

Continuous Adaptive Population Reduction (CAPR) for Differential Evolution Optimization

SLAS Technology
1–17
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DOI: 10.1177/2472630317690318
jals.sagepub.com/home/jala


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Abstract

Differential evolution (DE) has been applied extensively in drug combination optimization studies in the past decade. It allows for identification of desired drug combinations with minimal experimental effort. This article proposes an adaptive population-sizing method for the DE algorithm. Our new method presents improvements in terms of efficiency and convergence over the original DE algorithm and constant stepwise population reduction-based DE algorithm, which would lead to a reduced number of cells and animals required to identify an optimal drug combination. The method continuously adjusts the reduction of the population size in accordance with the stage of the optimization process. Our adaptive scheme limits the population reduction to occur only at the exploitation stage. We believe that continuously adjusting for a more effective population size during the evolutionary process is the major reason for the significant improvement in the convergence speed of the DE algorithm. The performance of the method is evaluated through a set of unimodal and multimodal benchmark functions. In combining with self-adaptive schemes for mutation and crossover constants, this adaptive population reduction method can help shed light on the future direction of a completely parameter tune-free self-adaptive DE algorithm.

Keywords

differential evolution, self-adaptation, population size, global optimization, artificial intelligence

Introduction

Differential evolution (DE) is a simple, reliable, and efficient population-based real-parameter function optimizer derived from the evolutionary algorithm (EA).^{1–4} A number of studies have pointed out that compared with other evolutionary-based algorithms, DE is more practical and exhibits much better performance on a wide variety of problems.^{5–9} Recently, the DE algorithm has been applied in combinatorial drug studies, in which multiple drugs with multiple dose levels are present and an optimal drug combination is required to develop desired treatment efficacy. To identify the optimal drug combinations from a large pool of drug candidates is traditionally considered a tedious and prohibitive task. With the advancement of technology in the emerging interdisciplinary field of combinatorial drug optimization, feedback system control strategies that were conventionally applied mainly in the engineering domain have gradually been adapted for biological complex systems. The hybrid of biological experimental advancements and engineering optimization platforms has paved the way for a paradigm shift for new drug development in various disease models.^{10–16} For instance, Ding et al.¹⁵ applied DE to identify the optimal drug combination to treat herpes simplex virus type 1 (HSV-1). Nowak-Sliwinska et al.¹⁶ demonstrated the application of DE to identify the optimal drug combination to

treat cancer angiogenesis. Tsutsui et al.¹⁷ adopted DE in their effort to identify the optimal drug combinations for long-term maintenance of human embryonic stem cells. Honda . et al.¹⁸ proved DE could quickly provide a solution to control the osteogenesis process of human mesenchymal stem cells. The success of DE is found to be due to an implicit self-adaptation contained within the algorithmic structure, which makes it highly explorative at the beginning of the evolution and subsequently becomes more exploitative in the later stage of the optimization.¹⁹

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Received Oct 8, 2016.

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The simplicity, ease of implementation, and the great performance of DE in terms of accuracy, convergence speed, and robustness make it attractive for a diverse domain of real-world optimization problems. DE has been extensively applied in engineering fields such as robotics,⁵ electronics,²⁰ engineering,²¹ financial planning,²² risk management,²³ and medical applications.²⁴ A review of DE applications has been presented by Plagianakos et al.²⁵

Although it is clear to the scientific community that DE is a powerful global optimization algorithm, there still remains considerable margin of improvement. This triggered extensive research efforts over the past decade, resulting in a wealth of variants designed to improve the performance of the original DE.^{5,6}

The performance of the original DE algorithm is mainly affected by three control parameters: the mutation factor F , the crossover constant CR , and the population size NP . Because these values have to be tuned to fit specific optimization applications, a major problem that researchers face is the choice of a right set of control parameters. This problem is amplified when DE is employed for handling various difficulties in real-world applications such as high dimensionality and noisy optimization problems. In view of this, a wealth of DE variants has been proposed to improve the robustness and efficiency through the application of adaptive or self-adaptive techniques.^{26–30}

Neri and Tirronen⁵ suggested that, among a selection of DE variants, population size reduction, dynNP-DE, proposed by Brest and Maucec,³¹ is one of the most effective algorithmic components in terms of robustness and efficiency, whereas the self-adaptive control parameter scheme (jDE) proposed by Brest and Maucec³² is superior in terms of robustness and versatility over a diverse benchmark functions.

In this work, we propose a new population reduction method that can dynamically and continuously reduce the population size in response to the optimization progress. Our new method presents improvements in terms of efficiency and convergence over dynNP-DE. The method is DE structure independent, so it can be integrated into any type of DE variant.

