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A Unified Framework for Symbiosis of Evolutionary Mechanisms with Application to Water Clusters Potential Model Design

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Abstract—This article presents a theoretic model for facilitating the emergence of productive search profiles transpiring from the symbiosis of gene (stochastic variation) and meme (lifetime learning) working in synergy. The *evolvability* measure of the symbiotic search profiles for each individual is quantified by means of statistical learning on distinct sample vectors encountered along the search. The most productive search profile inferred for an individual, as defined by *evolvability* measure, is subsequently used to work on it, leading to the self-configuration of solvers that acclimatizes to suit the given problem of interest. Empirical studies on representative problems are presented to reflect the characteristics of symbiotic evolution. Assessment made against several recent state-of-the-art evolutionary and adaptive search algorithms highlighted the efficacy of the theoretic formalism of evolutionary mechanisms in symbiosis for autonomic search. As the design of computationally cheap advanced empirical water models for the understanding of enigmatic properties of water remains an important and unsolved problem, the article presents an illustration of symbiotic evolution for the design of $(\text{H}_2\text{O})_n$ or water clusters potential model.

I. Introduction

In computational intelligence, it is well established that the core issue to designing of successful stochastic search lies in balancing well between generality (through stochastic variations) and problem specificity (through lifetime learning) [1, 2]. Taking fundamentals from Darwinian principles of natural evolution and Dawkins notion of a meme, for instance, many modern evolutionary algorithms in the field of computational intelligence have opted to incorporate domain expert knowledge, each designed and crafted specifically for addressing particular problems or domains, and with much success reported [3–7]. This usual practice on manual crafting of dedicated search algorithm to suit a given problem in hand, however, is evolving into self-configuring algorithms that acclimatize adaptively to suit the problem [8–10].

Today, the design of successful adaptive search algorithms has emerged as one of the great challenges of computational intelligence. One of the conventional topics pertinent to their design is to identify which individuals of the search population should undergo lifetime learning, where for instance fitness and distribution-based strategies have been investigated. On the question pertaining to how often lifetime learning should be used, [11] suggested to apply learning on every individual when the computational complexity of the lifetime learning procedure is low, while others indicated otherwise. Schemes to adapt the frequency of lifetime learning based on search diversity and fitness distribution criteria, both independently and simultaneously, have also been considered [12, 13]. In addition, the concept of local search chains to adapt the intensity of lifetime learning was also studied recently in [14]. There are also studies on adapting appropriate lifetime learning procedures or otherwise often referred in the literature as local heuristics, local search(es) or meme(s) to employ, when solving specific problems or domains, including vertical inheritance by means

of coevolution [15] and meme selection via heuristics [10]. To address the overall balance of stochastic variation and lifetime learning in search, a theoretical upper bound on the computational budget to allocate was also considered [16]. The bound provided a means to adapt various design issues of MA simultaneously, and at runtime, from which individuals that should undergo lifetime learning, to the amount of computational budget allocated for learning. To alleviate the potentially high intensity and computational budget incurred in lifetime learning, especially when dealing with real world complex problems plagued with computationally expensive cost functions, management schemes to adapt the use of approximation models or surrogates in lieu of the original objective functions [17] have also been considered.

To summarize, several adaptive search algorithms have been proposed in recent years, with many shown to solve a great variety of optimization problems more effectively and robustly than their canonical counterparts. Existing schemes proposed for performing the adaptations however, are mostly designed based on semi-ad-hoc or heuristic/ meta-heuristic methods that comes with little theoretical rigor. More importantly, few have explicitly modelled the dynamics of stochastic variations and lifetime learning in search. Further, in contrast to earlier efforts, the focus of the present article is on modeling the *symbiosis*¹ or synergy of genetic and memetic mechanisms in evolutionary search, which perhaps has the greatest influence on search performance, but has remained yet to be formally investigated with vigor. Taking this cue, we present a theoretic study on *symbiosis* in adaptive search and its practicality to complex optimization in the context of non-linear programming. In the study, we propose a unified evolutionary model that facilitates the emergence and

¹In biology, the term '*Symbiosis*' commonly refers to the interactions of two dissimilar organisms or species, living together [18].

In this study, we propose a unified evolutionary model that facilitates the emergence and self-configuration of productive search profiles, transpiring from the symbiosis of stochastic variation and lifetime learning.

self-configuration of productive search profiles, transpiring from the symbiosis of stochastic variation and lifetime learning. In particular, the image of an adaptive search algorithm is modeled here as a *symbiosis* of gene and meme, or more precisely in search, the *symbiosis* of genetic (through stochastic variation) and memetic mechanisms (through lifetime learning), working in sync on solving the given problem in hand. Last but not least, it is worth noting that to date the core interest of taking such a pursue of research on partnering species of memes and genes is nonetheless motivated by the potential benefits brought about from the constructive synergy of stochastic variation and lifetime learning in accelerating search performances.

