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Faculty of Electrical Engineering Department of Cybernetics

Bachelor's Thesis

Differential Evolution Crossover with Dependency Detection

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May 2021 Supervisor: Ing. Petr Pošík, Ph.D.



BACHELOR'S THESIS ASSIGNMENT

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II. Bachelor's thesis details

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Differential Evolution Crossover with Dependency Detection

Bachelor's thesis title in Czech:

Křížení pro diferenciální evoluci s detekcí závislostí

Guidelines:

Differential Evolution (DE) is a successfull black-box optimization algorithm for real-valued problems. Its weakness is a class of problems with dependent solution components, the exponential or binomial crossover operators conventionally used in DE are not suitable for them. The goal of this bachelor project is to design a new crossover operator based on the linkage tree known from the genetic algorithms with binary representation.

1. Familiarize yourself with the basic variants of differential evolution and the binomial and exponential crossover operators. 2. Learn about dependencies between solution components and about models used to describe them. Focus on the linkage tree model used to solve binary optimization problems.

3. Find or propose a new way of building a linkage tree-like model for real-valued representation. Propose a modified crossover operator for DE based on the model.

4. Evaluate the proposed algorithm on a set of benchmark functions and compare it with the basic DE, and other optimization algorithms.

Bibliography / sources:

[1] Storn, R., Price, K. Differential Evolution – A Simple and Efficient Heuristic for global Optimization over Continuous Spaces. Journal of Global Optimization 11, 341–359 (1997). https://doi.org/10.1023/A:1008202821328 [2] C. Olieman, A. Bouter and P. A. N. Bosman, "Fitness-based Linkage Learning in the Real-Valued Gene-pool Optimal Mixing Evolutionary Algorithm," in IEEE Transactions on Evolutionary Computation, doi: 10.1109/TEVC.2020.3039698 [3] Reshef, David N et al. "Detecting novel associations in large data sets." Science (New York, N.Y.) vol. 334,6062 (2011): 1518-24. doi:10.1126/science.1205438

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III. Assignment receipt

The student acknowledges that the bachelor's thesis is an individual work. The student must produce his thesis without the assistance of others, with the exception of provided consultations. Within the bachelor's thesis, the author must state the names of consultants and include a list of references.

Date of assignment receipt

Acknowledgement / Declaration

First of all, I would like to express my gratitude to my supervisor Ing. Petr Pošík, Ph.D. for his guidance, his helpful comments, and his patience with me.

Thank you!

Many thanks also belong to my family, present and future, and to all my friends for their support.

Love you!

I declare that the presented work was developed independently and that I have listed all sources of information used within it in accordance with the methodical instructions for observing the ethical principles in the preparation of university theses.

Prague, 20. May 2020

Abstrakt / Abstract

Diferenciální evoluce je považována za jeden z nejlepších evolučních algoritmů pro spojité black-box optimalizační problémy. Originální verze diferenciální evoluce používá náhodný uniformí operátor křížení, který nebere v potaz potencialní závislosti mezi částmi řešení a může tyto vazby narušovat.

Cílem této práce je poskytnout nový operátor křížení pro diferenciální evoluci, který bude vhodnější pro třídu problémů obsahující závislé komponenty řešení.

V této práci jsou prezentovány dvě metody, jak nalézt závislosti mezi proměnnými problému a dvě možnosti, jak modelovat strukturu vazeb. S užitím těhto metod byly navrženy čtyři nové operátory křížení.

Nově navržené algoritmy jsou vyhodnoceny na množině referenčních funkcí a jsou porovnány s dalšími optimalizačními algoritmy, včetně originalní diferenciální evoluce.

Výsledky ukazují, že nově navržené algoritmy dosahují výrazně lepšího výkonu a škálovatelnosti než původní diferenciální evoluce ve smyslu potřebného počtu vyhodnocení účelové funkce k nalezení globálního optima pro téměř všechny testované problémy. Něktré z nich dosahují podobné škálovatelnosti jako CMA-ES, jeden z nejmodernějších evolučních algoritmů.

Klíčová slova: Evoluční algoritmus, diferenciální evoluce, vazebný strom, mezní produkt, kontrola nelinearity, maximální informační koeficient, učení se závislostí.

Překlad titulu: Křížení pro diferenciální evoluci s detekcí závislostí Differential evolution is considered one of the best evolutionary algorithms for continuous black-box optimization problems. The original version of differential evolution uses a random uniform crossover operator, which does not take possible dependencies between parts of the solution into account and may even disrupt these linkages.

This work aims to propose a new crossover operator for differential evolution that is more suitable for the class of problems containing dependent solution components.

This work presents two methods of finding dependencies between problem variables and two possibilities of modeling the linkage structure. Moreover, those methods enable to design four new crossover operators.

The newly proposed algorithms are evaluated on a set of benchmark functions and then compared with other optimization algorithms, including the original differential evolution.

The results indicate that all of the four newly proposed algorithms achieve significantly enhanced performance and scalability compared to the original differential evolution in terms of fitness function evaluations, which are needed to find a global optimum for almost all analyzed problems. Moreover, some of them achieve comparable scalability to the state-of-the-art evolutionary algorithm CMA-ES.

Keywords: Evolutionary algorithm, differential evolution, linkage tree, marginal product, non-linearity check, maximal information coefficient, linkage learning.

Contents /

1 h	ntroduction1
2 E	volutionary algorithms $\ldots \ldots 2$
2.1	Components of evolutionary
	algorithms2
	2.1.1 Representation of indi-
	viduals2
	2.1.2 Objective function2
	2.1.3 Population3
	2.1.4 Parent selection
	2.1.5 Crossover operator $\dots 3$
	2.1.6 Mutation operator3
	2.1.7 Replacement strategy3
	2.1.8 Initialization3
	2.1.9 Termination condition3
2.2	General scheme4
2.3	Differential evolution4
	2.3.1 Representation
	2.3.2 Mutation
	2.3.3 Crossover
• •	2.3.4 Replacement strategy5
3 L	Inkage information modeling7
ა.1 ეკ	Family Of Subsets
3.4 2.2	Manginal product
ა.ა ⊿ ⊿	Intification of the linkage
- IL	tructure 10
41	Fitness-based method 10
4.2	Distribution-based method 11
5 E	xperiments
5.1	Algorithms 13
	5.1.1 Differential evolution
	variants $\dots \dots 13$
	5.1.2 Other algorithms 15
5.2	Test problems 15
	5.2.1 Sphere 16
	5.2.2 Levy 16
	5.2.3 Rastrigin 16
	5.2.4 Rosenbrock $\dots 17$
	5.2.5 SoREB 17
	5.2.6 OSoREB 17
5.3	Black Box Optimization
	Benchmarking problems 18
5.4	Setup 18
	5.4.1 Test problems specifics \dots 18
	5.4.2 BBOB problems
	specifics $\dots \dots \dots 18$

0
0
0
1
2
4
6
8
1
2
0

Tables / Figures

9	moroman	CVOIUIOII	varianus	•	1.4
				-	
	11101010100	0,010,0101011	10011001100	•	

5.2. MICE grid resolution *B*..... 15

Evolutionary algorithm pseu-
docode4
Differential evolution pseu-
docode
Linkage tree
Differential evolution with
dependency detection 14
Separable problems graphs 22
Block-separable problems
graphs
Non-separable problems
graphs
Ellipsoid separable function
graphs
Bent function graphs
Griewank-Rosenbrock F8F2
function graphs

Chapter **1** Introduction

Striving for the best solution to a particular problem is an essential part of many fields of human interest. The process of finding the best solution according to some criteria is called optimization.

There is an extensive number of engineering optimization problems in the real world whose input-output relationships are noisy and indistinct. Therefore, one cannot assume anything about the optimized function. However, it is possible to observe its outputs on given inputs. In this case, the function is called a black box function.

