Elliptical and Archimedean Copulas in Estimation of Distribution Algorithm with Model Migration

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Abstract: Estimation of distribution algorithms (EDAs) are stochastic optimization techniques that are based on building and sampling a probability model. Copula theory provides methods that simplify the estimation of a probability model. An island-based version of copula-based EDA with probabilistic model migration (mCEDA) was tested on a set of well-known standard optimization benchmarks in the continuous domain. We investigated two families of copulas – Archimedean and elliptical. Experimental results confirm that this concept of model migration (mCEDA) yields better convergence as compared with the sequential version (sCEDA) and other recently published copula-based EDAs.

1 INTRODUCTION

Estimation of distribution algorithms (EDAs) belong to a new class of evolutionary optimization methods that explore the search space by estimating and sampling an explicit probabilistic model of promising solutions. EDAs applied to discrete problems are described in the well-known papers UMDA (Pélikan and Mühlenbein, 1999b), BMDA (Pélikan and Mühlenbein, 1999a), MIMIC (De Bonet et al., 1997), and BOA (Pélikan et al., 1999). Solutions of the optimization problems in the real value domain can be found in (Larrañaga and Lozano, 2001). A very modern and accessible survey of the EDAs algorithm is presented in (Hauschild and Pelikan, 2011).

The main advantage of EDAs is its capacity to discover those variable linkages that yield a solution to a complex optimization problem. On the one hand this probability model-based approach has allowed EDAs to be applied to large and complex problems. On the other hand explicit probabilistic models are very time consuming. That was the reason for implementing various advanced EDAs to solve this problem. The well-known enhancement approaches include the parallelization of model building and sporadic model building (Hauschild and Pelikan, 2011).

In the last ten years a new approach has appeared to building an efficient probabilistic model that is based on copula theory (Mai and Scherer, 2012). Copulas are special probability distribution functions. Due to their properties it is possible to use them to model correlations within multivariate problems – the joint distribution is separated into the univariate marginal distributions and into the correlation structure that is expressed by the copula function. Copula theory has very often been used in finance and statistics works (Nelsen, 2006; Cherubini et al., 2004; Aas et al., 2009) (e.g. modeling health insurance data (Zimmer and Trivedi, 2006)).

Recently copulas have been utilized in the field of the machine learning (Rey and Roth, 2012; Póczos et al., 2012). More recently the copula theory has been applied to EDA probability models. The simplest case is the application with bivariate (2D) copulas: (Wang et al., 2009) – 2D Gaussian copula EDA, (Wang et al., 2010b) – 2D Clayton copula EDA, (Wang et al., 2010a) – 2D Gumbel copula EDA.

In the case of multivariate models bivariate copulas are used as local building blocks in various graph dependence structures: (Salinas-Gutiérrez et al., 2009) – MIMIC + Frank and Gaussian copula, (Méndez and Landa, 2012) – Bayesian network + Archimedean copulas, (Salinas-Gutiérrez et al., 2011) – D-vine + copulas, (Soto et al., 2012) – C-vine, D-vine + copulas.

The copula-based EDA starts with an estimation of the marginal distribution of each variable, then using a proper copula, the joint distribution is established. Given the margins and a copula, it is then possible to generate new solutions.
This paper deals with an efficient parallelization of island-based mCEDA with the goal to increase the convergence speed. After some experiments we chose the island-based structure with bidirectional ring topology. Instead of the often used migration of individuals we instantiated the migration of probability models. Note that the first experiments with this new concept were published in (delaOssa et al., 2004; Schwarz and Jaros, 2008) for the optimization in the discrete domain, the chief obstacle being an efficient combination of the probabilistic models, especially those having the dependence structure expressed by a graph. That is why we focused on the migration of probabilistic model parameters only.

The paper is organized as follows. In Section 2, the basis of copula theory is given. In Section 3, the utilization of copulas in EDA is described, and sampling algorithms for copulas are presented. In Section 4, the island-based model of evolution algorithm with copula-model migration is described. Our experiments are discussed in Section 5. The conclusions are given in Section 6.

