values than UMDA but neither can find the optimum of the function. The probabilistic model estimated by Copula MIMIC can not represent important dependences for the success of the optimization.

GCEDA, CVEDA and DVEDA do find the global optimum of Summation Cancellation. The correlation matrix estimated by GCEDA represents accurately the multivariate linear interactions between the variables. Thus, GCEDA has the best behavior in Summation Cancellation in terms of the number of function evaluations. The results of CVEDA closely

Algorithm	Success	Population	Evaluations	Best evaluation	CPU time
UMDA	30/30	81	3823.2	6.9e − 07	0.4
			±128.3	±2.3e − 07	±0.0
GCEDA	30/30	310	13082.0	6.5e − 07	0.9
			±221.4	±2.0e − 07	±0.0
CVEDA	30/30	104	4777.0	6.7e − 07	8.3
			±118.8	±1.8e − 07	±1.5
DVEDA	30/30	104	4787.4	6.7e − 07	8.2
			±100.2	±2.0e − 07	±1.1
Copula MIMIC	30/30	150	6495.0	6.9e − 07	468.8
			±209.0	±1.7e − 07	±62.9

Table 3: Results of 30 independent runs of UMDA, GCEDA, CVEDA, DVEDA and Copula MIMIC in the 10-dimensional Sphere problem with the critical population size.

Algorithm	Success	Population	Evaluations	Best evaluation	CPU time
UMDA	30/30	111	5224.4	6.6e − 07	0.5
			±231.2	±1.9e − 07	±0.0
GCEDA	30/30	355	15099.3	6.9e − 07	1.2
			±414.1	±1.8e − 07	±0.0
CVEDA	30/30	142	6579.3	7.0e − 07	9.3
			±389.9	±1.8e − 07	±2.0
DVEDA	30/30	150	6785.0	6.5e − 07	9.5
			±338.1	±2.4e − 07	±1.9
Copula MIMIC	30/30	188	8221.8	6.6e − 07	595.7
			±220.4	±1.8e − 07	±91.6

Table 4: Results of 30 independent runs of UMDA, GCEDA, CVEDA, DVEDA and Copula MIMIC in the 10-dimensional Griewank problem with the critical population size.

follow the ones of GCEDA and the latter has much better results than DVEDA. A C-vine provides a more appropriate modeling of the dependence structure between the variables of Summation Cancellation than a D-vine, since it is possible to find a variable that governs the interactions in the sample (González-Fernández 2011).

Rastrigin is not considered a problem where the interactions between the variables play an important role for the success of the optimization. It is often only used to assess the effect of multimodality. In spite of this, Rastrigin provides interesting results about dependence modeling in EDAs.

All the studied algorithms find the global optimum of Rastrigin, but not all require the same number of function evaluations. Neither assuming independence between all pairs of variables nor considering a multivariate linear dependence structure lead to the best results. The approach of DVEDA, that lies in the middle, performs better. DVEDA constructs a probabilistic model that uses bivariate normal copulas if the dependence is strong and product copulas in the other case. In Rastrigin, the combination of normal and product copulas in a single probabilistic model is better than assuming independence or a multivariate linear dependence structure.

Algorithm	Success	Population	Evaluations	Best evaluation	CPU time
UMDA	30/30	81	4997.7	8.1e − 07	0.6
			±88.0	±1.1e − 07	±0.0
GCEDA	30/30	279	15633.3	8.3e − 07	1.6
			±258.8	±1.1e − 07	±0.0
CVEDA	30/30	104	6330.1	8.1e − 07	10.6
			±163.2	±1.0e − 07	±1.8
DVEDA	30/30	111	6678.5	7.9e − 07	11.4
			±133.8	±1.4e − 07	±1.6
Copula MIMIC	30/30	188	10784.9	8.0e − 07	800.1
			±143.7	±1.2e − 07	±122.1

Table 5: Results of 30 independent runs of UMDA, GCEDA, CVEDA, DVEDA and Copula MIMIC in the 10-dimensional Ackley problem with the critical population size.