Due to these limited capabilities, all black box optimization algorithms are allowed to perform just these three steps:

- Create a candidate solution
- Check if a candidate is feasible or not
- Evaluate its fitness by using the objective function

In the mid-1950s [1-2], a new family of optimization algorithms called Evolutionary algorithms has been introduced. Evolutionary algorithms have proven [3] to be very effective in optimizing black box functions. Among the evolutionary algorithms, *Differential Evolution* (DE) [4] has achieved excellent results on real-valued black box functions.

However, a class of functions containing dependent solution components exists, and the recognition of those components may be a crucial task that could lead to significantly enhanced performance. Nevertheless, DE does not provide any tool capable of recognizing the dependent components of a solution. Thus, it can be argued that this particular class of functions is the weakness of DE.

This work aims to propose a way to find dependencies between parts of the solution and how to represent a dependency structure. It would lead to the proposal of a new crossover operator for DE well suited for functions with dependent solution components. This new operator could eliminate the weakness above-mentioned of DE.

Chapter **2** Evolutionary algorithms

Evolutionary algorithms (EAs) [5–8] is a set of stochastic metaheuristic optimization algorithms inspired by Darwin's theory of evolution by natural selection [9]. The theory describes the process of developing organisms over time as a result of changes in heritable traits. Changes that allow an organism to adapt to its environment better will help it survive and reproduce more offspring. This phenomenon is commonly called "Survival of the fittest", first used by Herbert Spencer [10].

In analogy to the natural environment, EA maintains a *population* of potential solutions (*individuals*) for the given problem. The population is iteratively evolved by encouraging the reproduction of fitter individuals. The fitness is usually the value of the objective function in the optimization problem being solved. New candidate solutions are created by combining existing individuals (*crossover*) or modifying an individual (*mutation*). The algorithm runs until a candidate solution with sufficient quality is found or a certain user-defined limit is reached.

2.1 Components of evolutionary algorithms

In this section, certain parts of evolutionary algorithms are discussed in detail. In general, EAs can be divided into various components, procedures, or operators, including:

- representation of individuals
- objective function
- population
- parent selection
- crossover operator
- mutation operator
- replacement strategy

To define a particular EA, it is necessary to specify these components. In addition, the initialization procedure and the termination condition must be defined to obtain a working algorithm.

2.1.1 Representation of individuals

Each individual is encoded in so-called *chromosomes*. The representation of chromosomes is called *genotype*. *Phenotype* refers to the interpretation of the genotype, in other words, how the objective function treats the genotype. The Representation also involves genotype-phenotype mapping. For instance, given an optimization problem on integers. If one decides to represent them by their binary code, 20 would be seen as a phenotype and 10100 as a genotype representing it.

2.1.2 Objective function

The role of the objective function is to represent the requirement to adapt to. The objective function defines what is the quality of an individual with respect to the problem in consideration. Technically, it is a function that takes an individual as input and produces a measure of the quality of a given individual as an output. The measure of quality is called *fitness*, and the objective function is called *fitness function*.

To remain with the example mentioned above, where the problem is to minimize x^2 on integers. The fitness of the individual represented by the genotype 10100 would be defined as a square of its corresponding phenotype: $20^2 = 400$.

2.1.3 Population

The population within an evolutionary algorithm means a set of individuals. A population can be specified only by setting the population size. In other words, the number of individuals in the population. This parameter is usually determined by the user.

2.1.4 Parent selection

During each generation (one iteration of the algorithm), a specific part of the population is selected to breed offspring. The choice is made similar to natural selection. Hence fitter individuals are preferred. Nevertheless, low quality individuals are given a small but positive chance to be selected. Otherwise, the EA could become too greedy and get stuck in the local optimum. *Parent selection*, along with the replacement strategy, pushes quality improvements. Parent selection, as well as other EA procedures, are usually stochastic. Individuals selected by parent selection are called *parents*.

2.1.5 Crossover operator

The *crossover* is a genetic operator used to combine typically two parents to generate new offsprings. The idea behind the crossover is that by mating two individuals with different but desirable features, it is possible to produce offsprings that combine both of those features. Similar to other genetic operators, the crossover is stochastic.

2.1.6 Mutation operator

The *mutation* is a unary genetic operator that changes parts of an individual's chromosome, typically randomly. The mutation is used to maintain and introduce diversity in the population.

2.1.7 Replacement strategy

Replacement strategy defines which individuals survive and become members of the subsequent generation. Typically, the decision is based on the quality of individuals, preferring those with higher fitness. The replacement strategy is similar to parent selection, as both are responsible for promoting quality improvement. However, parent selection is usually stochastic, while the replacement strategy is often deterministic.

2.1.8 Initialization

The *Initialization* procedure generates a defined number of individuals of the given representation, thereby creating the initial population. Initialization is often done randomly due to a lack of knowledge when optimizing black box functions.

2.1.9 Termination condition

The algorithm runs until the *termination condition* has been reached. Suppose the optimum of the optimized problem is known. In that case, reaching the optimum (with a given precision $\epsilon \geq 0$) is a natural termination condition. However, since EAs are stochastic, there is usually no guarantee to reach an optimum, and the condition would never be satisfied. Therefore, this condition is extended with the condition that stops the algorithm certainly, such as the limited number of fitness function calls.