2 COPULA THEORY

The copula concept was introduced by (Sklar, 1959) in order to separate the effect of dependence of variables from the effect of marginal distributions in a joint distribution. A copula is a function which joins the univariate distribution function and creates multivariate distribution functions. This approach allows us to transform multivariate statistic problems into the univariate problems with the relation represented by just the copula.

**Definition.** A copula $C$ is a multivariate probability distribution function for which the marginal probability distribution of each variable is uniform in $[0,1]$.

**Definition.** A copula is a function $C: [0,1]^d \to [0,1]$ with the following properties:

1. $C(u_1, u_2, \ldots, u_d) = 0$ for at least one $u_i = 0$
2. $C(1, 1, \ldots, 1, u_i, 1, \ldots, 1) = u_i$ for all $i = 1, 2, \ldots, d$
3. $C(u_1, u_2, \ldots, u_d)$ is $d$-increasing (see lit. for details)

**Theorem.** Sklar’s theorem: Let $F$ be a $d$-dimensional distribution function with margins $F_1, \ldots, F_d$. Then there exists a $d$-dimensional copula $C$ such that for all $(x_1, \ldots, x_d) \in \mathbb{R}^d$ it holds that

$$F(x_1, \ldots, x_d) = C(F_1(x_1), \ldots, F_d(x_d))$$

(1)

If $F_1, \ldots, F_d$ are continuous, then $C$ is unique. Conversely, if $C$ is a $d$-dimensional copula and $F_1, \ldots, F_d$ are univariate distribution functions, then the function $F$ defined via (1) is a $d$-dimensional distribution function.

In this paper we focus on two big copula families – Archimedean and elliptic.

Archimedean copulas are capable of capturing wide ranges of dependence. The definition of the Archimedean copula is based on the generator function. There are many existing Archimedean copulas and many more that could be created. The three copulas, i.e. Clayton, Gumbel and Frank appear regularly in statistics literature, they are popular because they model different patterns of dependence and have a relatively simple functional form. Fig. 1 shows scatterplots of these copulas.

The elliptical copulas are derived from the related elliptical distribution. The first example of elliptical copula is the Gaussian copula, which belongs to the normal distribution, the second example is the Student copula, which belongs to the t-distribution (see Fig. 2).
3 COPULA-BASED ESTIMATION OF DISTRIBUTION ALGORITHM

Estimation of distribution algorithms belongs to the advanced evolutionary algorithms. Solving the numerical optimization problem, vector \( \mathbf{x} = (x_1, \ldots, x_d) \) of the optimal solution is searched out.

The core of the canonical EDA consists of three main steps, see Algorithm 1.

Algorithm 1 The pseudocode of canonical EDA.

\[
\text{Generate initial population.}
\]

\[\text{WHILE} \quad (\text{termination criteria is false)}:\]

\[1. \text{ Select promising solutions into subpopulation from the current population.}\]

\[2. \text{ Create the probability model from the selected subpopulation.}\]

\[3. \text{ Sample the probability model and generate the new population.}\]

Step 1 is quite straightforward, the promising solutions are stated using the standard selection truncation. In the case of copula-based EDA it is necessary to choose the proper type of copula and derive the copula parameters and the marginal distribution parameters.

The principle of sampling schema for generating the new individuals using the copula model is described in Algorithm 2:

Algorithm 2 Sampling the copula and generating the new individuals.

\[1. \text{ Obtain the random copula sample } (u_1, \ldots, u_d) \sim C, \text{ where } u_i \in [0; 1].\]

\[2. \text{ Derive the vector } \mathbf{x} \text{ of the searched solution using inverse marginal distributions, } x_i = F_i^{-1}(u_i).\]

3.1 Identification of copula probability model

The copula-based probability model includes two parts: univariate marginal distributions and the copula function. Marginal distributions can be identified separately for each variable and the copula includes the correlation between variables.

For marginal distribution in each dimension \( i = 1, \ldots, d \) we used normal distribution, which is parameterized by the mean value \( \mu_i \) and standard deviation \( \sigma_i \).

For assessing the parameters of the copula we used the Kendall \( \tau \) correlation coefficient.