Algorithm	Success	Population	Evaluations	Best evaluation	CPU time
UMDA	0/30	2000	300000.0	−5.7e + 02	66.8
			±0.0	±3.4e + 02	±0.7
GCEDA	30/30	355	42434.3	−1.0e + 05	9.3
			±305.4	±1.3e − 07	±0.4
CVEDA	30/30	325	44622.5	−1.0e + 05	537.2
			±858.3	±1.3e − 07	±6.6
DVEDA	30/30	965	117408.3	−1.0e + 05	2367.3
			±959.4	±9.3e − 08	±20.0
Copula MIMIC	0/30	2000	300000.0	−2.3e + 04	10426.1
			±0.0	±2.7e + 04	±1054.3

Table 6: Results of 30 independent runs of UMDA, GCEDA, CVEDA, DVEDA and Copula MIMIC in the 10-dimensional Summation Cancellation problem with the critical population size.

Algorithm	Success	Population	Evaluations	Best evaluation	CPU time
UMDA	30/30	447	33614.4	6.7e − 07	1.7
			±2452.2	±2.3e − 07	±0.1
GCEDA	30/30	721	46095.9	6.8e − 07	2.8
			±2158.2	±1.8e − 07	±0.1
CVEDA	30/30	447	32914.1	6.6e − 07	44.8
			±2011.0	±1.7e − 07	±13.3
DVEDA	30/30	325	24710.8	7.3e − 07	31.3
			±1754.3	±1.7e − 07	±6.9
Copula MIMIC	30/30	386	27315.9	6.4e − 07	1431.7
			±1673.9	±2.1e − 07	±218.6

Table 7: Results of 30 independent runs of UMDA, GCEDA, CVEDA, DVEDA and Copula MIMIC in the 10-dimensional Rastrigin problem with the critical population size.

Algorithm	Success	Population	Evaluations	Best evaluation	CPU time
UMDA	0/30	2000	300000.0	8.0e + 00	72.0
			±0.0	±2.6e − 02	±0.1
GCEDA	0/30	2000	300000.0	7.5e + 00	74.3
			±0.0	±1.9e − 01	±0.4
CVEDA	0/30	2000	193866.6	7.5e + 00	1278.9
			±48243.4	±1.1e − 01	±532.0
DVEDA	0/30	2000	172200.0	7.5e + 00	961.4
			±35183.6	±1.5e − 01	±386.9
Copula MIMIC	0/30	2000	139000.0	7.6e + 00	6173.5
			±5139.4	±1.3e − 01	±820.5

Table 8: Results of 30 independent runs of UMDA, GCEDA, CVEDA, DVEDA and Copula MIMIC in the 10-dimensional Rosenbrock problem with the critical population size.

The chain dependence structure learned by Copula MIMIC is similar to a D-vine that only uses normal copulas in the first tree. This is why, Copula MIMIC also combines normal and product copulas, and attains the second best results in Rastrigin according to the number of function evaluations.

The results of CVEDA in Rastrigin are different than the ones of DVEDA. The model used by DVEDA allows a freer selection of the bivariate dependences that will be explicitly modeled, while the model used by CVEDA has a more restrictive structure. These characteristics prevent CVEDA from discovering the bivariate dependences DVEDA finds and its results are similar to the ones of UMDA.

Rosenbrock is generally recognized as a difficult problem for numerical optimization algorithms. Its global optimum is located inside a parabolic shaped flat region. It seems to be easy for algorithms to find the flat region, but convergence to the global optimum is difficult. This function presents nonlinear and even nonmonotone dependences between the variables. The normal copula can not account for this type of dependence and therefore the relationships between the variables are not properly represented. However, the algorithms that consider dependences find slightly better solutions than UMDA. A more appropriate representation of the relationships between the variables of the function might improve the behavior of copula-based EDAs in this problem.

The running time of Copula MIMIC is considerably greater than the running time of the other algorithms in all functions. This situation is due to the use of a numerical optimization algorithm for the estimation of the parameters of the copulas by maximum likelihood. In the context of EDAs, where copulas are fitted at every generation, the computational effort required to estimate the parameters of the copulas becomes an important issue. As was illustrated with the behavior of CVEDA and DVEDA, using the inversion of Kendall's tau is a viable alternative to maximum likelihood that requires much less CPU time.

The empirical investigation confirms the robustness of CVEDA and DVEDA in both weakly strongly and correlated problems. Nonetheless, the flexibility afforded by these algorithms comes with an increased running time when compared to UMDA or GCEDA, since the interactions between the variables have to be discovered during the learning step.

A general result of this empirical study is that copula-based EDAs should use copulas other

than the product only when there is evidence of dependence in the sample of the selected population. Otherwise, the EDA will require larger populations and hence a greater number of function evaluations to accurately determine the values of the parameters of the copulas that correspond to independence.