The present article is organized as follows: Section II introduces the present research with a treat on the theoretical modeling of *Symbiosis* in adaptive search. The propensity of symbiotic search profile composing of stochastic variation and lifetime learning, in creating viable or “potentially favorable” individuals that lead towards the global optimum, is then defined using the concept of *evolvability*. Section III proceeds to discuss on Symbiotic Evolution (SE) as a realization of the proposed theory on symbiosis in the context of evolutionary computation, for solving complex problems. Taking a data-centric paradigm in the spirit of Optinformatics [19], SE performs the statistical learning of *evolvability*, at runtime, to infer the most productive symbiotic search profile for use on a given solution individual, leading to a self-configuring solver that adapts to search on the given problem in hand. Section IV presents a numerical study on the search performance of SE while Section V analyzes the performances of SE with assessment made against several recent state-of-the-art modern evolutionary methods, adaptive and hybrid approaches. Further, Section VI illustrates Symbiotic Evolution for optimizing the OSS2 potential model that describes $(\text{H}_2\text{O})_n$ water clusters when no prior knowledge of suitable search profile on the problem is available. Finally, Section VII concludes the present study with a brief discussion.

II. A Theoretic Modeling of Symbiosis for Adaptive Search

In this section, the theoretical modeling of *symbiosis* in adaptive search is presented. In particular, we begin by first quantifying the roles of gene (stochastic variations) and meme (lifetime learning) in symbiosis, using the concept of *evolvability*. Subsequently an illustration of successful symbiosis that benefits search is given.

A. Gene and Meme in Symbiosis

The image of modern adaptive algorithms in computational intelligence can be established as a *symbiosis* of gene and meme,

or more precisely in evolutionary search, the *symbiosis* of genetic (through its stochastic variation) and memetic mechanisms (through lifetime or individual learning²), working in sync on the given problem in hand. In most research work on adaptive evolutionary algorithms, the symbiosis of meme and gene are

generally studied as separate independent entities consisting of the variation and individual learning phases, which is evident in the works of Hinterding *et al.* [20] and Ong *et al.* [21]. Until now, existing schemes proposed for performing the adaptations however, are mostly designed based on semi-ad-hoc or heuristic/ meta-heuristic methods that comes with little theoretical rigor. More importantly, few have explicitly constructed a formal modeling on the combined behaviors of stochastic variations and lifetime learning in search.

Here, we model the solver’s behavior that emerged from the *symbiosis* of gene and meme in search as a directed graph that defines the *connectivity probability* of local optimum solutions, more precisely, the probability of “jumping” from one local optimum to another as determined by the stochastic variation and individual learning used [22]. Figure 1 depicts an example where the connectivity of local optimums exhibited by three adaptive search algorithms is depicted on the contour plot of a search problem landscape. The symbiotic search profiles, as defined by the interactions of unique stochastic variation and lifetime learning mechanisms, are then represented by broken and/or continuous directed edges³ in Figure 1(a), (b), and (c), respectively. In the figures, search profile \mathbb{Y} (represented by continuous line) is depicted as more effective for finding good quality solutions that are close to the global optimum faster than profile \mathbb{X} (represented by broken line), while the latter is shown as more effective in converging to the precise global optimum, although more hops (denoting the computational effort incurred) are required. Thus profiles \mathbb{X} and \mathbb{Y} display strength in solution precision and efficiency, respectively. The emergent behavior resulting from the interactions by unique stochastic variations and lifetime learning mechanisms working in symbiosis, i.e., search profiles $\mathbb{X} + \mathbb{Y}$, as depicted in Figure 1(c), if appropriately harvested, would lead to a higher probability of discovering the global optimum at high precision and efficiency in search, thus forms the core motivation of the present study.

B. Evolvability of Symbiotic Search Profile

In this subsection, we introduce the concept on the “*Evolvability*” of symbiotic search profile as the basis for adaptation. Since the term “*Evolvability*” has been used in different contexts⁴, it is

²Note that the term *lifetime learning* is used interchangeable with *individual learning* throughout this paper.

³Note that only the edge with highest probability of reaching a minimum among all others is depicted.

⁴In [23], “*evolvability*” is defined as the genome’s ability to produce adaptive variants when acted upon by the genetic system. Others have generally refer the term to the ability of stochastic or random variations to produce improvement for adaptation to happen [21].