In the case of Archimedean copulas the following relations hold for the parameter \( \theta \) (in the case of \( d \)-variate copulas, \( d \geq 3 \), we use average \( \tau \); for \( d = 2 \) the standard pairwise \( \tau \) is used):

- for the Clayton copula \( \theta_{\text{Clayton}} = \frac{2\tau}{\tau - 1} \).
- for the Gumbel copula \( \theta_{\text{Gumbel}} = \frac{1}{1 - \tau} \).
- for the Frank copula (approximation) \( \theta_{\text{Frank}} \approx \frac{1}{\log(\tau - 1)} e \).

Elliptical copulas are parameterized by correlation matrix \( R \). Elements \( R_{ij} \) are adapted from Kendall’s \( \tau \) for each pair of dimensions \( i, j \) using formula \( R_{ij} = \sin \frac{1}{2} \pi \tau_{ij} \).

3.2 Copula sampling algorithms

Now we specify step 1 from Alg. 2 for each type of copulas in more details.

The algorithm for sampling Archimedean copulas uses a random value \( J \), which is obtained from the distribution given by the inverse of Laplace transform \( L^{-1} \) of generator (Mai and Scherer, 2012; Aas, 2004; Melchiori, 2006), see Alg. 3.

Algorithm 3 Archimedean copula sampling.

\[1. \text{ generate value } J \sim L^{-1}[\phi(t)]\]

\[2. \text{ generate uniformly distributed random numbers } z_i \sim U(0, 1) \quad (\text{for } i = 1, \ldots, d)\]

\[3. \text{ return } u_i = \phi \left( \frac{-\log(z_i)}{J} \right) \quad (\text{for } i = 1, \ldots, d)\]

According to (Aas, 2004; Melchiori, 2006) the value of \( J \) can be derived:

- for the Clayton copula by Gamma distribution \( J \sim \text{Gamma} \left( \frac{d}{2}, \theta \right) \).
- for the Gumbel copula by Levy skew alpha-Stable distribution \( J \sim \text{Stable} \left( \frac{d}{2}, 1, (\cos \frac{\pi}{2d})^{\theta}, 0 \right) \).
- for the Frank copula by logarithmic series distribution \( J \sim \text{Logarithmic} \left( 1 - e^{-\theta} \right) \).

The sampling scheme for Gaussian and Student copulas (Mai and Scherer, 2012) (see Alg. 4, 5) uses the Cholesky decomposition of the given correlation matrix \( R \) to obtain the lower triangular matrix \( L \). The Student copula is further specified by degrees of freedom, we use \( v = (N - 1)d \) (where \( N \) is population size and \( d \) number of dimensions).
Algorithm 4 Gaussian copula sampling
1. compute $L$
2. generate random numbers $z_i \sim N(0,1)$ with standard normal distribution (for $i = 1, \ldots, d$)
3. calculate $s_i = \sum_{j=1}^{i} L_{i,j} z_j$ (for $i = 1, \ldots, d$)
4. return $u_i = \Phi(s_i)$ (for $i = 1, \ldots, d$)

Algorithm 5 Student copula sampling
1. compute $L$
2. generate $V \sim \chi^2(v)$
3. generate random numbers $z_i \sim N(0,1)$ with standard normal distribution (for $i = 1, \ldots, d$)
4. calculate $s_i = \sqrt{v} \sum_{j=1}^{i} L_{i,j} z_j$ (for $i = 1, \ldots, d$)
5. return $u_i = t_v(s_i)$ (for $i = 1, \ldots, d$)

4 ISLAND-BASED COPULA-EDA

The principal motivation for the proposal of a concept of copula-based EDA parallelization is to discover the efficiency of the transfer of probabilistic parameters instead of the traditional transfer of individuals. The main goal is to improve algorithm convergence. In the case of EDAs only a few papers deal with the discrete probability model migration ( delaOssa et al., 2004; delaOssa et al., 2005) and (Hyrš and Schwarz, 2014) in the case of copula-based EDA.

4.1 EDA with migration

With the concordance of experimental work done in (Schwarz and Jaroš, 2008), and according to our experimental results, we used the island-based communication model with bidirectional ring topology. This topology provides good local interaction and in a few steps allows the propagation of information along the ring.

The evolution process on every island runs independently. When the migration condition is met the communication (transfer of model parameters) is activated, see Alg. 6.