This article is organized as follows. The next section reviews the background of the original DE algorithm and surveys recent work on different variants of DE. The third section describes the mechanism of the self-adaptive control parameter DE scheme. The section also provides the detailed mechanism and properties of our new population-based method, which we termed the *continuous adaptive population reduction* (CAPR) method. The fourth section presents experimental results on the comparisons of the performance between our new method and the well-studied population reduction scheme dynNP-DE, by testing with well-known benchmark functions under a wide range of dimensions. The fifth section discusses the experimental results. The sixth section concludes this work.

Related Works

Most of the DE variants proposed in the literature are based on either adaptation or self-adaptation of the crossover and mutation rate, namely, F and CR .^{26,29,32–35} These variants of DE have been shown to greatly improve the robustness and efficiency by dynamically adjusting the control parameters.

Liu and Lampinen³³ proposed a fuzzy adaptive DE algorithm that uses fuzzy logic controllers to adapt the search parameters for the mutation and crossover operations. Brest et al.²⁷ proposed a self-adaptive scheme (jDE) in which the control parameters F and CR are assigned to each agent in the population. Better agents, resulted from better control parameters, are more likely to produce better offspring to survive the selection process. These offspring in turn enhance the likelihood for the better parameter values to propagate. Das et al.³⁶ modified the original mutation scheme in DE by involving both global and local neighbors, which are defined as the entire population and a portion of the nearby agents in the population, respectively. The combined contributions between these two parts are weighted self-adaptively. Neri and Tirronen³⁵ proposed a scale factor local search DE, which applied a local search with certain probability to the scale factor F , corresponding to the offspring with higher performance, during the generation of an offspring.

Besides the variants that focused on the adaptation and self-adaptation of the control parameters, others focused on the adaptation of various mutation strategies or hybridization with other strategies. Fan and Lampinen³⁷ proposed the trigonometric differential evolution (TDE) in which the mutation operation is replaced by a trigonometric mutation scheme with a prefixed probability. Qin and Suganthan²⁹ proposed a self-adaptive DE (SaDE) algorithm in which different mutation strategies are allowed to switch between each other while F and CR are allowed to self-adapt without any predefinition. Rahnamayan et al.³⁸ proposed an opposition-based DE that applies the logic of opposition points to generate initial population. The method improves the convergence properties of DE on noisy and large-scale problems. Mezura-Montes et al.³⁹ conducted a comparison study on the different DE variants.

Besides controlling the mutation and crossover parameters, it should be obvious that varying the population size during the optimization process could also be a highly rewarding approach. However, population size has so far not been studied as much as the other two control parameters. In contrast, in the context of EAs, population-sizing schemes have long been investigated in a number of works, such as Genetic Algorithm with Varying Population Size (GAVaPS),⁴⁰ Adaptive Population size Genetic Algorithm,⁴¹ Random Variation of Population Size GA,⁴² and Population Resizing on Fitness Improvement GA.⁴³ Lobo and Lima⁴⁴ surveyed a variety of population-sizing schemes for EAs.

The effect of population size NP on the DE algorithm is analogous to the EAs in which too small a population could cause premature convergence and too large a population could lead to stagnation.⁴⁵ In the context of DE, there exist a few works that focused on the population size. Teo³⁴ made the first attempt by self-adapting NP using an absolute and relative encoding scheme which was improved by Teng et al.⁴⁶ Neri et al.²⁴ proposed an integration of fitness diversity into the DE structure where population size and the other parameters encoded within each agent are self-adapted based on a measurement of the fitness diversity. Brest and Maucec³¹ proposed a population size reduction scheme in which the population size is reduced in a step-wise fashion during the optimization process, so as to avoid DE stagnation with high dimensional problems. The idea is shown to significantly improve robustness for large-scale problems.^{31,47}

In addition, several new variants of population-resizing mechanisms have been proposed recently in the framework of DE. Zhang et al.⁴⁸ recently incorporated the lifetime and extinction mechanisms of GaVAPS to regulate the population size in an adaptive manner. Dziedzic⁴⁹ proposed a clustering-based population size reduction method in which only the best specimens from each of the resulting clusters are transferred to the next generation. Wang and Zhao⁵⁰ proposed a self-adaptive population-resizing mechanism, SapsDE, in which the population size can be adjusted dynamically by eliminating a fixed amount of poorest performing population based on some online solution-search status. Zamuda et al.⁵¹ proposed a structured population size reduction algorithm in which dynNP-DE is combined with multiple population size-dependent mutation strategies using a structured population.