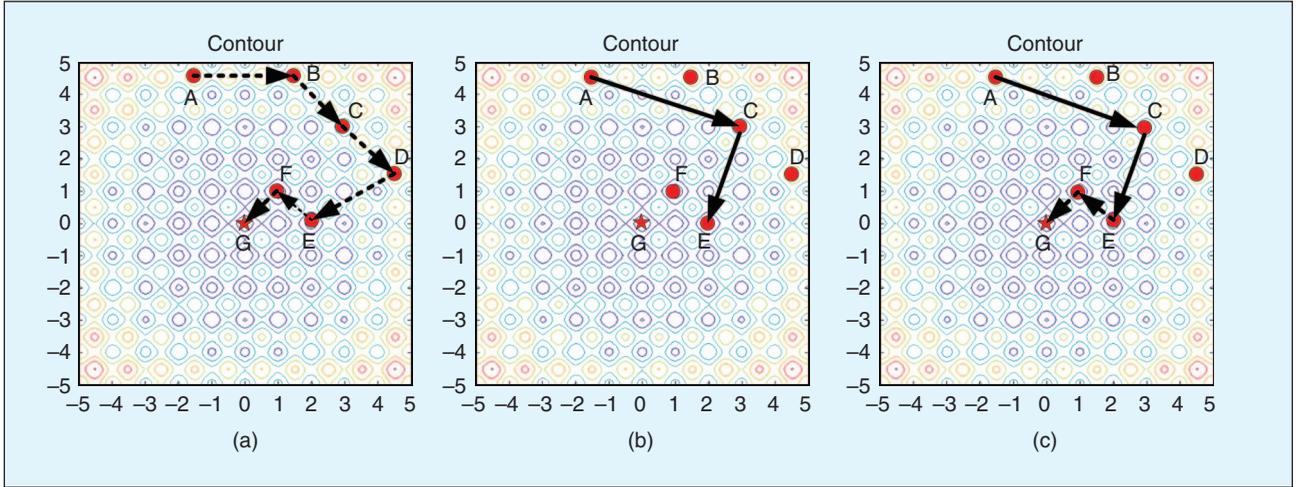


FIGURE 1 Symbiosis of stochastic variation and lifetime learning. In particular, the search behaviors of the stochastic variation and lifetime learning are depicted as directed graphs that models the connectivity probability of local optimum solutions on the contour plot. (a) Connectivity Search Profile of \mathbb{X} (b) Connectivity Search Profile of \mathbb{Y} (c) Connectivity Search Profile of $\mathbb{X} + \mathbb{Y}$. From the graphs, the search path from solution A to the global optimum G is likely to be $A \rightarrow B \rightarrow C \rightarrow D \rightarrow E \rightarrow F \rightarrow G$ when profile \mathbb{X} (“dotted line”) is used. However, when both profiles work together effectively (profile $\mathbb{X} + \mathbb{Y}$), the path becomes shorter as defined by $A \rightarrow C \rightarrow E \rightarrow F \rightarrow G$. Note that the “circle” and “star” symbols in Figure 1 denotes the local optimum and global optimum, respectively. (a) Profile X (High Solution Precision), (b) Profile Y (High Efficiency), and (c) Profile Z (High Precision + High Efficiency).

worth highlighting that here our concept of *evolubility* generalizes from that of learnability in machine learning [24] where an evolutionary process is regarded as “evoluble” on a given optimization problem if the progress in search performance is observed for some moderate number of generations. Hence *evolubility* of a symbiotic search profile is referred here to the propensity of the stochastic variation and lifetime learning in creating viable or “potentially favorable” individuals that lead to the global optimum.

The *evolubility* of search profile ID for a given solution \mathbf{x} , denoted here as E_{ID} , may be defined using a variety of criteria or cost functions. An intuitive and common quantitative measure of *evolubility* in search would be to consider the expected fitness improvement (FI) with respect to the expected computational cost (C) incurred. Without loss of generality, we consider minimization problems throughout this paper. Let a search profile ID be defined as a pair of stochastic variation V and lifetime learning L , i.e., $ID = (V, L)$. The *evolubility* of symbiotic search profile $E_{ID}(\mathbf{x}, t)$, for a potential solution \mathbf{x} in population P^t , may be formulated in terms of (FI) and (C) as follows:

$$E_{ID}(\mathbf{x}, t) = \frac{FI(\mathbf{x}, t)}{C(\mathbf{x}, t)} \quad (1)$$

$$FI(\mathbf{x}, t) = E[\Delta f | P^t, \mathbf{x}] = \iint \Delta f \times P(\mathbf{y} | P^t, \mathbf{x}) P(\mathbf{z} | \mathbf{y}) d\mathbf{y} d\mathbf{z} \\ = \int_{\mathbf{y}} P(\mathbf{y} | P^t, \mathbf{x}) \times \int_{\mathbf{z}} \Delta f \times P(\mathbf{z} | \mathbf{y}) d\mathbf{z} d\mathbf{y} \quad (2)$$

$$C(\mathbf{x}, t) = E[\Delta C | P^t, \mathbf{x}] = \iint \Delta C \times P(\mathbf{y} | P^t, \mathbf{x}) P(\mathbf{z} | \mathbf{y}) d\mathbf{y} d\mathbf{z} \\ = \int_{\mathbf{y}} P(\mathbf{y} | P^t, \mathbf{x}) \times \int_{\mathbf{z}} \Delta C \times P(\mathbf{z} | \mathbf{y}) d\mathbf{z} d\mathbf{y}, \quad (3)$$

where

- $f(\mathbf{x})$ = Objective or fitness function
- P^t = Reproduction pool at generation t
- \mathbf{x} = Solution individual in the reproduction pool, i.e., $\mathbf{x} \in P^t$
- \mathbf{y} = Offspring produced by stochastic variation V , i.e., $\mathbf{y} = V(\mathbf{x}, P^t)$
- \mathbf{z} = Resultant individual from offspring through lifetime learning, i.e., $\mathbf{z} = L(\mathbf{y})$
- $P(\mathbf{z} | \mathbf{y})$ = Density function of individual learning L applied on offspring \mathbf{y}
- $P(\mathbf{y} | P^t, \mathbf{x})$ = Density function of variation operator V applied on parent \mathbf{x}
- Δf = Fitness improvement $f(\mathbf{x}) - f(\mathbf{z})$ on minimization problem
- ΔC = Computational cost incurred.