Algorithm	1:	Evo	lutionary	algorithm
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 \begin{array}{l} \textbf{Result: best individual in } Population(t) \\ t \leftarrow 0; \\ Population(t) \leftarrow initialization(); \\ fitnessFunctionEvalutation(Population(t)); \\ \textbf{while } termination\_condition \ not \ met \ \textbf{do} \\ \\ \hline Parents \leftarrow parentSelection(Population(t)); \\ Offspring \leftarrow crossover(Parents); \\ Offspring \leftarrow mutation(Offspring); \\ evaluate(Offspring); \\ Population(t+1) \leftarrow replacementStrategy(Population(t), Offspring); \\ t \leftarrow t+1; \\ \end{array}  end
```

Figure 2.1. General scheme of an evolutionary algorithm

2.2 General scheme

In the previous section, the main parts of an EA were introduced individually. By merging the above-mentioned components, the evolutionary algorithm is formed. This section describes the way the EA works as a whole.

Firstly, an initial population is generated by an initialization procedure. The fitness function subsequently evaluates the population. Then a generational process starts and is repeated until the termination condition is not satisfied. The generational process starts with parent selection, usually based on fitness. A portion of individuals is chosen to seed the new generation. The chosen individuals are combined by a crossover operator to produce offsprings, which are then modified by the mutation operator. A fitness function subsequently evaluates offsprings, and the generational process ends by creating a new population. Creating a new population is done with respect to the replacement strategy that selects some newly created offsprings to replace some members of the old population.

The algorithm returns the best individual found so far, eventually some statistics concerning the run of the algorithm. The pseudocode is shown in figure 2.1.

2.3 Differential evolution

Differential evolution was introduced by Storn and Price [4] as an efficient evolutionary algorithm initially designed for multidimensional real-valued spaces.

DE [7] utilizes a population of real vectors. The initial population is chosen randomly. After initialization, for each member \vec{x}_i of a population P is generated a so-called *mutant* vector. The mutant vector is generated by adding the weighted difference between two individuals $(\vec{x}_{r_2}, \vec{x}_{r_3})$ to a third individual (\vec{x}_{r_1}) . These three individuals are mutually exclusive. The offspring \vec{o}_i is then created by crossing over the mutant vector with \vec{x}_i .

Note that the impact of the mutant vector is largely based on the actual variance in the population. The mutant vector will make major changes if the population is spread. On the other hand, the mutant vector will be small if the population is condensed in a particular region. Thus, DE belongs to the family of adaptive mutation algorithms.

Lastly, the newly created offspring is compared to its parent using the greedy criteria. If the offspring is better than its parent, it replaces its parent in the population. Formally, the standard DE is defined by specifying the components of an EA, as done in the paragraphs below.

2.3.1 Representation

Individuals are represented by real-valued vectors:

$$\vec{x_i} = \{x_{i,0}, x_{i,1}, \dots, x_{i,D-1}\}, \forall j : x_{i,j} \in \mathbb{R},$$

where i represents the individual's index in the population P and D stands for the dimension of the optimized function. The population is represented as follows:

$$P = \{\vec{x}_0, \vec{x}_1, \dots, \vec{x}_{NP-1}\}, NP \ge 4,$$

where NP is the size of the population.

2.3.2 Mutation

For each individual in the population $\vec{x}_i, i = 0, 1, ..., NP - 1$, DE generates mutant vector \vec{m}_i as following:

$$\vec{m}_i = \vec{x}_{r_1} + F \cdot (\vec{x}_{r_2} - \vec{x}_{r_3}),$$

with random, mutually exclusive indexes $r_1, r_2, r_3 \in \{0, 1, ..., NP - 1\}$, which are also chosen to be different from the running index *i*. *F*, called *differential weight*, is a constant factor $\in [0, 2]$, representing the amplification of the random deviation $(\vec{x}_{r_2} - \vec{x}_{r_3})$.

2.3.3 Crossover

After the mutation, the mutant vector \vec{m}_i undergoes a crossover with its relevant individual \vec{x}_i to generate the offspring \vec{o}_i . Standard DE us binomial crossover, where the offspring is generated as follows:

$$\vec{o_i} = \{o_{i,0}, o_{i,1}, \dots, o_{i,D-1}\},\$$

$$\forall j: o_{i,j} = \begin{cases} m_{i,j} & \text{if } j = R \lor rand(0,1) < CR,\\ x_{i,j} & \text{otherwise,} \end{cases}$$

where: $R \in [0, D]$ is a random integer, rand(0, 1) represents a random number between zero and one, and CR denotes the probability of crossover. Since \vec{x}_i is the parent of \vec{o}_i , it can be seen that each individual in the population generates an offspring. In other words, the parent selection chooses all individuals from the population.

2.3.4 Replacement strategy

To decide which individuals become members of the subsequent generation, DE compares offspring $\vec{o_i}$ to its relevant parent $\vec{x_i}$ using the greedy criterion. Thus, if $\vec{o_i}$ is better than $\vec{x_i}$, the offspring $\vec{o_i}$ will replace the parent $\vec{x_i}$ and enter the population of the next generation. Algorithm 2: Differential evolution

 Result: best individual found so far

 Generate initial population of size NP;

 Evaluate population by fitness function;

 while termination_condition not met do

 for each i individual in population do

 Generate integers $r_1, r_2, r_3 \in [1, NP]$, with $r_1 \neq r_2 \neq r_3 \neq i$ (transitively);

 Generate integer $R \in [0, D - 1]$;

 for each j dimension do

 $o_{i,j} = \begin{cases} x_{r_1,j} + F \cdot (x_{r_2,j} - x_{r_3,j}), & \text{if } j = R \text{ or } rand(0,1) < CR \\ x_{i,j}, & \text{otherwise} \end{cases}$

 end

 if \vec{o}_i is better than \vec{x}_i then

 Replace \vec{x}_i with \vec{o}_i ;

 end

 end

Figure 2.2. General scheme of the differential evolution

Chapter **3** Linkage information modeling

It is worth noting that DE, as was described in the previous chapter, uses random, uniform crossover. The crossover has no assumptions about the structure of the optimized function. The original DE does not take possible dependencies between specific parts of the solution into account.

However, a whole class of problems with dependent solution components exists. DE using uniform crossover does not take possible dependencies into consideration and often disrupts linkages between strongly connected components.

The aim of this work is to propose a new crossover operator capable of finding dependencies and taking them into account when generating new offsprings. This chapter proposes two possible representations of the dependency structure.

3.1 Family Of Subsets

Both representations of the dependency structure are based on the Family Of Subsets (FOS) [11]. FOS is a way to model linkage information that describes presumed dependencies between variables. FOS $\mathcal{F} = \{\mathcal{F}_1, \mathcal{F}_2, ...\}$ represents a subset of a power set $\mathcal{P}(\mathcal{I})$ of \mathcal{I} , where $\mathcal{I} = \{0, 1, ..., D - 1\}$ stands for a set of indices and D is a number of problem variables (dimension of the fitness function). Each block $\mathcal{F}_j \in \mathcal{F}$ contains the indices of those variables that are considered dependent.

3.2 Linkage tree

Many FOS structures exist, and any of them can be used to model the linkage structure. However, this work focuses on two of them. The first of them is the *linkage tree* (LT).

"The Linkage Tree is the hierarchical cluster tree of the problem variables using an agglomerative hierarchical clustering algorithm with a dependency measure \mathcal{M} . The dependency measure $\mathcal{M}(X_1, X_2)$ measures the degree of dependency between two sets of variables X_1 and X_2 ." [12]

More potential dependency measures $\mathcal{M}(X_1, X_2)$ exist. However, in this work, two dependency measures are used. They are described in detail in the following chapter (4).

The linkage tree is a tree with D leaf nodes and D-1 inner nodes, where D is the number of problem variables. Each node of the LT represents a specific set of variables \mathcal{F}_j . The key property of the LT is that each \mathcal{F}_j , which contains more than one variable, is the union of two other sets \mathcal{F}_k , $\mathcal{F}_l \in \mathcal{F}$, where $j \neq k \neq l$ (transitively). Formally, for any subset \mathcal{F}_j , where $|\mathcal{F}_j| > 1$, subsets $\mathcal{F}_k, \mathcal{F}_l$, for which the following applies, exist:

1) $\mathcal{F}_k, \mathcal{F}_l \neq \emptyset$ 2) $\mathcal{F}_k \cap \mathcal{F}_l = \emptyset$ 3) $\mathcal{F}_k \cup \mathcal{F}_l = \mathcal{F}_j$ The hierarchical clustering procedure starts by assigning each problem variable to a separate block in random order. The procedure proceeds top-down. Therefore, the tree is initialized with these univariate blocks as leaves. In each step, a new node is created by merging two nodes of the tree determined, by a given dependency measure \mathcal{M} , as the most dependent. It is important to mention that each node can be merged only once. The merging process stops when no more merges are possible. In other words, the root node has been created. Due to the way the procedure works, the root node has to be a set of all problem variables. The tree itself contains multiple levels of dependency. From the univariate level at the height of zero to the complete dependency between all variables at a depth of zero. [12]



Figure 3.1. Example of the linkage tree [13]

The DE using the LT structure (DE_LT) builds the LT in every generation. Once the tree is built, DE_LT traverses the tree in the opposite order of merging.

3.3 Marginal product

The second introduced FOS structure is marginal product (MP) [14]. The MP is defined as set \mathcal{F} , where for each $\mathcal{F}_k, \mathcal{F}_l \in \mathcal{F}$ holds that $\mathcal{F}_k \cap \mathcal{F}_l = \emptyset$. When all variables are independent, MP is called univariate FOS and $\mathcal{F} = \{\{0\}, \{1\}, ..., \{D-1\}\},$ where D is number of problem variables. On the contrary, when all variables are considered mutually dependent, MP is called compact FOS. Before introducing the *MP* building procedure, it is necessary to define the strength of block $S_{\mathcal{M}}(\mathcal{F}_j)$, which determines the dependency rate within a certain block \mathcal{F}_j according to the given dependency measure \mathcal{M} . The strength of blocks is defined as follows:

$$\mathcal{S}_{\mathcal{M}}(\mathcal{F}_i) = \begin{cases} \frac{G}{D-1} \sum_{v \in \mathcal{V}} \mathcal{M}(\mathcal{F}_i, \{v\}) & \text{if } |\mathcal{F}_i| = 1, \\ \frac{1}{|\mathcal{F}_i|(|\mathcal{F}_i|-1)} \sum_{u \in \mathcal{F}_i} \sum_{v \in \mathcal{F}_i} \mathcal{M}(\{u\}, \{v\}) & \text{otherwise,} \end{cases}$$

where $G \ge 0$ is a user-specified factor defining the degree of strength of univariate blocks, and \mathcal{V} denotes the set of all problem variables.

The MP building procedure starts by initializing MP \mathcal{F} as univariate FOS and by assigning the strength of block to each block. In each step, new block \mathcal{F}_n is created by merging two blocks $\mathcal{F}_a, \mathcal{F}_b \in \mathcal{F}$, which are determined as the most dependent by the given dependency measure \mathcal{M} . Then \mathcal{F}_n is assigned its strength of block. If the newly created block meets the following conditions:

1) $S_{\mathcal{M}}(\mathcal{F}_n) \ge \theta_1, \theta_1 \in \mathbb{R}$ 2) $S_{\mathcal{M}}(\mathcal{F}_n) \ge Kmax(S_{\mathcal{M}}(\mathcal{F}_a), S_{\mathcal{M}}(\mathcal{F}_b))$ 3) $|\mathcal{F}_n| \le \theta_2, \theta_2 \in \mathbb{N}$

Where thresholds $\theta_1 > 0$, $\theta_2 \in [1, D]$ and factor $K \in (0, 1]$ are defined by the user, then \mathcal{F}_n is inserted into the FOS \mathcal{F} , and $\mathcal{F}_a, \mathcal{F}_b$ are removed from \mathcal{F} . The procedure runs until a newly created block \mathcal{F}_n has not met mentioned conditions or until MP has become the compact FOS.

The DE using the MP FOS structure (DE_MP) builds the MP in every generation. After building the MP, DE_MP traverses FOS in the opposite order of merging, in other words, from the last one added to FOS to the first one.

Chapter **4** Identification of the linkage structure

In the previous chapter, two possible representations of the dependency structure were introduced. In order to represent the dependency structure, it is necessary to determine the degree of dependence between each pair of variables and between each pair of sets of variables. The tool used to measure the degree of dependency is called the dependency measure and is denoted as \mathcal{M} .

Formally, \mathcal{M} is a function that takes two sets of variables as input and produces a real, positive number as output. \mathcal{M} is defined as follows [12]:

$$\mathcal{M}(X_i, X_j) = \frac{1}{|X_i| |X_j|} \sum_{u \in X_i} \sum_{v \in X_j} p_{u,v},$$

where X_i and X_j are sets of variables and $p_{u,v}$ is an element of the *dependency matrix* \mathcal{P} at position u, v.

The dependency matrix

$$\mathcal{P} = \begin{pmatrix} p_{0,0} & p_{0,1} & \dots & p_{0,D-1} \\ p_{1,0} & p_{1,1} & & \vdots \\ \vdots & & \ddots & \vdots \\ \vdots & & & \ddots & \vdots \\ p_{D-1,0} & \dots & \dots & p_{D-1,D-1} \end{pmatrix} \in \mathbb{R}^{D \times D}$$

is a symmetric and positive semidefinite matrix. The dependency matrix captures the dependency between each pair of variables. The element $p_{i,j}$ denotes the pairwise dependency strength between i-th and j-th problem variables. Diagonal elements of \mathcal{P} are defined as zeros, i.e $\forall i = 0, 1, ..., D - 1 : p_{i,i} = 0$.

Several methods of constructing the dependency matrix \mathcal{P} exist. Nevertheless, this work focuses only on two of them.

4.1 Fitness-based method

The first method, called *non-linearity check* (NC) [15–16], defines whether two variables interact directly based on fitness values. The method works under the assumption that non-linear interactions may exist only between dependent variables. It classifies a pair of variables, either separable or non-separable, by comparing the difference in overall fitness while making the exact same change for a particular pair of chromosomes of a given individual $x_{i,j}$ for different values of $x_{i,k}, k \neq j$. Nevertheless, checking only one individual is not convincing enough because there may exist linearity between a dependent pair of variables in some context. Therefore, more individuals must be checked. In this work, m best individuals from the population are checked. The set of indices of m best individuals in the population is denoted as C. For each of chosen individuals $\vec{x}_i, i \in C$ and each pair of variables j, k, a pairwise dependency $d_{i,j,k}$ is calculated. The overall pairwise dependency between those variables is determined by aggregating those values as follows:

$$p_{j,k} = \frac{1}{m} \sum_{i \in C} d_{i,j,k}$$

In order to calculate $d_{i,j,k}$, four individuals are picked by combining all possible points that can be created by picking two different values for each $x_{i,j}$ and $x_{i,k}$ [17]. The absolute value of differences in the overall fitness value for those points is used to calculate the potential dependence between *j*-th and *k*-th variables. It is done by determining whether the adjustment to $x_{i,k}$ affects the change in fitness caused by modification to $x_{i,j}$. Define $\Delta_{i,j,k}$ as:

$$\Delta_{i,j} = |(f(\vec{x}_i)|x_{i,j} = a_j, x_{i,k} = a_k) - (f(\vec{x}_i)|x_{i,j} = a_j + b_j, x_{i,k} = a_k)|,$$

$$\Delta_{i,j,k} = |(f(\vec{x}_i)|x_{i,j} = a_j, x_{i,k} = a_k + b_k) - (f(\vec{x}_i)|x_{i,j} = a_j + b_j, x_{i,k} = a_k + b_k)|,$$

where f denotes fitness function, and a_j, a_k, b_j, b_k can be any real value, so that for every variable j: a_j and $a_j + b_j$ remain within the bound for j-th variable inside the current population, formally:

$$\forall j : \max_{\vec{x}_i \in P} (x_{i,j}) \ge a_j \ge \min_{\vec{x}_i \in P} (x_{i,j}),$$
$$\forall j : \max_{\vec{x}_i \in P} (x_{i,j}) \ge a_j + b_j \ge \min_{\vec{x}_i \in P} (x_{i,j}).$$

Nevertheless, the values that have been empirically found for [17] are used in this work, those values are

$$a_{j} = \min_{\vec{x}_{i} \in P} (x_{i,j}) + (\max_{\vec{x}_{i} \in P} (x_{i,j}) - \min_{\vec{x}_{i} \in P} (x_{i,j})) \cdot 0.35,$$
$$b_{j} = (\max_{\vec{x}_{i} \in P} (x_{i,j}) - \min_{\vec{x}_{i} \in P} (x_{i,j})) \cdot 0.35.$$

Finally, *j*-th and *k*-th variables are said to be dependent when $|\Delta_{i,j} - \Delta_{i,j,k}| \ge 0$, the pairwise dependency $d_{i,j,k}$ is defined as:

$$d_{i,j,k} = \begin{cases} 1 - \frac{\Delta_{i,j,k}}{\Delta_{i,j}} & \text{if } \Delta_{i,j} \ge \Delta_{i,j,k}, \\ 1 - \frac{\Delta_{i,j}}{\Delta_{i,j,k}} & \text{otherwise.} \end{cases}$$

Note that $d_{i,j,k}$ as well as $p_{j,k}$ lie within [0, 1) with zero indicating independent variables.

4.2 Distribution-based method

The second method of constructing the dependency matrix \mathcal{P} is called the *maximal in-formation coefficient* (MIC) [18]. More methods used to identify dependencies between a pair of variables based on the distribution of the population exist [14, 17]. However, MIC achieved better accuracy in comparison to other methods [18–19].