DE and Related Algorithms

DE is a stochastic, population-based algorithm developed for real-valued function optimization problems.² It operates by having a population of agents (\mathbf{x} vector) that move around in the search space by recombining through crossover and mutation with other existing agents in the population. Through an aggressive selection process, a newly generated agent is accepted as part of the population if the new agent \mathbf{x} is an improvement; otherwise, it is discarded. This iteration process is repeated to find a vector \mathbf{x} that optimizes a function $f(\mathbf{x})$.

A brief description of the original DE algorithm² iteration procedures is as follows:

1. Generate a population of D -dimensional target vectors $\mathbf{x}_{i,G} = \{x_{1i,G}, x_{2i,G}, \dots, x_{Di,G}\}$, $i = 1, 2, \dots, NP$ from the solution space S . D is the dimensionality of the function f . $S \subseteq R^D$ is the D -dimensional search space for the problem. NP is the population size, and

G is the iterative generation. The initial population is selected randomly from a uniform distribution between upper and lower bounds, $x_{j,low}$ and $x_{j,upp}$, defined for each variable x_j , $j \in \{1, \dots, D\}$.

2. Generate a trial vector $\mathbf{u}_{i,G+1}$ for each vector $\mathbf{x}_{i,G}$ in turn by employing mutation, crossover, and selection procedures as follows, until either a value to reach (VTR) or maximum number function evaluations (MaxFES) criterion is reached:

- a. Mutation: Generate a mutant vector $\mathbf{v}_{i,G}$ using DE/rand/1 strategy for each vector $\mathbf{x}_{i,G}$:

$$\mathbf{v}_{i,G+1} = \mathbf{x}_{r1,G} + F \cdot (\mathbf{x}_{r2,G} - \mathbf{x}_{r3,G}) \quad (1)$$

where $r1, r2, r3 \in \{1, \dots, NP\}$ are random indexes and are mutually different from each other and i . F is the amplification factor $\in [0, 1]$, which controls the amplification of the differential variation $(\mathbf{x}_{r2,G} - \mathbf{x}_{r3,G})$.

- b. Crossover: Perform binomial crossover:

$$u_{ji,G+1} = \begin{cases} v_{ji,G+1}, & \text{if } \text{rand}(j) \leq CR \\ x_{ji,G}, & \text{otherwise.} \end{cases} \quad (2)$$

where CR is the crossover control parameter.

- c. Selection: Perform selection between the trial vector and target vector using a greedy selection criterion:

$$\mathbf{x}_{i,G+1} = \begin{cases} \mathbf{u}_{i,G}, & \text{if } f(\mathbf{u}_{i,G+1}) \leq f(\mathbf{x}_{i,G}) \\ \mathbf{x}_{i,G}, & \text{otherwise.} \end{cases} \quad (3)$$

3. Output the results of the best target vector.

Self-adaptive DE algorithms eliminate the manual tuning of F and CR for different types of functions. To facilitate the sole comparison with an existing dynamic population reduction algorithm, we used the same self-adaptive schemes and parameter settings as presented in Brest et al.⁵² This self-adaptive scheme has been shown to provide enhanced robustness and great performance for large-scale problems,⁴⁸ constrained optimization,⁵³ and multi-objective problems⁵⁴ and has been extensively discussed.^{5,6}

The method allows a self-tuning of the control parameters, F and CR , of each individual agent in the population in each iteration. $F_{i,G+1}$ and $CR_{i,G+1}$ are updated according to the following scheme:

$$F_{i,G+1} = \begin{cases} F_i + \text{rand}_1 \cdot F_u, & \text{if } \text{rand}_2 < \tau_1 \\ F_{i,G}, & \text{otherwise.} \end{cases} \quad (4)$$

$$CR_{i,G+1} = \begin{cases} rand_3, & \text{if } rand_4 < \tau_2 \\ CR_{i,G}, & \text{otherwise.} \end{cases} \quad (5)$$

where $rand_j, j \in \{1, 2, 3, 4\}$, are uniformly distributed random values between 0 and 1; τ_1 and τ_2 are constant values, 0.1, which represent the probabilities that the control parameters F and CR are updated, respectively. F_l and F_u are constant values, 0.1 and 0.9, respectively, which represent the minimum and maximum values that F can take. This allowed $F_{i,G+1}$ and $CR_{i,G+1}$ to take a value from [0.1, 1.0] and [0, 1], respectively, in a random manner. These parameters are renewed before each trial vector generation and are used during the mutation, crossover, and selection steps during the creation of each offspring $x_{i,G+1}$.