Let $\text{Gain}(\mathbf{y}) = \int_{\mathbf{z}} \Delta f \times P(\mathbf{z} | \mathbf{y}) d\mathbf{z}$ and $\text{Cost}(\mathbf{y}) = \int_{\mathbf{z}} \Delta C \times P(\mathbf{z} | \mathbf{y}) d\mathbf{z}$ then Eqn. (2) and (3) becomes

$$FI(\mathbf{x}, t) = \int_{\mathbf{y}} P(\mathbf{y} | P^t, \mathbf{x}) \times \text{Gain}(\mathbf{y}) d\mathbf{y} \quad (4)$$

$$C(\mathbf{x}, t) = \int_{\mathbf{y}} P(\mathbf{y} | P^t, \mathbf{x}) \times \text{Cost}(\mathbf{y}) d\mathbf{y}. \quad (5)$$

With the substitution of Eqns. (4) and (5) into Eqn. (1), we arrive at

$$E_{ID}(\mathbf{x}, t) = \frac{\int_{\mathbf{y}} P(\mathbf{y} | P^t, \mathbf{x}) \times \text{Gain}(\mathbf{y}) d\mathbf{y}}{\int_{\mathbf{y}} P(\mathbf{y} | P^t, \mathbf{x}) \times \text{Cost}(\mathbf{y}) d\mathbf{y}}. \quad (6)$$

Evolubility measure of a symbiotic search profile $E_{ID}(\mathbf{x}, t)$ indicates the expectation of how a developed offspring, after undergoing individual learning, is improved over its initial

Evolvability measure of a symbiotic search profile

$E_{ID}(\mathbf{x}, t)$ indicates the expectation of how a developed offspring, after undergoing individual learning, is improved over its initial parent with the computational cost taken into consideration.

parent with the computational cost taken into consideration. Given a multitude of search profiles composing of stochastic variation and lifetime learning working on a minimization problem, the most productive profile can then be defined as having the highest evolvability measure, i.e., $\max E_{ID}(\mathbf{x}, t)$.

III. Symbiotic Evolution

In Section II, the proposed theoretical modeling of *Symbiosis* in adaptive search using the concept of evolvability has been presented. However, since realistic problems are seldom tractable and possess fitness landscapes that are highly complex in practice, a theoretic formulation may be deemed inappropriate. To deal with complex search problems, we introduce next in the present section the concept of *Evolvability Learning* in Symbiotic Evolution.

A. Statistical Learning of Evolvability

Taking a data-centric paradigm [19], here we propose a statistical approach on the *evolvability learning* of symbiotic search profiles during runtime. In consistence with the definition of *evolvability* in Eqn. (6), the statistical learning on the *evolvability* of symbiotic search profile ID on solution individual \mathbf{x} at generation t , $E_{ID}(\mathbf{x}, t) \approx \tilde{E}_{ID}(\mathbf{x}, t)$, is *quantitatively* estimated from *distinct* data pairs $\Phi_{ID} = \{(\mathbf{y}_1, \mathbf{z}_1), \dots, (\mathbf{y}_m, \mathbf{z}_m), \dots, (\mathbf{y}_M, \mathbf{z}_M)\}$ using Algorithm 1. Note that Φ_{ID} denotes the database containing the vectors of solution individuals and their associated fitness uncovered along the evolution and $\mathbf{y}_i \neq \mathbf{y}_j$ if and only if $i \neq j$.

Algorithm 1 Statistical Evolvability Learning SEVL(ID)

- 1: Query archived data ($\mathbf{y}_j \rightarrow \mathbf{z}_j, \text{Cost}$) of search profile $ID = (V, L)$
- 2: Model density distribution $P(\mathbf{y}|\mathbf{x}, P^t)$ of variation operator $V(\cdot)$, based on P^t and \mathbf{x}
- 3: Calculate weight $w_i = P(\mathbf{y}_i|P^t, \mathbf{x})$ for each sample \mathbf{y}_i
- 4: **if** $\sum w_i < \epsilon$ **then**
- 5: $w_i = 0$ (No relevant data is available)
- 6: **return** $\tilde{E}_{ID}(\mathbf{x}, t) = -\infty$
- 7: **else**
- 8: Normalize $w_i = w_i / (\sum w_i)$
- 9: **return** $\tilde{E}_{ID}(\mathbf{x}, t) = \sum_{i=1}^M w_i \times \text{Gain}(\mathbf{y}_i) / \sum_{i=1}^M w_i \times \text{Cost}(\mathbf{y}_i)$ (Eqn. (10))
- 10: **end if**