MIC is based on the idea that a relationship between a pair of variables can be captured by a grid on the scatterplot of the two variables that partitions the data to encapsulate that relationship. 4. Identification of the linkage structure

In order to calculate MIC, all possible grids up to maximal grid resolution are considered. Note that maximal grid resolution depends on the sample size. For each pair of integers (x, y), the largest possible mutual information (MI) [20], achievable by any x-by-y grid applied to the data, is computed. Those mutual information values are then normalized by the logarithm of the minimum of x and y. Finally, MIC is defined as the maximum of those highest normalized mutual information values [18]. Formally:

$$MIC_{i,j} = \max_{(x,y):x \le B, y \le B} \left(\max_{g:G_{x,y}} \left(\frac{MI_{i,j}|_g}{\log\min(x,y)} \right) \right),$$

where B is a user-specified value defining maximal grid resolution, $G_{x,y}$ denotes a set of all possible x-by-y grids, and $MI_{i,j}|_g$ stands for mutual information of *i*-th and *j*-th variables achieved by application of grid g.

As was mentioned above, MIC achieved good results in various comparisons. However, a big limitation of MIC is its high computational cost. Therefore, several algorithms for approximating the MIC have been published [18–19, 21]. In this work, MICE minepy implementation [22–23] is used.

In this work, MICE is not calculated from the whole population, but only a subset C of all individuals from the current population is considered. The dependency matrix \mathcal{P} is then formally calculated as follows:

$$p_{i,j} = \text{MICE}_{i,j}|_C.$$

Chapter 5 Experiments

In section 2.3, the standard differential evolution was introduced. It was also noted that DE does not have any tool to recognize or model the linkage information between certain parts of the solution. In chapter 3, two possible representations of the dependency structure were introduced assuming known pairwise dependencies, and in chapter 4, two ways to find pairwise dependencies and thereby build the dependency matrix \mathcal{P} were presented.

Based on those methods, it is possible to propose a modified DE with dependency detection. The modified version differs from the original in two factors. Firstly, in every generation, the dependency matrix \mathcal{P} and FOS structure based on it is built. Secondly, the crossover is modified to respect dependent blocks. The block $\mathcal{F}_j \in \mathcal{F}$ divides the set of all variables into two mutually exclusive subsets of variables \mathcal{F}_j and $\mathcal{F} \setminus \mathcal{F}_j$. Variables within those subsets are crossed over together [11].

Formally, within the crossover, for each individual \vec{x}_i , each block \mathcal{F}_j is iteratively considered in random order (crossover probability CR = 1). For each block \mathcal{F}_j , a new mutant vector \vec{m}_i is randomly generated in the same way as it is generated within the standard mutation. Suppose mutant's values for variables contained in \mathcal{F}_j are different from those contained in its parent \vec{x}_i . In that case, these values are overwritten in the parent \vec{x}_i . It produces \vec{x}_{new} , which is then evaluated by the fitness function. New individual \vec{x}_{new} is only accepted if it has a better or equal fitness value than the original \vec{x}_i . Changes in DE pseudocode are captured in figure 5.1.

The main goal of the experiments is to study the performance of various types of DE with dependency detection differing in creating the matrix \mathcal{P} , or in the building of FOS \mathcal{F} . Compare them with each other and with standard DE and other optimization algorithms.

5.1 Algorithms

5.1.1 Differential evolution variants

Within the experiments, seven types of differential evolution are compared. The original DE, as was introduced in section 2.3. (DE_UNIFORM). The remaining six variants of DE are divided into three pairs according to how they create the dependency matrix \mathcal{P} . The first variant uses the linkage tree (LT) and the second the marginal product (MP) within each pair. The first pair uses the non-linearity check to create \mathcal{P} (DE_LT_NC and DE_MP_NC). The second pair takes advantage of the maximal information coefficient (DE_LT_MIC and DE_MP_MIC). The third pair are DE variants with full prior knowledge of pairwise dependencies. Therefore, they build optimal \mathcal{P} , which is a (0, 1)-matrix with zeros for independent pairs and ones for dependent pairs (DE_LT+ and DE_MP+), before starting the generational process.

It is important to note that all newly proposed variants of DE create \mathcal{P} and build the FOS structure in every second generation instead of every generation in order to speed up the computation.

Algorithm 3: Differential evolution with dependency detection

Result: best individual found so far Generate initial population of size NP; Evaluate population by fitness function; while termination_condition not met do Create dependency matrix \mathcal{N} ; Build FOS \mathcal{F} based on \mathcal{N} ; for each $\vec{x_i}$ individual in population do for each block $\mathcal{F}_k \in \mathcal{F}$ in opposite order of merging \mathbf{do} $\vec{x}_{new} = \vec{x}_i;$ Generate integers $r_1, r_2, r_3 \in [1, NP]$, with $r_1 \neq r_2 \neq r_3 \neq i$ (transitively); for each $j \in \mathcal{F}_k$ do $x_{new,j} = x_{r_1,j} + F \cdot (x_{r_2,j} - x_{r_3,j});$ end if \vec{x}_{new} is better than \vec{x}_i then Replace \vec{x}_i with \vec{x}_{new} ; end end end end

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	Non-linearity check	Max. inf. coeff.	Optimal
Linkage tree	DE_LT_NC	DE_LT_MIC	DE_LT+
Marginal product	DE_MP_NC	DE_MP_MIC	DE_MP+

 Table 5.1. Overview of newly proposed variants of the differential evolution.

All the above-mentioned DE variants share the following:

- Initialization of individuals $\sim \mathcal{N}(\mathbf{0}, 100 \cdot \mathbf{I}_D)$, where \mathcal{N} is multivariate normal distribution, $\mathbf{0}$ stands for the zero vector, and \mathbf{I}_D represents $D \times D$ identity matrix.
- The differential weight F = 0.7

Other parameters:

- The crossover probability for DE_UNIFORM: CR = 0.9
- The degree of strength of univariate blocks:

$$G = \begin{cases} 1 & \text{for DE_MP+,} \\ 2 & \text{otherwise.} \end{cases}$$

• Threshold θ_1 defining the minimal strength of block to be accepted:

$$\theta_1 = \begin{cases} 10^{-1} & \text{for DE_MP_MIC,} \\ 10^{-8} & \text{otherwise.} \end{cases}$$

- Maximal size of blocks: $\theta_2 = 6$
- Maximum potential degree of strength of block reduction during merging

$$K = \begin{cases} 0.8 & \text{for DE}_{MP+}, \\ 0.4 & \text{for DE}_{MP}_{NC}, \\ 0.7 & \text{for DE}_{MP}_{MIC}. \end{cases}$$

- Number of checked individuals within non-linearity check method: $m = [0.15 \cdot NP]$
- The subset used to calculate MICE $C = C_b \cup C_r$, where C_b is set of $\lceil 0.3 \cdot NP \rceil$ best individuals in population and C_r is a set of $\lceil 0.1 \cdot NP \rceil$ randomly chosen individuals from the remaining.
- The maximal MICE grid resolution *B* is set according to table 5.2 (rounded to the nearest integer in an upward direction).

Number of samples	B parameter
C < 25	$ C ^{0.85}$
$25 \le C < 50$	$ C ^{0.8}$
$50 \le C < 250$	$ C ^{0.75}$
$250 \le C < 500$	$ C ^{0.7}$
$500 \le C < 1000$	$ C ^{0.65}$
$1000 \le C < 2500$	$ C ^{0.60}$
$2500 \le C < 5000$	$ C ^{0.55}$

Table 5.2. The dependence of the cardinality of C on the parameter B, taken from [22].

■ Th MICE parameter c, which determines how many more clumps there will be than columns in every partition, was set default value 15 [22].

All values mentioned above were found empirically unless otherwise stated.

5.1.2 Other algorithms

The Covariance matrix adaptation evolution strategy (CMA-ES) belongs to the class of evolutionary algorithms. CMA-ES is considered state-of-the-art in evolutionary computation and has very quickly become the standard tool for continuous optimization [24–26]. In this work, Hansen's implementation of CMA-ES with default parameters is used [27].

The last considered algorithm is the Nelder-Mead simplex algorithm [28], An optimization algorithm, which is not an evolutionary algorithm. Nevertheless, it uses only function values to find the optimum. Therefore, it may be used for black box optimization. The Scipy implementation, called FMIN, is used [29]. The minimal absolute difference in the candidate solution between iterations (*xtol*) as well as the minimal absolute difference in fitness function values between iterations (*ftol*) is set to 10^{-12} . Independent restarts are allowed.

5.2 Test problems