In this section, we introduce our CAPR scheme. We have mentioned in the previous section that two control parameters, F and CR , can be self-adapted within each individual agent during each iteration run, through a self-adaptive DE scheme (jDE).²⁷ To further improve the efficiency of the DE algorithm, we propose a new dynamic population size reduction scheme that eliminates the manual tuning of the third control parameter, NP . The method gradually reduced the population size according to the change of gradient of the fitness value. A new NP is calculated after one cycle of function evaluations for all agents in the population:

$$NP_{G+1} = \begin{cases} \sqrt[\alpha]{\Delta_G / \Delta_{G-1}}, & 0 < \Delta_G / \Delta_{G-1} < 1 \\ NP_G, & \text{otherwise} \end{cases} \quad (6)$$

$$NP_{G+1} = \begin{cases} NP_{G+1}, & NP_{G+1} > NP_{min} \\ NP_{min}, & NP_{G+1} \leq NP_{min} \end{cases} \quad (7)$$

where

$$\Delta_G = \frac{f_{ave}(x_G) - f_{ave}(x_{G-1})}{f_{ave}(x_G)}, \Delta_{G-1} = \frac{f_{ave}(x_{G-1}) - f_{ave}(x_{G-2})}{f_{ave}(x_{G-1})} \quad (8)$$

After one cycle of evaluation of all agents in the population (i.e., NP_G function evaluations), the evaluated function values of all agents in the population are averaged to be $f_{ave}(x_G)$. This value, together with that from the previous evaluation cycle, is used to calculate the normalized gradient value Δ_G (8). Δ_{G-1} is calculated in a similar fashion using the previous average function evaluation value, $f_{ave}(x_{G-1})$, and the one before the previous, $f_{ave}(x_{G-2})$. If the ratio Δ_G / Δ_{G-1} is within the range of [0, 1], then NP is reduced by a fraction equal to the α -th root of the ratio of Δ_G / Δ_{G-1} . The reason for taking a root of the ratio is to slow down the population size reduction rate. Unless stated otherwise, the parameter α takes a value of 100.

The design behind our population reduction scheme was inspired by dynNP-DE proposed by Brest and Maucec.³¹ In their method, population reduction was

performed in a stepwise fashion a few times throughout the whole optimization process. The numbers of function evaluations are distributed evenly for each population size. More specifically, the algorithm was predefined to reduce the population by $pmax$ number of times. After each size reduction, the new population size is always equal to half of the previous population size. During the population reduction, one individual from each half of the current population is compared based on their fitness values, and the better one becomes the survivor for the next generation. For example, if the total number of function evaluations is predefined as 100,000, $pmax = 4$, and initial population = 200, the population size for each generation will be $NP_i \in \{200, 100, 50, 25\}$, and each generation will last for $100,000/pmax/NP_i = \{125, 250, 500, 1000\}$ number of function evaluations. This stepwise population size reduction mechanism allows us to wonder about the possibility of a continuous, instead of stepwise, population size reduction scheme that may more efficiently and interactively reduce the population size.

In CAPR, the population size reduction rate is dependent on the gradient of optimization performance. Compared with dynNP-DE, in which the population is always reduced by half of the previous population for a predefined number of times, the population reduction size in CAPR is not a constant but a variable based on the performance of the current and previous iterations. The population is reduced only if the gradient of the current generation, Δ_G , is lower than the gradient of the previous generation, Δ_{G-1} . As is for all population-based evolutionary algorithms, a large pool of diverse populations is required at the beginning of the optimization process for exploration reasons. In the later stages of the evolutionary process, exploitation should take place to improve the best-so-far individuals. Exploitation should start only when exploration starts to slow down. Therefore, an increase in the gradient simply means the optimization process is still in the exploration phase, and therefore, reduction of population size should not be carried out. For the same reason, if the current gradient has an opposite sign of the previous gradient, which means the performance of the current iteration is worse than the previous iteration, the population will also not be reduced.

Moreover, because of the fast population reduction rate of CAPR, we do not perform any sorting or comparison, which keeps only the best individuals in the reduced NP population. Instead, we simply randomly truncate the excessive agents in the population. This prevents the method from always picking the best individuals, which may trap the optimization into local optimum. This also avoids any addition on the time complexity to the algorithm.

We have limited the minimum population size, NP_{min} , to be the same as the dimension. This is higher than the minimum requirement of standard DE, which is 4 ($r1, r2, r3$, and i itself), for the crossover step. We found that the higher NP_{min} is helpful to our algorithm. As we will notice

Table I. Unimodal and Multimodal Benchmark Functions f_1 to f_{13} .