5. Concluding remarks

We have developed **copulaedas** aiming to provide in a single package not only publicly available implementations of EDAs based on copulas but also utility functions to study these algorithms. In this paper, we illustrate how to run the copula-based EDAs implemented in the package, how to implement new algorithms and how to perform an empirical study to compare a group of EDAs. We hope that these functionalities help the research community to improve EDAs based on copulas by getting a better insight of their strengths and weaknesses and also help practitioners to find new applications of these algorithms to real-world problems.

References

Aas K, Czado C, Frigessi A, Bakken H (2009). "Pair-Copula Constructions of Multiple Dependence." *Insurance: Mathematics and Economics*, **44**(2), 182–198.

Akaike H (1974). "A New Look at Statistical Model Identification." *IEEE Transactions on Automatic Control*, **19**, 716–723.

Arderí RJ (2007). *Algoritmo con estimación de distribuciones con cópula gaussiana*. Bachelor thesis, University of Havana, Cuba.

Azzalini A (1981). "A Note on the Estimation of a Distribution Function and Quantiles by a Kernel Method." *Biometrika*, **68**(1), 326–328.

Baluja S (1994). "Population-Based Incremental Learning: A Method for Integrating Genetic Search Based Function Optimization and Competitive Learning." *Technical Report CMU-CS-94-163*, Carnegie Mellon University, USA.

Barba-Moreno S (2007). *Una propuesta para algoritmos de estimación de distribución no paramétricos*. Master's thesis, Center for Research in Mathematics, Mexico.

Bedford T, Cooke RM (2001). "Probability Density Decomposition for Conditionally Dependent Random Variables Modeled by Vines." *Annals of Mathematics and Artificial Intelligence*, **32**(1), 245–268.

Bengoetxea E, Miquélez T, Lozano JA, Larrañaga P (2002). "Experimental Results in Function Optimization with EDAs in Continuous Domain." In P Larrañaga, JA Lozano (eds.), *Estimation of Distribution Algorithms. A New Tool for Evolutionary Computation*, pp. 181–194. Kluwer Academic Publisher.

Berg D, Aas K (2007). "Models for Construction of Multivariate Dependence." *Note SAMBA/23/07*, Norwegian Computing Center, NR, Norway.

Bosman PAN, Thierens D (2006). "Numerical Optimization with Real-Valued Estimation of Distribution Algorithms." In M Pelikan, K Sastry, E Cantú-Paz (eds.), *Scalable Optimization via Probabilistic Modeling. From Algorithms to Applications*, pp. 91–120. Springer-Verlag.

Brechmann EC (2010). *Truncated and Simplified Regular Vines and Their Applications*. Diploma thesis, University of Technology, Munich, Germany.

Chambers J (2008). *Software for Data Analysis: Programming with R*. Springer-Verlag. ISBN 978-0-387-75935-7.

Chen Yp, Lim MH (eds.) (2008). *Linkage in Evolutionary Computation*. Springer-Verlag. ISBN 978-3-540-85067-0.

Cuesta-Infante A, Santana R, Hidalgo JI, Bielza C, Larrañaga P (2010). "Bivariate Empirical and n-variate Archimedean Copulas in Estimation of Distribution Algorithms." In *Proceedings of the IEEE Congress on Evolutionary Computation (CEC 2010)*, pp. 1355–1362.

Davy M, Doucet A (2003). "Copulas: A New Insight Into Positive Time-Frequency Distributions." *IEEE Signal Processing Letters*, **10**(7), 215–218.

De Bonet JS, Isbell CL, Viola P (1997). "MIMIC: Finding Optima by Estimating Probability Densities." In M Mozer, M Jordan, T Petsche (eds.), *Advances in Neural Information Processing Systems*, volume 9, pp. 424–430. The MIT Press.

Demarta S, McNeil AJ (2005). "The t Copula and Related Copulas." *International Statistical Review*, **73**(1), 111–129.

Devroye L (1986). *Non-Uniform Random Variate Generation*. Springer-Verlag. ISBN 0-387-96305-7.

Gao Y (2009). "Multivariate Estimation of Distribution Algorithm with Laplace Transform Archimedean Copula." In W Hu, X Li (eds.), *Proceedings of the International Conference on Information Engineering and Computer Science (ICIECS 2009)*.