4.2 Model combination

According to the island-based topology we have decomposed the migration process into pairwise interactions of two islands – one of them is the resident island specified by resident probabilistic model $M_R$ and the other one is the immigrant island whose probabilistic model $M_I$ is transferred to a new resident model.

The combination of the immigrant model with the model of the resident island is described in more details. In general, the modification of the resident model by the immigrant model can be formalized by (Schwarz and Jaroš, 2008):

$$M_R^\text{new} = (1 - \beta) M_R + \beta M_I$$ (2)

where the coefficient $\beta \in [0;1]$ specifies the influence of the immigrant model.

We have proposed the following model combination rules according to (Frühwirth-Schnatter, 2006):

- Learning the mean value $\mu_i$ of each univariate marginal distribution $F_i(x_i)$
  $$\mu_i^\text{new} = (1 - \beta) \mu_i^R + \beta \mu_i^I$$ (3)

- Learning the standard deviation $\sigma_i$ of each univariate marginal distribution $F_i(x_i)$
  $$\sigma_i^\text{new} = \sqrt{(1 - \beta) \left( (\mu_i^\text{new} - \mu_i^R)^2 + (\sigma_i^R)^2 \right) + \beta \left( (\mu_i^\text{new} - \mu_i^I)^2 + (\sigma_i^I)^2 \right) }$$ (4)

- Learning the correlation matrix value $R_{ij}$
  $$R_{ij}^\text{new} = (1 - \beta) R_{ij}^R + \beta R_{ij}^I$$ (5)

We have chosen the coefficient $\beta$ as

$$\beta = \begin{cases} \frac{f_{it}^R}{f_{it}^R + f_{it}^I} & f_{it}^R \leq f_{it}^I \\ 0.1 & \text{otherwise} \end{cases}$$ (6)

where $f_{it}^R$ or $f_{it}^I$ represents the fitness value of the resident or the immigrant model.
5 EXPERIMENT AND RESULTS

We used standard benchmark problems to compare island-based copula-EDA (mCEDA) with the sequential one (sCEDA).

5.1 Benchmarks

The shifted variants of several well-known benchmarks from the area of numerical optimization are used. All these functions have been adapted such that the task is minimization with optimal fitness value 0 and with shifted optima position.

- **Elliptic Function:**
  \[ f(x) = \sum_{i=1}^{d} \left(10^6 \frac{x_i}{\pi} \right)^{2/5} + 100; x_i \in [-100; 100] \]

- **Rastrigin’s Function:**
  \[ f(x) = \sum_{i=1}^{d} (x_i^2 - 10 \cos(2\pi x_i) + 10), x_i \in [-5; 5] \]

- **Ackley’s Function:**
  \[ f(x) = -20 e^{-0.2 \sqrt{\frac{1}{d} \sum_{i=1}^{d} x_i^2}} - e^{\frac{1}{d} \sum_{i=1}^{d} \cos(2\pi x_i)} + 20 + e, \quad x_i \in [-32; 32] \]

- **Schwefel’s Problem 1.2:**
  \[ f(x) = \sum_{i=1}^{d} x_i \left(\sum_{j=1}^{d} x_j \right)^2, \quad x_i \in [-100; 100] \]

- **Rosenbrock’s Function:**
  \[ f(x) = \sum_{i=1}^{d} \left(100(x_{i+1}^2 - x_i^2) + (x_i - 1)^2\right), \quad x_i \in [-100; 100] \]

- **Summation Cancellation:**
  \[ f(x) = 10^5 \sum_{i=1}^{d} \frac{1}{\left|\sum_{j=i}^{d} x_j\right|}, \quad x_i \in [-1; 1] \]

We used the shifted optima position in the form \( f(x') = f(x' - 0.25(x_{\text{max}} - x_{\text{min}})), \quad i = 1, \ldots, d \). We have chosen the following settings:

- **Problem size:** 10 variables/dimensions for all problems.
- **Population size of each island:** 500.
- **Selection:** We used truncation selection, with a selection proportion of 0.2, i.e. 100 individuals.
- **Number of islands:** 10.
- **Migration rate:** after every 20 generations.
- **Maximum number of fitness evaluations:** 500000 (i.e. 100 generations for the island-based model and 1000 generations for the sequential variant).
- **Number of independent runs:** 20.