Based on $P(\mathbf{y}|P^t, \mathbf{x})$, using a weighted sampling approach, each distinct sample pair of solution individuals $\{\mathbf{y}_i, \mathbf{z}_i\}$ is then associated with some weight w_i , which defines the probability of it being selected in the estimation of E_{ID} , i.e., the relevancy of $\{\mathbf{y}_i, \mathbf{z}_i\}$ in *evolvability* learning. By considering $\{(\mathbf{y}_1, \mathbf{z}_1), (\mathbf{y}_2, \mathbf{z}_2), \dots, (\mathbf{y}_M, \mathbf{z}_M)\}$ as *distinct* samples of $P(\mathbf{y}|P^t, \mathbf{x})$ with *arbitrarily small* bins, the weights w_i associated with sample \mathbf{y}_i satisfy the equations: $\sum w_i = 1$ and $w_i \sim \int_{V(\mathbf{y}_i)} P(\mathbf{y}_i|P^t, \mathbf{x}) d\mathbf{y}$ (i.e., proportional to), where $V(\mathbf{y}_i)$ denotes the arbitrarily small bin around \mathbf{y}_i . Since the integration $\int_{V(\mathbf{y}_i)} P(\mathbf{y}|P^t, \mathbf{x}) d\mathbf{y}$ is computationally expensive, without significant loss of precision, the weight w_i is estimated by Eqn. (7).

$$w_i \approx \frac{P(\mathbf{y}_i|P^t, \mathbf{x})}{\sum_{i=1}^M P(\mathbf{y}_i|P^t, \mathbf{x})} \quad (7)$$

Note that the conditional density function $P(\mathbf{y}|P^t, \mathbf{x})$ in Eqn. (7) is derived based on the characteristic of variation operators used, in order to reflect the current state of the search. Details of this step (Line 2 of Algorithm 1) in our current implementation will be provided in Section IV-A. From the M archived sample pairs $\{\mathbf{y}_i, \mathbf{z}_i\}$, $FI(\mathbf{x}, t)$ and $C(\mathbf{x}, t)$ are then estimated using a weighted sampling approach defined by w_i as follows:

$$FI(\mathbf{x}, t) = \int_{\mathbf{y}} P(\mathbf{y}|P^t, \mathbf{x}) \times \text{Gain}(\mathbf{y}) d\mathbf{y} \approx \sum_{i=1}^M w_i \times \text{Gain}(\mathbf{y}_i) \quad (8)$$

$$C(\mathbf{x}, t) = \int_{\mathbf{y}} P(\mathbf{y}|P^t, \mathbf{x}) \times \text{Cost}(\mathbf{y}) d\mathbf{y} \approx \sum_{i=1}^M w_i \times \text{Cost}(\mathbf{y}_i). \quad (9)$$

Using Eqns. (6), (8) and (9), the *evolvability* of symbiotic search profile ID is estimated by Eqn. (10)

$$E_{ID}(\mathbf{x}, t) \approx \tilde{E}_{ID}(\mathbf{x}, t) = \frac{\sum_{i=1}^M w_i \times \text{Gain}(\mathbf{y}_i)}{\sum_{i=1}^M w_i \times \text{Cost}(\mathbf{y}_i)}. \quad (10)$$

B. Symbiotic Evolution for Non-Linear Programming

Next, the proposed novel Symbiotic Evolution, labelled here as SE, for solving non-linear programming problems is presented. The essential ingredients of our framework are composed of stochastic variation V and lifetime learning L procedures that are governed by the *evolvability* of symbiotic search profiles. Let Ψ denote the set of symbiotic search profiles (*Stochastic Variation, Lifetime Learning*) considered in the SE. Based on the statistical evolvability learning scheme described in Section III-A, SE adapts the search by inferring the most productive symbiotic search profile (i.e., that would lead to good search performances) to use on each individual while the search progresses online, as outlined in Algorithm 2.

In the first step, a population of individuals is initialized either randomly or using design of experiment techniques such as Latin hypercube sampling. The evaluated population of individuals then undergoes natural selection, for instance,

via fitness-proportional or tournament selection. The *evolvability* of symbiotic search profiles with respect to each individual in the population is then estimated probabilistically using the vectors of solution individuals uncovered and archived along the search. Subsequently, each individual is evolved using their respective statistically inferred productive symbiotic search profile for generating the next population of solution individuals. The entire process repeats until the specified stopping criteria is satisfied. For the sake of brevity, a summary of the Symbiotic Evolution is depicted in Figure 2.

IV. Empirical Study

In this section, a numerical study of the proposed SE on several commonly used continuous parametric benchmark functions is presented. To ensure a comprehensive study, diverse pairs of unique stochastic variations and individual learning procedures are also considered.