Genest C, Quessy JF, Rémillard B (2007). "Asymptotic Local Efficiency of Cramér-von Mises Tests for Multivariate Independence." *The Annals of Statistics*, **35**, 166–191.

Genest C, Rémillard B (2004). "Tests of Independence or Randomness Based on the Empirical Copula Process." *Test*, **13**(2), 335–369.

Genest C, Rémillard B (2008). "Validity of the Parametric Bootstrap for Goodness-of-Fit Testing in Semiparametric Models." *Annales de l'Institut Henri Poincaré: Probabilités et Statistiques*, **44**, 1096–1127.

González-Fernández Y (2011). *Algoritmos con estimación de distribuciones basados en cópulas y vines*. Bachelor thesis, University of Havana, Cuba.

González-Fernández Y, Soto M (2011a). ***copulaedas**: Estimation of Distribution Algorithms Based on Copulas*. R package version 1.1.0, URL http://CRAN.R-project.org/package=copulaedas.

González-Fernández Y, Soto M (2011b). ***vines**: Multivariate Dependence Modeling with Vines*. R package version 1.0.3, URL http://CRAN.R-project.org/package=vines.

Hauschild M, Pelikan M (2011). "An Introduction and Survey of Estimation of Distribution Algorithms." *Swarm and Evolutionary Computation*, **1**, 111–128.

Hering C, Hofert M, Mai JF, Scherer M (2010). "Constructing Hierarchical Archimedean Copulas with Lévy Subordinators." *Journal of Multivariate Analysis*, **101**, 1428–1433.

Joe H (1996). "Families of m-variate Distributions with Given Margins and $m(m-1)/2$ Bivariate Dependence Parameters." In L Rüschendorf, B Schweizer, MD Taylor (eds.), *Distributions with fixed marginals and related topics*, pp. 120–141.

Joe H (1997). *Multivariate Models and Dependence Concepts*. Chapman & Hall.

Kern S, Müller SD, Hansen N, Büche D, Ocenasek J, Koumoutsakos P (2003). "Learning Probability Distributions in Continuous Evolutionary Algorithms – A Comparative Review." *Natural Computing*, **3**, 77–112.

Kojadinovic I, Yan J (2010). "Modeling Multivariate Distributions with Continuous Margins Using the **copula** R Package." *Journal of Statistical Software*, **34**(9), 1–20. URL http://www.jstatsoft.org/v34/i09/.

Larrañaga P, Etxeberria R, Lozano JA, Peña JM (1999). "Optimization by Learning and Simulation of Bayesian and Gaussian Networks." *Technical Report EHU-KZAA-IK-4/99*, University of the Basque Country.

Larrañaga P, Etxeberria R, Lozano JA, Peña JM (2000). "Optimization in Continuous Domains by Learning and Simulation of Gaussian Networks." In *Proceedings of the Workshop in Optimization by Building and Using Probabilistic Models in the Genetic and Evolutionary Computation Conference (GECCO 2000)*, pp. 201–204.

Larrañaga P, Lozano JA (eds.) (2002). *Estimation of Distribution Algorithms. A New Tool for Evolutionary Computation*. Kluwer Academic Publisher.

Larrañaga P, Lozano JA, Bengoetxea E (2001). "Estimation of Distribution Algorithms Based on Multivariate Normal and Gaussian Networks." *Technical Report EHU-KZAA-IK-1/01*, University of the Basque Country.

McNeil AJ (2008). "Sampling Nested Archimedean Copulas." *Journal of Statistical Computation and Simulation*, **78**(6), 567–581.

Mühlenbein H, Paaß G (1996). "From Recombination of Genes to the Estimation of Distributions I. Binary Parameters." In *Parallel Problem Solving from Nature — PPSN IV*, pp. 178–187. Springer-Verlag.

Nelsen RB (2006). *An Introduction to Copulas*. 2 edition. Springer-Verlag. ISBN 978-0387-28659-4.

Pelikan M (2005). *Hierarchical Bayesian Optimization Algorithm. Toward a New Generation of Evolutionary Algorithms*. Springer-Verlag.

Pelikan M, Goldberg DE, Lobo F (2002). "A Survey of Optimization by Building and Using Probabilistic Models." *Computational Optimization and Applications*, **21**, 5–20.

R Development Core Team (2011). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria. ISBN 3-900051-07-0, URL http://www.R-project.org/.