The first set of benchmarking problems is called Test problems. These six optimization problems to minimize are considered to study the impact of various types of linkage learning on the performance of DE and to benchmark the considered algorithms.

Before introducing the Test problems, it is important to state the property of functions, called *additive separability*. Additively separable function F is defined as:

$$F(x_0, x_1, \dots, x_{D-1}) = f_0(x_0) + f_1(x_1) + \dots + f_{D-1}(x_{D-1}),$$

where $f_0, f_1, ..., f_{D-1}$ are functions of one variable. It is crucial that the optimum of a D-dimensional additively separable function may be obtained by performing D independent one-dimensional optimizations along each dimension, formally:

$$\min_{[x_0, x_1, \dots, x_{D-1}] \in \mathbb{R}^{\mathbb{D}},} F(x_0, x_0, \dots, x_{D-1}) = \min_{x_0 \in \mathbb{R}} f_0(x_0) + \min_{x_1 \in \mathbb{R}} f_1(x_1) + \dots + \min_{x_{D-1} \in \mathbb{R}} f_{D-1}(x_{D-1}).$$

It can be seen that the standard DE, which optimizes each dimension independently, would be suitable for optimizing additively separable functions. Additively separable functions are exactly those functions without dependencies.

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5.2.1 Sphere

The first benchmark function is the sphere function, also known as De Jong F1 [30]. It is presumable the easiest continuous domain optimization problem. It is convex, separable, and has one local minimum.

Definition of the sphere function:

$$f_{sphere}(\vec{x}) = \sum_{i=0}^{D-1} x_i^2.$$

Global minimum:

$$f_{sphere}(\vec{x}_{min}) = 0,$$

 $\vec{x}_{min} = [0, 0, ..., 0].$

5.2.2 Levy

The second considered benchmark problem is the Levy function [31]. Like the sphere, it is a separable function. Nevertheless, the Levy function is considered more challenging to optimize.

The Levy function is defined as follows:

$$f_{Levy}(\vec{x}) = \sin^2(\pi v_0) + \sum_{i=0}^{D-2} \left[(v_i - 1)^2 (1 + 10\sin^2(\pi v_i + 1)) \right] + (v_{D-1} - 1)^2 (1 + \sin^2(2\pi v_{D-1})),$$

where $v_i = 1 + \frac{x_i - 1}{4}$, for all i = 0, 1, ..., D - 1.

Global minimum:

$$f_{Levy}(\vec{x}_{min}) = 0,$$

 $\vec{x}_{min} = [1, 1, ..., 1].$

5.2.3 Rastrigin

The Rastrigin function [32–33] is the third benchmark problem. Like the previous functions, this one is also separable. It is a difficult function to optimize. Due to regular "noise", it has many regularly distributed local minima. The Rastrigin function is defined as:

$$f_{Rastrigin}(\vec{x}) = 10 \cdot D + \sum_{i=0}^{D-1} \left[x_i^2 - 10\cos(2\pi x_i) \right].$$

Global minimum:

$$f_{Rastrigin}(\vec{x}_{min}) = 0,$$
$$\vec{x}_{min} = [0, 0, ..., 0].$$

5.2.4 Rosenbrock

The Rosenbrock function [34], also known as the Banana function, is the first nonseparable function because it has overlapping dependencies. Each pair of consecutive variables is dependent. The Rocenbrock function contains a narrow parabolic valley, where the global minimum is located. However, even though this valley is easy to find, convergence to the minimum is difficult [35]. The definition of Rosenbrock function is as follows:

$$f_{Rosenbrock}(\vec{x}) = \sum_{i=0}^{D-2} \left[100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2 \right].$$

Global minimum:

 $f_{Rosenbrock}(\vec{x}_{min}) = 0,$ $\vec{x}_{min} = [1, 1, ..., 1].$

5.2.5 **Soreb**

The Sum of Rotated Ellipsoid Blocks, abbreviated SoREB [14] is defined as follows:

$$f_{Ellipsoid}(\vec{x}) = \sum_{i=0}^{l-1} \left[10^{\frac{6i}{l-1}} x_i^2 \right],$$

$$f_{SoREB}(\vec{x},k) = \sum_{i=0}^{D/k-1} \left[f_{Ellipsoid} \left(R_{\theta}([x_{ki},...,x_{k(i+1)-1}]) \right) \right],$$

where R_{θ} defines the rotation of a vector around the origin by the angle of θ , and k is the size of blocks. Rotated blocks of variables that enter to $f_{ellipsoid}$ as an input creates strongly connected components. Variables within the block have strong dependencies but are entirely independent of any variables outside their block. This feature is called block-separability.

Within comparison, four types of the SoREB function differing in the size of blocks (2, 3, 4, 5) were considered. The rotation of $\theta = \pi/8$ is used. Global minimum:

$$f_{SoREB}(\vec{x}_{min}, k) = 0; k \in \mathbb{N}$$
$$\vec{x}_{min} = [0, 0, ..., 0].$$

5.2.6 OSoREB

The SoREB function contaions only non-overlapping, non-decomposable blocks of size k. In [14] the overlapping version of this problem was defined as OSoREB (Overlapping Sum of Rotated Blocks). In addition to the original SoREB problem, SoREB blocks of length 2 for every pair of successive variables belonging to other original blocks are used. For OSoREB is used k = 5 and $\theta = \pi/8$. Definition of OSoREB:

$$f_{OSoREB}(\vec{x},k) = f_{SoREB}(\vec{x},k) + \sum_{i=1}^{D/k-1} \left[f_{Ellipsoid} \left(R_{\theta}([x_{ki-1}, x_{ki}]) \right) \right].$$

Global minimum:

$$f_{OSoREB}(\vec{x}_{min}, k) = 0; k \in \mathbb{N}$$

 $\vec{x}_{min} = [0, 0, ..., 0].$

5.3 Black Box Optimization Benchmarking problems

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Black Box Optimization Benchmarking (BBOB) problems are the second considered set of benchmark problems. A set of 24 noise-less real-parameter single-objective benchmark functions are defined in [36] as Real-Parameter Black-Box Optimization Benchmarking 2009 Noiseless Functions. Those functions were used for the BBOB workshop 2009. The BBOB problems were selected with the intention to evaluate the performance of algorithms with regard to standard difficulties that occur in continuous domain search. So they definitely should, at least to a certain extent, reflect the problems that are dealt with in practice. All BBOB problems are to be minimized.

It is important to note that since BBOB problems cover a wide range of possible optimization problems, the proposed DE variants may be unsuitable for some of them. BBOB problems consist of separable and non-separable ones.

5.4 Setup

All the experimental results that are described in this work measure the first time a global optimum was hit. In other words, the number of fitness function calls needed to reach the small enough neighborhood of the global optimum for the first time within the run. The toleration is 10^{-8} .

5.4.1 Test problems specifics

For each problem, each algorithm, and each dimension, twenty-five independent runs are performed. The performance is considered successful if at least 24 runs converged to the global optimum or a predefined sufficiently close approximation within 300 000 $\cdot D$ calls of the fitness function.

The associate population size of evolutionary algorithms is the smallest possible size so that the algorithm's performance is considered successful. It is determined by starting from the smallest possible population and letting the algorithm run 25 times. If the performance has not been successful, the population size for the next trial will increase by s. This procedure is repeated until the successful population size is found or a population size reaches the upper limit T. If the successful population size is found, the optimal population size is searched for by performing a bisection search between the current population size and the previous size. Otherwise, the algorithm is considered unable to optimize a certain problem and dimension. Parameters s and T are set as follows:

$$s = \begin{cases} 10 & \text{for DE_LT_MIC and DE_MP_MIC,} \\ 4 & \text{for otherwise.} \end{cases}$$
$$T = \begin{cases} 50 + 6 \cdot D & \text{for DE_LT_MIC and DE_MP_MIC,} \\ 50 & \text{for otherwise.} \end{cases}$$

5.4.2 BBOB problems specifics

The setup for BBOB problems is partially determined by the authors of BBOB problems in [37]. For each algorithm, dimension, and optimized function, five different function *instances* are used, each of them three times. The number of fitness function calls is limited to $1000000 \cdot D$. The population size is set to 25, except for algorithms using MIC, for which it is increased to 50. For BBOB problems, algorithms DE_LT+ and DE_MP+ are not considered. BBOB problems evaluation and results visualization are provided by COCO (COmparing Continuous Optimizers) platform [38].

Chapter **6** Results

In this chapter, the results of the experiments introduced in the previous chapter are presented. The results are divided into two sections.

6.1 Test problems

Firstly, results of the performance of the algorithms introduced in section 5.1 for the Test problems. Results are visualized in the form of graphs, which show the dependence of the number of fitness function calls on the dimension of a certain problem. These graphs are called scalability graphs. They show the most important facets of the algorithm's performance. Moreover, they provide a prediction regarding the performance on higher-dimensional problems.