A. Stochastic Variations: Mutation & Crossover

The density distribution $P(\mathbf{y}|P^t, \mathbf{x})$ of some common stochastic variation in EA, also sometimes referred to as genetic variations, are derived and described in what follows. In the present experimental study, the stochastic variation operators considered include the conventional Gaussian mutation and the two-point crossover, which have been used widely in real-coded genetic evolution. Our motivation of using simple variation operators in this current work is to provide a simple illustration of Symbiotic Evolution. It is worth noting that other real-parameter mutation or crossover operators, such as that discussed in [25], can also be considered within the framework.

In real-coded Gaussian mutation, for instance, each individual vector is perturbed with a multivariate Gaussian distribution $\mathbf{r} \sim \mathbf{N}(\mathbf{0}, \mathbf{C})$, i.e., $\mathbf{x}' = \mathbf{x} + \mathbf{r}$. In this case, the density function of mutation operator is given in [26] as

$$P(\mathbf{y}|P^t, \mathbf{x}) = \frac{1}{(2\pi)^{n/2} |\mathbf{C}|^{1/2}} \times \exp\left(-\frac{1}{2}(\mathbf{y} - \mathbf{x})^T \mathbf{C}^{-1}(\mathbf{y} - \mathbf{x})\right). \quad (11)$$

Although there exists many variations of crossover operators in real-coded representation, such as the uniform and arithmetic crossovers, it is worth highlighting all these variations share common property of the resultant offspring \mathbf{y} bounded by $\min_{j=1 \dots N}\{\mathbf{x}_j^{(i)}\}$ and $\max_{j=1 \dots N}\{\mathbf{x}_j^{(i)}\}$ for each dimension⁵, i.e., $\forall i = 1 \dots n$.

Hence the density distribution of crossover operator can be modelled as a uniform distribution of bounds

$$\mathbf{R} = [\min_{j=1 \dots N}\{\mathbf{x}_j^{(i)}\}, \max_{j=1 \dots N}\{\mathbf{x}_j^{(i)}\}]_{i=1 \dots n}$$

⁵If $\mathbf{x}_1, \mathbf{x}_2$ and \mathbf{y} denote the parents and the offspring then each locus of the offspring \mathbf{y} satisfies the inequality

$$\min\{\mathbf{x}_1^{(i)}, \mathbf{x}_2^{(i)}\} \leq \mathbf{y}^{(i)} \leq \max\{\mathbf{x}_1^{(i)}, \mathbf{x}_2^{(i)}\}, \forall i = 1 \dots n$$

Algorithm 2 Symbiotic Evolution

```

1: Generate an initial population
2: while Stopping conditions are not satisfied do
3:   Evaluate all individuals in the population
4:   Update reproduction pool size
5:   Select individuals for the reproduction pool  $\Omega$ 
6:   for each individual  $x$  in  $\Omega$  do
7:     for each  $ID = (V, L) \in \Psi$  do
8:        $\tilde{E}_{ID}(x, t) = SEVL(ID)$  on  $x$  (see Algorithm 1)
9:     end for
10:    if  $\tilde{E}_{ID}(x, t) < 0 \forall ID$  then
11:      Select symbiotic profile  $ID$  randomly
12:    else
13:      Select symbiotic profile  $ID$  with optimal  $\tilde{E}_{ID}(x, t)$ 
14:    end if
15:    Evolve  $x$  according to stochastic variation operator  $V(\cdot)$ 
16:    Perform individual learning via operator  $L(\cdot)$ 
17:    Proceed in the spirit of Lamarckian learning
18:  end for
19: end while

```

defined in Eqn. (12), where $Vol(\mathbf{R})$ denotes the hyper-volume of hyper-rectangle \mathbf{R} . Note that since \mathbf{R} reduces as the search progresses, the probabilistic model of crossover operator reflects well on the refinement of the search space by crossover and selection pressure. In particular, Eqn. (12) models the density distribution of the coordinated-based crossover considered in the present study.

$$P(\mathbf{y}|P^t, \mathbf{x}) = \text{UniformDist}(\mathbf{R}) = \begin{cases} \frac{1}{Vol(\mathbf{R})} & \text{if } \mathbf{y} \in \mathbf{R} \\ 0 & \text{otherwise} \end{cases}. \quad (12)$$

B. Lifetime Learning

In the present study, a comprehensive set of representative lifetime learning schemes is considered. These include the zero-order derivative *Davies, Swann, and Campey with Gram-Schmidt orthogonalization* (DSCG) [27], 1st-order derivative *Davidon, Fletcher and Powell* strategy (DFP) [28], and stochastic *Evolution Strategy* ($1 + n$) (ES).