Rosenkrantz DJ, Stearns RE, Lewis II PM (1977). "An Analysis of Several Heuristics for the Traveling Salesman Problem." *SIAM Journal on Computing*, **6**(3), 563–581.

Rousseeuw P, Molenberghs G (1993). "Transformation of Nonpositive Semidefinite Correlation Matrices." *Communications in Statistics: Theory and Methods*, **22**, 965–984.

Salinas-Gutiérrez R, Hernández-Aguirre A, Villa-Diharce E (2009). "Using Copulas in Estimation of Distribution Algorithms." In *Proceedings of the Eight Mexican International Conference on Artificial Intelligence (MICAI 2009)*, pp. 658–668.

Salinas-Gutiérrez R, Hernández-Aguirre A, Villa-Diharce E (2010). "D-vine EDA: A New Estimation of Distribution Algorithm Based on Regular Vines." In *Proceedings of the Genetic and Evolutionary Computation Conference (GECCO 2010)*, pp. 359–365.

Salinas-Gutiérrez R, Hernández-Aguirre A, Villa-Diharce E (2011). "Dependence Trees with Copula Selection for Continuous Estimation of Distribution Algorithms." In *Proceedings of the Genetic and Evolutionary Computation Conference (GECCO 2011)*, pp. 585–592.

Santana R, Bielza C, Larrañaga P, Lozano JA, Echegoyen C, Mendiburu A, Armañanzas R, Shakya S (2010). "**Mateda-2.0**: A MATLAB Package For the Implementation and Analysis of Estimation of Distribution Algorithms." *Journal of Statistical Software*, **35**(7), 1–30. URL http://www.jstatsoft.org/v35/i07/.

Schwarz G (1978). "Estimating the Dimension of a Model." *The Annals of Statistics*, **6**, 461–464.

Silverman BW (1986). *Density Estimation for Statistics and Data Analysis*. Chapman & Hall.

Sklar A (1959). "Fonctions de répartition à n dimensions et leurs marges." *Publications de l'Institut de Statistique de l'Université de Paris*, **8**, 229–231.

Soto M, González-Fernández Y (2010). "Vine Estimation of Distribution Algorithms." *Technical Report ICIMAF 2010-561*, Institute of Cybernetics, Mathematics and Physics, Cuba. ISSN 0138-8916.

Soto M, Ochoa A, Arderí RJ (2007). "Gaussian Copula Estimation of Distribution Algorithm." *Technical Report ICIMAF 2007-406*, Institute of Cybernetics, Mathematics and Physics, Cuba. ISSN 0138-8916.

Soto M, Ochoa A, González-Fernández Y, Milanés Y, Álvarez A, Carrera D, Moreno E (2012). "Vine Estimation of Distribution Algorithms with Application to Molecular Docking." In S Shakya, R Santana (eds.), *Markov Networks in Evolutionary Computation*, volume 14 of *Adaptation, Learning, and Optimization*, pp. 209–225. Springer-Verlag. ISBN 978-3-642-28899-9.

Tierney L, Rossini AJ, Li N, Sevcikova H (2011). ***snow***: *Simple Network of Workstations*. R package version 0.3-6, URL http://CRAN.R-project.org/package=snow.

Wang L, Zeng J, Hong Y (2009a). "Estimation of Distribution Algorithm Based on Archimedean copulas." In *Proceedings of the first ACM/SIGEVO Summit on Genetic and Evolutionary Computation (GEC 2009)*, pp. 993–996.

Wang L, Zeng J, Hong Y (2009b). "Estimation of Distribution Algorithm Based on Copula Theory." In *Proceedings of the IEEE Congress on Evolutionary Computation (CEC 2009)*, pp. 1057–1063.

Ye B, Gao H, Wang X, Zeng J (2010). "Estimation of Distribution Algorithm Based on Nested Archimedean Copulas Constructed with Lévy Subordinators." In *Proceedings of the Eleventh International Conference on Computer-Aided Industrial Design & Conceptual Design (CAIDCD 2010)*, pp. 1586–1590.

Affiliation:

Yasser González-Fernández
Institute of Cybernetics, Mathematics and Physics
Calle 15 No. 551 e/ C y D, Vedado. La Habana, Cuba.
E-mail: ygonzalezfernandez@gmail.com

Marta Soto
Institute of Cybernetics, Mathematics and Physics
Calle 15 No. 551 e/ C y D, Vedado. La Habana, Cuba.
E-mail: mrosa@icimaf.cu