Name	Function	Range	$f_{optimal}$
Sphere function	$f_1(x) = \sum_{i=1}^D x_i^2$	[-100, 100]	0
Schwefel's problem 2.22	$f_2(x) = \sum_{i=1}^D x_i + \prod_{i=1}^D x_i $	[-10, 10]	0
Schwefel's problem 1.2	$f_3(x) = \sum_{i=1}^D \left(\sum_{j=1}^i x_j \right)^2$	[-100, 100]	0
Schwefel's problem 2.21	$f_4(x) = \max \{ x_i , 1 \leq i \leq D \}$	[-100, 100]	0
Rosenbrock's function	$f_5(x) = \sum_{i=1}^{D-1} \left[100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2 \right]$	[-30, 30]	0
Step function	$f_6(x) = \sum_{i=1}^D (x_i + 0.5)^2$	[-100, 100]	0
Quartic function	$f_7(x) = \sum_{i=1}^D i x_i^4 + \text{random}[0,1)$	[-1.28, 1.28]	0
Schwefel's problem 2.26	$f_8(x) = \sum_{i=1}^D -x_i \sin(\sqrt{ x_i })$	[-500, 500]	-12,569.5
Rastrigin's function	$f_9(x) = \sum_{i=1}^D [x_i^2 - 10 \cos(2\pi x_i) + 10]$	[-5.12, 5.12]	0
Ackley's function	$f_{10}(x) = -20 \exp \left(-0.2 \sqrt{\frac{1}{D} \sum_{i=1}^D x_i^2} \right) - \exp \left(\frac{1}{D} \sum_{i=1}^D \cos 2\pi x_i \right) + 20 + e$	[-32, 32]	0
Griewank function	$f_{11}(x) = \frac{1}{4000} \sum_{i=1}^D x_i^2 - \prod_{i=1}^D \cos \left(\frac{x_i}{\sqrt{i}} \right) + 1$	[-600, 600]	0
Penalized functions	$f_{12}(x) = \frac{\pi}{D} \{ 10 \sin^2(\pi y_1) + \sum_{i=1}^{D-1} (y_i - 1)^2 [1 + 10 \sin^2(\pi y_{i+1})] + (y_D - 1)^2 \} + \sum_{i=1}^D u(x_i, 10, 100, 4)$ $y_i = 1 + \frac{1}{4} (x_i + 1),$ $u(x_i, a, k, m) = \begin{cases} k(x_i - a)^m, & x_i > a, \\ 0, & -a \leq x_i \leq a \\ k(-x_i - a)^m, & x_i < -a \end{cases}$	[-50, 50]	0
Penalized functions	$f_{13}(x) = 0.1 \left\{ \sin^2(3\pi x_1) + \sum_{i=1}^{D-1} (x_i - 1)^2 [1 + \sin^2(3\pi x_{i+1})] + (x_D - 1)^2 [1 + \sin^2(2\pi x_D)] \right\} + \sum_{i=1}^D u(x_i, 5, 100, 4)$	[-50, 50]	0