5.2 Results and discussion

We carried out a comparison of two variants of the copula-based EDA algorithm: sequential variant sCEDA specified in Sec. 3 and island-based algorithm with model migration mCEDA (Sec. 4) – both of them with the same classes of copulas.

We used the so-called weak model of parallelization, the population size in sCEDA is equal to the population of one island in mCEDA. The total population in mCEDA is thus ten-times bigger than in sCEDA. To retain the same computational cost, we increased the number of generations ten-times for sCEDA according to mCEDA, thus the total computational cost measured by fitness evaluations is the same.

In Tables 1–6 the convergence of the proposed sCEDA and mCEDA algorithms is presented. The mean values related to specified evaluation epochs are listed.

It can be seen that mCEDA performs better than sCEDA for most benchmarks. (Only in the case of Ackley’s benchmark the sCEDA is better, the cause is under our investigation.) The sCEDA is able to find a relatively good local solution quite fast but then it loses its diversity and no further improvement is obtained. The mCEDA converges slowly but it has the capability to find near optimal solution. We suppose that this performance is caused by the phenomenon of the proposed model migration.

In the case of Rosenbrock’s and Summation Cancellation problems, only mCEDA using elliptic copulas is able to achieve some progress during the evolution process. Neither Archimedean copulas nor sCEDA have this capacity.

Besides the comparison of sCEDA and mCEDA the influence of each copula type in mCEDA is worth discussing. In the case of Rosenbrock’s and Summation Cancellation, only elliptical copulas are able to perform well. In the case of Rastrigin’s and Elliptic functions, Archimedean copulas perform better than elliptic ones. In the case of Ackley’s and Schwefel’s 1.2 functions, there is no significant difference between the two copula families.

From the observations it follows that the success rate of the both versions of mCEDA is almost identical. But in the case of Archimedean mCEDA the drawback appears in tendency to become stuck on local optima, see Table 3.

In Tables 7–9 we arranged a comparison (mean fitness values) of mCEDA using the Frank copula (mCEDA-F) and the Gaussian copula (mCEDA-G) (as members of Archimedean and elliptic families) with the other published algorithms that used different versions of copulas. The comparison is done for the same number of fitness evaluations for the same subset of benchmarks with 10 dimensions.

In Table 7 a comparison with the algorithm using the Copula Bayesian network (Méndez and Land, 2013)
### Table 1: Experimental results (mean fitness) for Rastrigin’s function.

<table>
<thead>
<tr>
<th>fit. eval.</th>
<th>Clayton</th>
<th>Gumbel</th>
<th>Frank</th>
<th>Gauss</th>
<th>Student</th>
</tr>
</thead>
<tbody>
<tr>
<td>island based</td>
<td>8.40e+00</td>
<td>8.40e+00</td>
<td>8.57e+00</td>
<td>8.13e+00</td>
<td>8.27e+00</td>
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<tr>
<td>sequential</td>
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<td>8.27e+00</td>
<td>8.13e+00</td>
<td>8.14e+00</td>
<td>7.63e+04</td>
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### Table 2: Experimental results (mean fitness) for Rosenbrock’s function.

<table>
<thead>
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<th>Gumbel</th>
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### Table 3: Experimental results (mean fitness) for Summation Cancellation function.

<table>
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<tr>
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### Table 4: Experimental results (mean fitness) for Elliptic function.

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<tbody>
<tr>
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### Table 5: Experimental results (mean fitness) for Ackley’s function.

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### Table 6: Experimental results (mean fitness) for Schwefel’s 1.2 function.

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Table 7: Comparison (mean fitness) of mCEDA with Copula Bayesian Network (CBN) from (Méndez and Landa, 2012).

<table>
<thead>
<tr>
<th></th>
<th>Rastr.</th>
<th>Ack.</th>
<th>Schw. 1.2</th>
<th>Rosen.</th>
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</tr>
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Table 8: Comparison (mean fitness) of mCEDA with: Copula EDA (cE), Copula EDA of Dynamic K-S test (cE-KS) from (Zhao and Wang, 2012); Clayton (Cl), Gumbel (Gu), Sn-EDA (Sn) from (Jia et al., 2013).