C. Numerical Results of Symbiotic Evolution on Representative Complex Benchmark Problems

To instill further understanding on symbiotic evolution, various aspects of the proposed framework are investigated on a comprehensive collection of unimodal/multimodal, epistatic/non-epistatic, continuous/discontinuous and noisy benchmark problems used in literature [29]. The benchmark test functions are tabulated with their notable characteristics in Table 1. In particular, here we focus on the potential of symbiotic

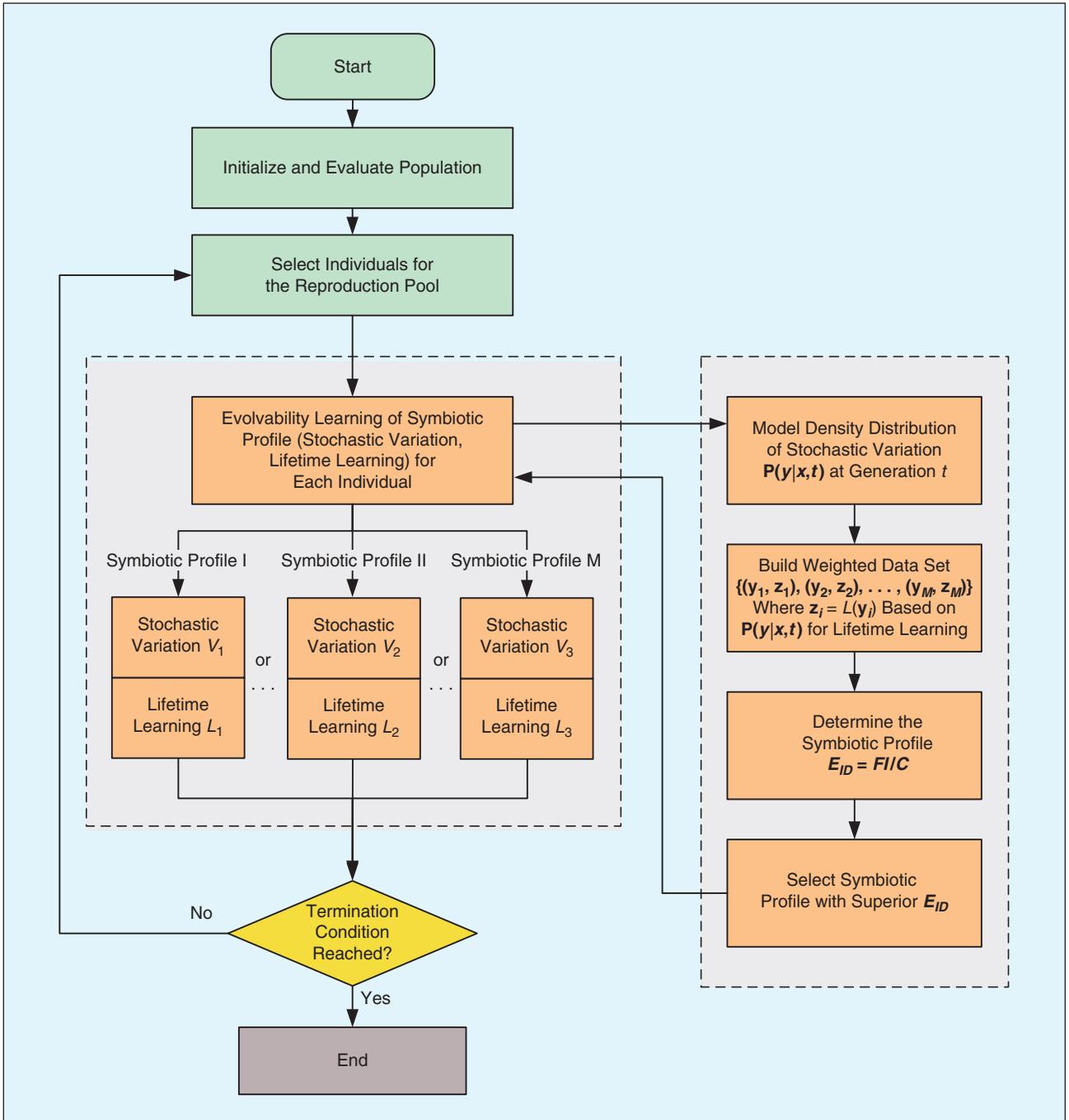


FIGURE 2 Symbiotic Evolution (SE) Framework.

evolution in providing high quality solution and efficiency across different problem types and the amount of additional computational effort incurred over and above the canonical EA hybrids.

1. Search Quality & Efficiency

The parametric configurations of the experiments are summarized in Table 2. From the configurations of stochastic variations (i.e., Gaussian mutation or coordinated-based crossover) and lifetime learning procedures (i.e., DSCG, DFP or

ES) considered, note that six potential combinations or unique configurations of symbiotic search profiles can transpire in the Symbiotic Evolution.