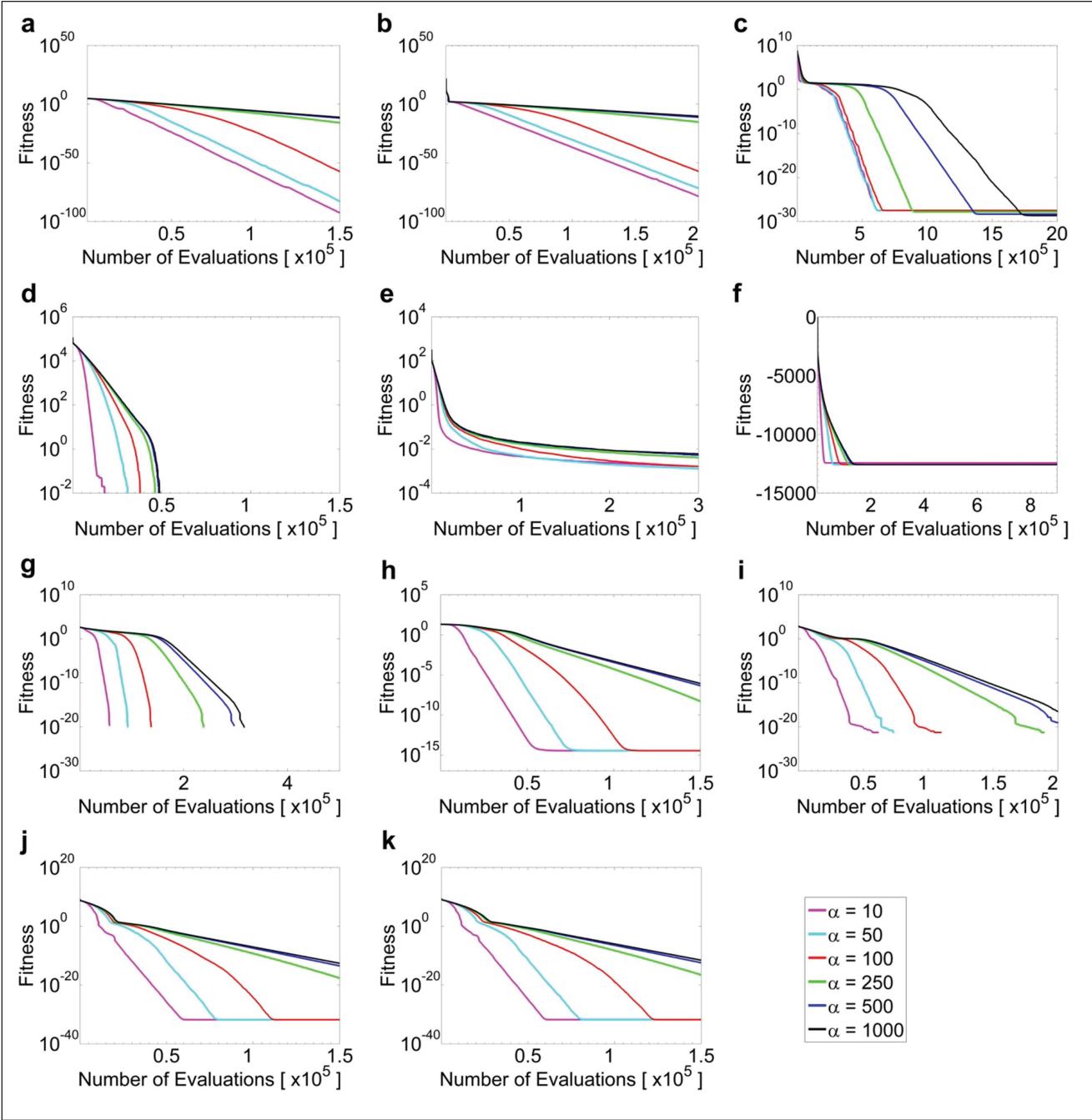


Figure 1. Average fitness value of all performing agents averaged over 100 independent experiments for f_1 (a), f_2 (b), f_5 (c), f_6 (d), f_7 (e), f_8 (f), f_9 (g), f_{10} (h), f_{11} (i), f_{12} (j), and f_{13} (k) at $D = 30$ at different α values (see legends).

be seen from the parametric study shown in **Table 5**. Nonetheless, the graphs present a robust performance and improved convergence efficiency of CAPR.

Figure 3 presents the comparison between CAPR and dynNP-DE on the iteration dynamics of the average fitness and NP values at $D = 60$ and 90 with $NP_{init} \in \{200,$

$400\}$. Both the curves of best fitness and NP values are plotted. Same as **Table 6** and **Figure 3**, $pmax = 4$ is used for $NP_{init} = 200$ and $pmax = 5$ is used for $NP_{init} = 400$ for the dynNP-DE algorithm. The other control parameter settings remain unchanged as the previous experiments. For all functions, CAPR reaches optimal fitness faster than