Each data point is the median of successful runs. In order to display data over a very wide range of values in a compact way and get clearer results, a base-10 logarithmic scale is used for both axes of graphs. It is also worth noting that the y-axis does not start at zero.

The Test results may be divided into three groups according to separability into separable problems (sphere, Levy, Rastrigin), block-separable problems (SoREB), and non-separable problems (Rosenbrock, OSoREB).

6.1.1 Separable problems

The results on separable problems are shown in figure 6.1.

Both algorithms with full prior knowledge (DE_LT+, DE_MP+) perform very similarly for all three separable problems. DE_LT+ is a bit better for the easiest function (sphere). Nevertheless, DE_MP+ achieves a little better results for more difficult problems than DE_LT+ (for Levy and Rastrigin).

Since separable problems do not contain any dependencies between variables, it is not surprising that there is almost no difference in DE_LT_MIC and DE_LT+ performance because, for separable problems, all possible linkage trees should be equally good. Therefore, it does not matter what dependency matrix \mathcal{P} DE_LT_MIC finds and subsequently what linkage tree it builds. The linkage tree would be just as good as the one built by DE_LT+.

The DE_MP_MIC is slightly worse than DE_LT+, DE_MP+, and DE_LT_MIC, especially for higher dimensions. It is tough to recognize separability by MIC because the DE selection operator aligns individuals with the fitness contours. Therefore, DE_MP_MIC may determine some variables as dependent and build suboptimal MP-FOS, which results in worse performance.

Although both algorithms using non-linearity check (DE_LT_NC, DE_MP_NC) correctly recognize the separability of the problem and build the optimal FOS, they have achieved significantly worse results than other newly-introduced variants of DE. The difference is mainly caused by the fact that DE_LT_NC and DE_MP_NC use fitness function evaluations to find dependencies, in contrast to DE_LT+, DE_MP+, and DE_LT_MIC, which also build optimal FOS but do not waste fitness function evaluations.

It also provides an explanation of why DE_LT_NC outperforms DE_MP_NC. Since DE_LT_NC, DE_MP_NC build optimal FOS, the DE_LT_NC performs comparably to DE_LT+ within the crossover. Similar to DE_MP_NC and DE_MP+. Moreover, since DE_LT+ and DE_MP+ perform similarly, DE_LT_NC and DE_MP_NC use a comparable number of fitness function evaluations within the crossover. It is a fact that LT FOS has a necessarily higher cardinality than MP FOS for the same dimension. Therefore, DE_LT_NC finds the optimum within a fewer number of generations than DE_MP_NC. Since the dependency matrix is built in every second generation, DE_MP_NC uses more fitness function calls to find dependencies, resulting in decreased performance in comparison to DE_LT_NC.

CMA-ES achieved interesting results. For the sphere function, CMA-ES is a constant factor better than DE_LT+, DE_MP+, DE_LT_MIC, and DE_MP_MIC. Nevertheless, as the difficulty of optimization of functions grows, the performance of CMA-ES decreases. For the Levy function, CMA-ES performs similarly to the four mentioned algorithms, and for the hardest function (Rastrigin), CMA-ES is significantly worse and achieves results comparable to DE_LT_NC and DE_MP_NC. However, it is worth noting that CMA-ES scales better than NC variants of DE.

Finally, FMIN outperforms all algorithms for low dimensions of the sphere. Nevertheless, it scales very badly and gets outperformed by all algorithms in higher dimensions. FMIN is unable to find optimum, even for low dimensions, of harder functions such as Levy and Rastrigin. It is not surprising that FMIN is not able to find the global optimum of multimodal problems since FMIN performs the downhill simplex algorithm, which is a local optimizer rather than a global one.

6.1.2 Block-separable problems

The results on block-separable problems are shown in figure 6.2.

The separable problems are represented by the SoREB function with variable sizes of blocks (2, 3, 4, 5). The relationships between particular pairs of DE variants that use the same technique to build the dependency matrix are worth noting.

Firstly, DE_MP+ is a constant factor better than DE_LT+. It is not surprising since the block-separable structure of a problem may be represented by MP FOS very well.

However, for the second pair, which uses the non-linear check, it can be seen that the LT variant (DE_LT_NC) outperforms the MP variant (DE_MP_NC). Although DE_MP_NC builds the same FOS as DE_MP+, which perfectly captures the problem's structure, it cannot achieve better results than DE_LT_NC. It points to the fact that worse performance within the crossover is compensated by a lower number of fitness function evaluations used to find dependencies.

Lastly, MIC variants (DE_LT_MIC, DE_MP_MIC) perform almost similarly for block sizes two and three. For k = 4 and k = 5, DE_LT_MIC achieves better results than DE_MP_MIC for lower dimensions. Nevertheless, the dependent blocks are easier to recognize for the higher dimensions, and the DE_MP_MIC outperforms DE_LT_MIC.

The relationship between MIC variants and NC variants is also worth noting. It can be seen that for k = 2, both MIC variants perform similarly to DE_LT+ and better than NC variants. However, as the size of blocks increases, more dependencies occur. Hence NC variants outperform MIC variants. It is caused by the weaker ability of MIC to recognize dependencies.



Figure 6.1. Scalability graphs of separable problems. Each point is the median of successful runs.

The original DE_UNIFORM performance shows up as the worst of all considered algorithms for block-separable problems. For bigger sizes of blocks, DE_UNIFORM is even worse.

CMA-ES performs similarly for all SoREB variants, regardless of the size of blocks, in terms of the required number of evaluations. Since other algorithms need more evaluations for SoREB with bigger blocks, CMA-ES outperforms all algorithms except DE_MP+ for k = 5. Nevertheless, DE_LT+ and DE_MP+ outscale CMA-ES, with scalability comparable to DE_LT_NC and DE_MP_NC.

Last considered algorithm FMIN shows the best results for small dimension, but the worst scalability of all algorithms and the inability to find the optimum for higher dimensions.

Lastly, note that DE_LT+ and DE_LT_NC need, on average, more evaluations to find optimum for D = 5 than for D = 8 if k = 5. It shows certain limitations of LT when all variables are pairwise dependent.

6.1.3 Non-separable problems

The results on non-separable problems are shown in figure 6.3.

Firstly, it is worth noting that no DE variant that builds MP-FOS is capable of finding the optimum of the presented non-separable problems, even for a small dimension. It is probably caused by the overlapping dependency structure of both problems, which is impossible to model well enough by MP-FOS.



Figure 6.2. Scalability graphs of block-separable problems. Each point is the median of successful runs.

DE_LT+ and DE_LT_MIC perform almost identically. The same trend may be observed in figure 6.1, which represents results for separable functions. For the Rosenbrock, DE_LT+ and DE_LT_MIC scale better than DE_LT_NC. Nevertheless, for OS-oREB, DE_LT+ and DE_LT_MIC are only a constant factor better than DE_LT_NC. The slightly better relative scalability of DE_LT_NC for OSoREB towards DE_LT+ and DE_LT_MIC corresponds to the results obtained in figure 6.2 because OSoREB is in a sense closer to the block-separable problem than Rosenbrock, and the dependency structure of OSoREB may be captured better within LT-FOS than the structure of Rosenbrock. Therefore the impact of correct recognition of dependencies, which DE_LT_NC does, increases.

The same phenomenon may be seen in the performance of DE_UNIFORM, which is a constant factor better than DE_LT_NC for Rosenbrock, which is the function with a relatively small number of dependencies. Nevertheless, OSoREB contains more dependencies between variables than Rosenbrock. Therefore, as the number of dependencies increases in OSoREB, the scalability of DE_UNIFORM decreases and DE_UNIFORM is unable to find the optimum of OSoREB in higher dimensions.

On the other hand, the opposite trend can be viewed in the performance of CMA-ES, which outperforms all other algorithms. Nevertheless, for the Rosenbrock, the difference is less significant, and DE_LT+ and DE_LT_MIC seemed to scale better than CMA-ES.

Non-separable problems



Figure 6.3. Scalability graphs of non-separable problems. Each point is the median of successful runs.