<table>
<thead>
<tr>
<th></th>
<th>Ellip./sphere</th>
<th>Rastrigin’s</th>
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<td>1.94e+00</td>
<td>2.41e-01</td>
<td>6.46e+00</td>
</tr>
</tbody>
</table>

Table 9: Comparison (mean fitness) of mCEDA with MIMIC\textsuperscript{Gaussian} and TREE\textsuperscript{Gaussian} copula model from (Salinas-Gutiérrez et al., 2011).

<table>
<thead>
<tr>
<th></th>
<th>Schwefel’s 1.2</th>
<th>Elliptic</th>
</tr>
</thead>
<tbody>
<tr>
<td>MIMIC</td>
<td>9.96e-01</td>
<td>1.15e+00</td>
</tr>
<tr>
<td>TREE</td>
<td>7.74e-01</td>
<td>3.99e-01</td>
</tr>
<tr>
<td>mCEDA-F</td>
<td>2.20e-03</td>
<td>3.42e-01</td>
</tr>
<tr>
<td>mCEDA-G</td>
<td>2.85e-03</td>
<td>2.78e+01</td>
</tr>
</tbody>
</table>

In Table 8 a comparison with the other suite of algorithms (Zhao and Wang, 2012; Jia et al., 2013) is carried out on the level of 300,000 evaluations. In the case of Rosenbrock’s function the results are comparable. In Table 9 a comparison with the algorithm using the MIMIC\textsuperscript{Gaussian} and TREE\textsuperscript{Gaussian} copula models (Salinas-Gutiérrez et al., 2011) after 100,000 evaluations is shown. For the case of Rastrigin’s, Ackley’s and Schwefel’s 1.2 functions mCEDA-F and mCEDA-G are evidently better, for Rosenbrock’s function the results are comparable.

In 2012) after 100,000 evaluations is shown. For the case of Rastrigin’s, Ackley’s and Schwefel’s 1.2 functions mCEDA-F and mCEDA-G are evidently better, for Rosenbrock’s function the results are comparable.

In Table 8 a comparison with the other suite of algorithms (Zhao and Wang, 2012; Jia et al., 2013) is carried out on the level of 300,000 evaluations. In the case of Rosenbrock’s function the results are comparable, for Rastrigin’s and the Sphere functions (the Sphere function is a simplified version of Elliptic problem) our algorithm mCEDA-F is better, but mCEDA-G is worse.

In Table 9 a comparison with the algorithm using the MIMIC\textsuperscript{Gaussian} and TREE\textsuperscript{Gaussian} copula models (Salinas-Gutiérrez et al., 2011) after 100,000 evaluations is shown. In the case of Schwefel’s 1.2 function mCEDA-F and mCEDA-G achieve evidently better behavior. In the case of the Elliptic problem mCEDA-F is better than TREE and MIMIC versions, on the other hand mCEDA-G is worse than the TREE and MIMIC versions. Unfortunately (Salinas-Gutiérrez et al., 2011) have used 12 dimensions and the variable domain is narrower than in our case, so the mutual comparison is only partly true.

## 6 CONCLUSION

In this paper we have introduced the utilization of multivariate elliptic and Archimedean copulas as cases of the probability model in the Estimation of Distribution Algorithm with model migration (mCEDA). We have presented the main theoretical basis and an effective approach of constructing and sampling both classes of copulas.

In order to illustrate the performance of the island-based mCEDA algorithm, a few known benchmarks of optimization were used. From the experimental results it follows:

1. mCEDA with model migration performs evidently better than the sequential sCEDA.
2. mCEDA using the elliptic copulas performs better than the Archimedean version of mCEDA.

We have also compared the performance of our mCEDA algorithm with other published copula EDA algorithms (Méndez and Landa, 2012; Zhao and Wang, 2012; Jia et al., 2013; Salinas-Gutiérrez et al., 2011). Our mCEDA algorithm is evidently better in most cases.

Our future research will be focused on the utilization of different implementations of univariate marginal distributions and their modification during the evolution process. An additional problem seems to be the tuning of the whole learning process during model combination in the migration mode.

## ACKNOWLEDGEMENTS

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## REFERENCES