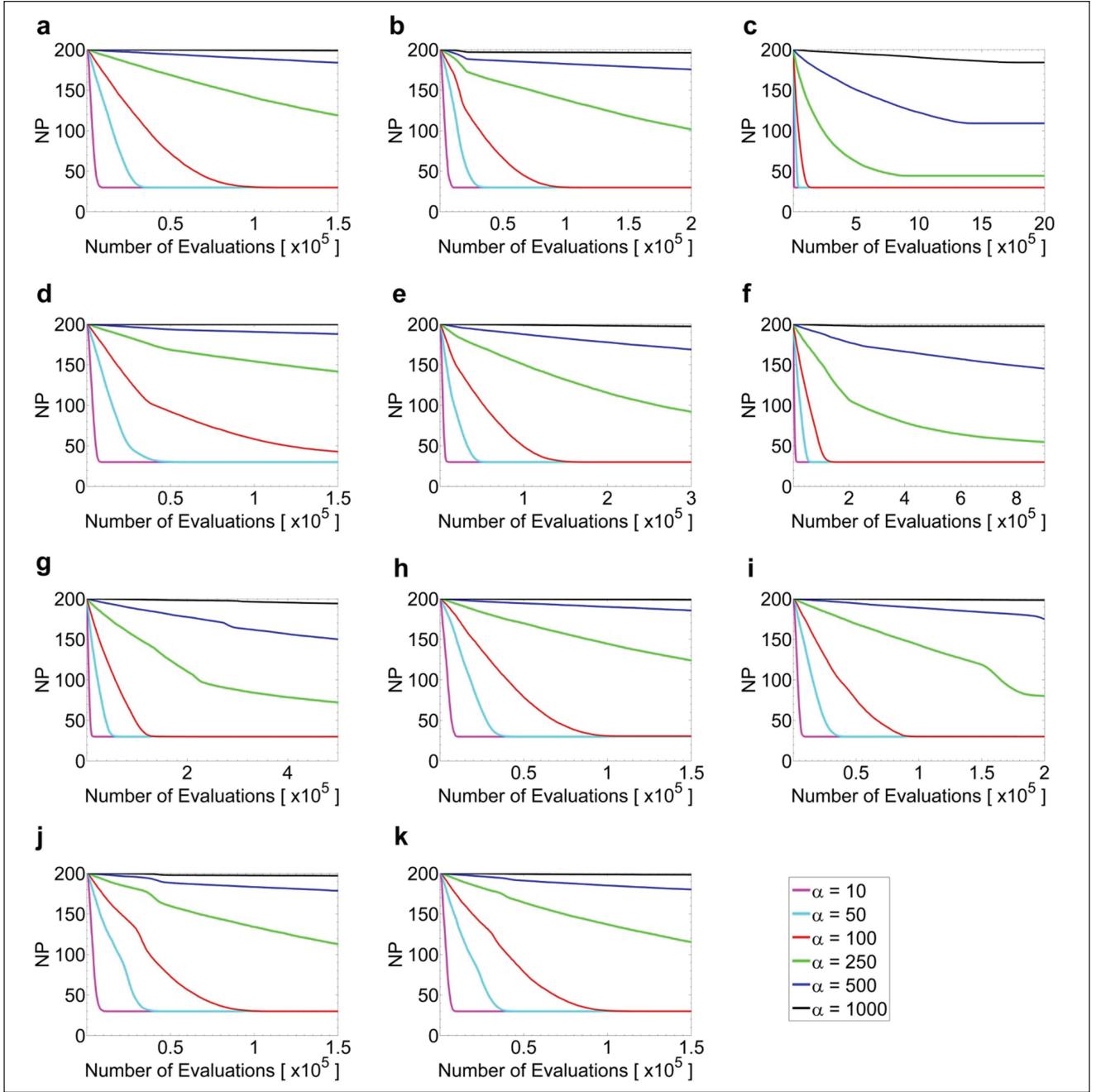


Figure 2. Average population size of all performing agents averaged over 100 independent experiments for f_1 (a), f_2 (b), f_5 (c), f_6 (d), f_7 (e), f_8 (f), f_9 (g), f_{10} (h), f_{11} (i), f_{12} (j), and f_{13} (k) for $D = 30$ at different α values (see legends).

dynNP-DE when comparing to figs. 15 to 25 in Brest and Maucec.³¹

We also tested some low-dimensional functions, f_{14} to f_{21} , which have only a few local minima.⁵⁴ Because the dimension D is much lower than the previous experiments, we lowered NP_{init} to 50 as suggested previously, where NP_{init} should be chosen to be about $5 \times D$ to $10 \times D^2$. Moreover, NP_{min} is also lowered to 4. **Table 7** shows the

comparison of performance of CAPR with dynNP-DE and the original DE.

CAPR shows slightly better performance than dynNP-DE for most functions, except f_{14} and f_{15} . Other than f_{15} , all three methods can reach the same global optimal values with CAPR showing the best in terms of standard deviations. Considering the fact that even the original DE can reach the global optimal values, which is not the case for f_1