For non-separable problems, similarly, as for others, FMIN shows up as the best algorithm for low dimensions but scales the worst. Therefore, it is almost useless for higher dimensions.

6.2 **BBOB problems**

The results on BBOB problems are presented by graphs of Empirical cumulative distribution functions (ECDFs) [39]. These ECDFs show on the y-axis the proportion of cases for which the number of fitness function evaluations needed to find the optimum was smaller than the value given on the x-axis. For the x-axis, a base-10 logarithmic scale is used, and the total number of fitness function evaluations is divided by dimension. Each graph also shows the performance of the best algorithm of BBOB workshop 2009 for a certain problem, which is noted as *best 2009*.

All results in this section were obtained by the COCO platform. Complete results contains 25 function for various dimensions (2, 3, 5, 10, 20, 40). Complete results are shown in Appendix B. In this section, only selected functions of dimensions 5 and 20 are shown. These functions were chosen to represent the characteristic trend seen for more functions.

Firstly, the set of functions on which all DE variants perform similar but worse than CMA-ES and best 2009. This set is represented by the so-called Ellipsoid separable function in figure 6.4.

Secondly, for a number of functions, MP variants of DE are outperformed by other DE variants, especially for higher dimensions. Nevertheless, LT and UNIFORM variants are outperformed by CMA-ES and by best 2009. An example of such a function may be seen in figure 6.5.

The third observed trend within BBOB functions is a significantly worse performance of DE variants against CMA-ES and best 2009. DE variants are unable to find the global optimum for the majority of these functions, especially in higher dimensions. Note that



Figure 6.4. Graphs of the empirical cumulative distribution functions of the introduced algorithms on the Ellipsoid separable function for dimensions 5 and 20.



Figure 6.5. Graphs of the empirical cumulative distribution functions of the introduced algorithms on the Bent function for dimensions 5 and 20.



Figure 6.6. Graphs of the empirical cumulative distribution functions of the introduced algorithms on the Griewank-Rosenbrock F8F2 function for dimensions 5 and 20.

these functions are mainly Multi-modal functions with a weak global structure. This trend is captured in figure 6.6.

Chapter **7** Conclusion

To conclude, the main goal of this work was to propose a crossover operator with dependency detection for DE.

Two representations of the dependency structure were introduced in chapter 3. First is the linkage tree (LT), which contains multiple levels of dependency, from univariate level to complete dependency, and the second is the marginal product (MP), which contains every problem variable exactly once.

Two approaches to finding pairwise dependencies between variables were introduced in chapter 4. Firstly, the fitness-based approach, called non-linearity check (NC), determines the possible dependency between a pair of variables according to the fitness values. Secondly, the distribution-based approach, known as maximal information coefficient (MIC), identifies dependencies based on the distribution of the population.

Subsequently, six new variants of DE differing in the crossover operator were proposed in section 5.1. Except for four regular variants using the above-mention methods (DE_LT_NC, DE_MP_NC, DE_LT_MIC, DE_MP_MIC), two artificial variants with full prior knowledge of the dependency structure (DE_LT+, DE_MP+) were also designed.

According to the results presented in section 6.1, newly proposed methods, as baselines, achieve fair scalability. All of them achieved greater scalability compared to the original DE (DE_UNIFORM) for almost all tested problems, independently of the dependency structure. They also showed enhanced scalability in comparison to the FMIN algorithm. Moreover, some of them exhibited greater scalability than the state-of-theart evolutionary algorithm CMA-ES in some cases. The application of any of the four proposed regular variants of DE would result in increased performance in comparison to the original one.

According to the results from the previous chapter, it may be concluded that linkage tree representation, thanks to its robustness, seems to be a better choice than marginal product representation.

It is worth noting that the results obtained by the NC methods should be compared to the MIC results with careful consideration. For instance, while NC methods can easily recognize the separability of two variables, the same task is challenging for MIC ones because the DE selection operator aligns individuals with the fitness contours. On the other hand, MIC variants, in contrast to NC ones, do not need any fitness function evaluations to find dependencies. The limitation of MIC is that DE usually takes advantage of relatively small populations. However, MIC achieves better results with more samples because it is a statistical method. On the other hand, MIC would probably be more noise resistant than NC. Nevertheless, so far, no experiments have not been presented to substantiate this assumption. Hence there is space for future work to prove or refute this hypothesis.

Although all four regular variants of DE enhance the performance of the original DE, they have some limitations which could be reduced by further adjustments.

For instance, *incremental dependency updating* described in [17] could significantly reduce the amount of fitness function evaluations used by NC methods to find depen-

dencies and decrease the difference in performance between NC methods and methods with full prior knowledge.

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Lastly, how to deal with problems containing overlapping sub-components remains unanswered. Because neither LT nor MP is able to represent these types of structures clearly. Moreover, the optimal linkage structure of these problems is unknown. Hence it would be very interesting to find the optimal structure for these problems.

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Appendix **A** Abbreviations

BBOB	Black box optimization benchmarking
CMA-ES	Covariance matrix adaptation evolution strategy
COCO	Comparing continuous optimizers
DE	Differential evolution
DE_LT	Differential evolution which uses the linkage tree to represent the structure
	of a problem
DE_LT+	Differential evolution which uses the linkage tree to represent the structure
	of a problem and has full prior knowledge of pairwise dependencies
DE_LT_MIC	Differential evolution which uses the linkage tree to represent the structure
	of a problem and finds dependencies by maximal information coefficient
DE_LT_NC	Differential evolution which uses the linkage tree to represent the structure
	of a problem and finds dependencies by non-linearity check
DE_MP	Differential evolution which uses the marginal product to represent the
	structure of a problem
DE_MP+	Differential evolution which uses the marginal product to represent the
	structure of a problem and has full prior knowledge of pairwise dependen-
	cies
DE_MP_MIC	Differential evolution which uses the marginal product to represent the
	structure of a problem and finds dependencies by maximal information
	coefficient
DE_MP_NC	Differential evolution which uses the marginal product to represent the
	structure of a problem and finds dependencies by non-linearity check
DE_UNIFORM	The original version of differential evolution
EA	Evolutionary algorithm
ECDFs	Empirical cumulative distribution functions
FOS	Family of subsets
LT	Linkage tree
MI	Mutual information
MIC	Maximal information coefficient
MP	Marginal product
NC	Non-linearity check
OSoREB	Overlapping Sum of Rotated Ellipsoid Blocks function
SoREB	Sum of Rotated Ellipsoid Blocks function

Appendix **B** Complete BBOB results



















.











best 2009

CMA-ES

UNIFORM

MP NC

MP NC

LT NC

TT MIC

МР МІС













Appendix **C** Implementation and content of attachments

Here, a brief description of the program used to generate results 6 is provided. All source codes together with README.txt file are on the enclosed CD. The program offers two functionalities for users.

Firstly, the procedure of finding the population size of chosen algorithms for chosen problems and dimensions, as was described in section 5.4.1.

Secondly, finding the median of successful runs of the selected algorithm for selected problem and dimension.

The content of attachments:

- BcThesis.pdf
- comparison.c
- \blacksquare comparison.h
- fitnessFunctions.c
- \blacksquare fitnessFunctions.h
- ∎ main.c
- Makefile
- mine.c [23]
- mine.h [23]
- parameters.c
- parameters.h
- README.txt
- search.c
- search.h
- utils.c
- utils.h