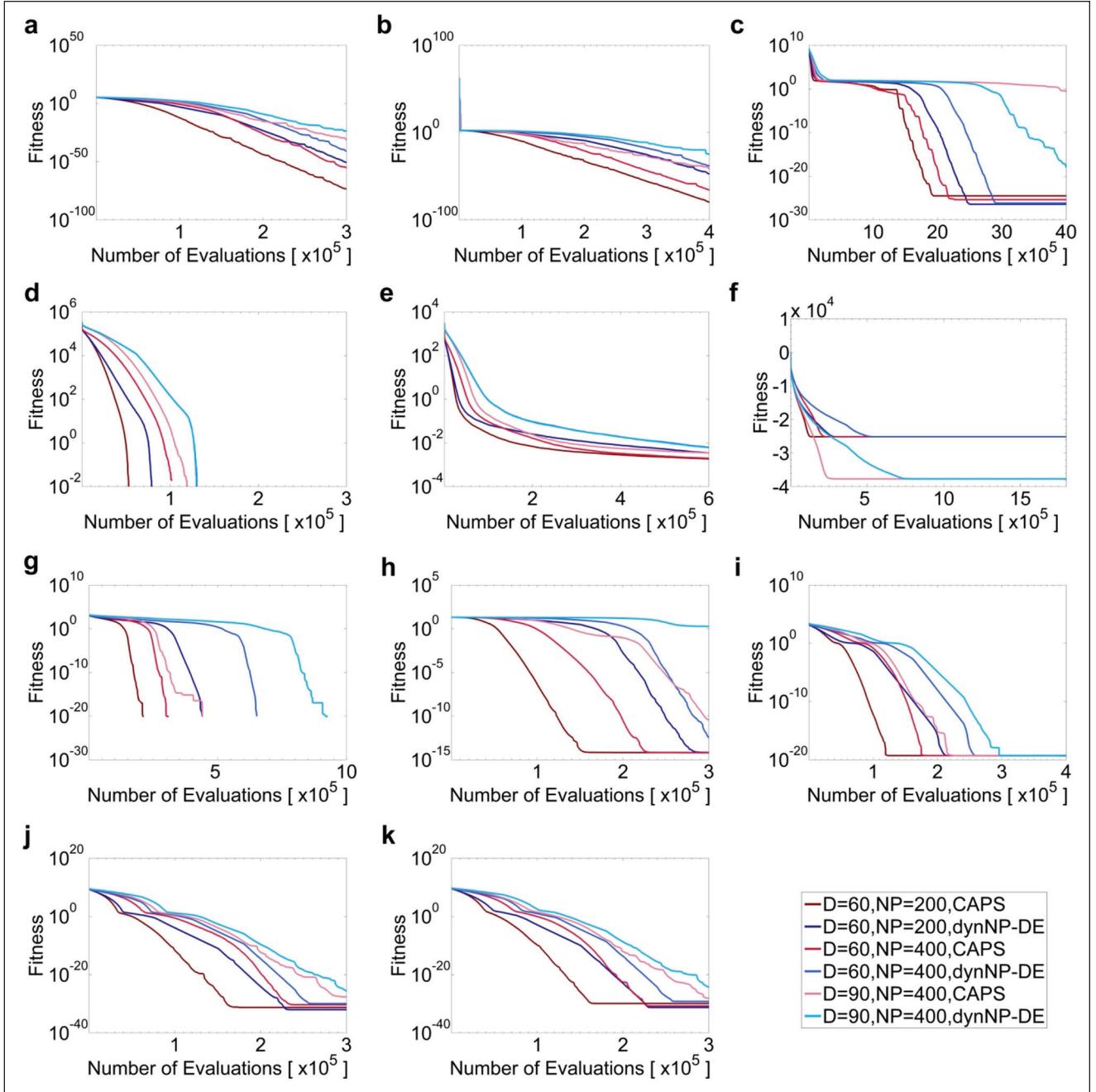


Figure 3. Comparison of average fitness values of all performing agents averaged over 100 independent experiments for f_1 (a), f_2 (b), f_5 (c), f_6 (d), f_7 (e), f_8 (f), f_9 (g), f_{10} (h), f_{11} (i), f_{12} (j), and f_{13} (k) between CAPR (red color-based lines) and dynNP-DE algorithms (blue color-based lines; see legends).

exploration-exploitation stage in the evolutionary process is an effective way to enhance the DE convergence efficiency.

One important feature of our population reduction scheme is that we limit the population reduction to happen only when the gradient ratio (Δ_G/Δ_{G-1}) is between 0 and 1. This limits exploitation (refining the best population) to occur only when improvement starts to slow down. If the

gradient ratio of the current iteration is greater than 1 (much better performance than previous iteration) or worse than that in the previous generation, no population reduction will take place.

It is always desirable to have an optimization algorithm be both effective and robust. CAPR improves, besides the final fitness values, significantly on the speed

Funding

The authors disclosed receipt of the following financial support for the research, authorship, and/or publication of this article: This work was supported by National Natural Science Foundation of China (81301293) and National Science and Technology Major Projects for “Major New Drugs Innovation and Development” (2014ZX09507008).

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