The average convergence search trends across 50 independent runs, attained by means of symbiotic evolution and canonical evolution represented by the six EA hybrids, when solving the representative 30-dimension shifted rotated Ackley, Rastrigin, Griewank, shifted Rosenbrock and noisy shifted Schwefel functions are depicted in Figures 3(a)–7(a), respectively. Here, each run continues until the global optimum was

TABLE 1 Benchmark functions for real-parameter optimization. In the equations, n is the dimensionality, \mathbf{x} is the vector of design variables to be optimized. In order to avoid any biased of the search algorithms on exploiting this symmetric property of the benchmark functions, the design variables are shifted. Vector \mathbf{o} is the shifted global optimum and $\mathbf{z} = \mathbf{x} - \mathbf{o}$ is the vector of shifted variables. For rotated problems, including of Problem 5, 7, 8, 10, 11 and 12, \mathbf{M} is the rotation matrix and $\mathbf{z} = \mathbf{M} \times (\mathbf{x} - \mathbf{o})$ is the vector of shifted rotated design variables.

| FUNC | BENCHMARK TEST FUNCTIONS | RANGE OF X | MULTI* | NON-SEP* |
|------|---|---------------------|--------|----------|
| 1 | $F_{\text{Sphere}} = \sum_{i=1}^n (z_i^2)$ | $[-100, 100]^n$ | NO | NO |
| 2 | $F_{\text{Step}} = 6n + \sum_{i=1}^n z_i $ | $[-5.12, 5.12]^n$ | NO | NO |
| 3 | $F_{\text{Schwefel1.2}} = \sum_{i=1}^n \left(\sum_{j=1}^i z_j \right)^2$ | $[-100, 100]^n$ | NO | YES |
| 4 | $F_{\text{Schwefel1.2-Noise}} = \left(\sum_{i=1}^n \left(\sum_{j=1}^i z_j \right)^2 \right) \times (1 + 0.4 N(0, 1))$ | $[-100, 100]^n$ | NO | YES |
| 5 | $F_{R\text{-Elliptic}} = \sum_{i=1}^n (10^6)^{((i-1)/(n-1))} z_i^2$ | $[-100, 100]^n$ | NO | YES |
| 6 | $F_{\text{Rosenbrock}} = \sum_{i=1}^{n-1} (100 \times (z_{i+1} - z_i^2)^2 + (1 - z_i)^2)$ | $[-2.048, 2.048]^n$ | YES | YES |
| 7 | $F_{R\text{-Ackley}} = 20 + e - 20e^{-0.2\sqrt{((1/n)\sum_{i=1}^n z_i^2) - \sum_{i=1}^n z_i^2 \cos(2\pi z_i)}}$ | $[-32, 32]^n$ | YES | YES |
| 8 | $F_{R\text{-Griewank}} = 1 + \sum_{i=1}^n z_i^2/4000 - \prod_{i=1}^n \cos(z_i/\sqrt{i})$ | $[-600, 600]^n$ | YES | YES |
| 9 | $F_{\text{Rastrigin}} = 10n + \sum_{i=1}^n (z_i^2 - 10 \cos(2\pi z_i))$ | $[-5, 5]^n$ | YES | NO |
| 10 | $F_{R\text{-Rastrigin}} = 10n + \sum_{i=1}^n (z_i^2 - 10 \cos(2\pi z_i))$ | $[-5, 5]^n$ | YES | YES |
| 11 | $F_{R\text{-Weierstrass}} = \sum_{i=1}^n \left(\sum_{k=0}^{k_{\max}} (a^k \cos(2\pi b^k (z_i + 0.5))) \right) - n \sum_{k=0}^{k_{\max}} (a^k \cos(\pi b^k))$ | $[-0.5, 0.5]^n$ | YES | YES |
| 12 | $F_{R\text{-ExpandedScaffer}} = \sum_{i=1}^n F(z_i, z_{i+1}), z_{n+1} = z_1$ $F(x, y) = 0.5 + \frac{\sin^2(\sqrt{x^2 + y^2}) - 0.5}{(1 + 0.001(x^2 + y^2))^2}$ | $[-100, 100]^n$ | YES | YES |
| 13 | $F_{\text{GrieRos}} = \sum_{i=1}^D F_{\text{Griewank}}(F_{\text{Rosenbrock}}(z_i, z_{i+1})), z_{D+1} = z_1$ | $[-3, 1]^n$ | YES | YES |

found or a maximum of 300,000 function evaluations were reached. In addition, the average frequency of each symbiotic profile that is inferred as most productive on the solution individuals along the search are depicted in Figures 3(b)–7(b) for the respective problems considered.

Statistical results in Figures 3(a)–7(a) indicated that by adaptively configuring the symbiotic search profile along the search, Symbiotic Evolution exhibits search performance that outwits all the canonical EA hybrids. It is worth noting that the search traces in Figures 3(a)–7(a) revealed interesting trends of slower convergence rate exhibited by symbiotic evolution during the initial stage of the search as compared to the other canonical evolutions on all the test problems. This denotes the initial learning phase of the SE in acquiring sufficient data and knowledge about the search profile before evolvability learning begins to bite. Note that when the database $\Phi_{ID} = \{(y_i, z_i)\}$ containing data pairs that represents each search profile gets sufficiently populated, the statistical evolvability learning kicks in to select the most productive search profile for each unseen individual solution, leading to a

faster convergence to the precise global optimum than other canonical MAs considered.

From Figure 3(b), search improvement in Symbiotic Evolution on the rotated Ackley function can be inferred as contributed mainly by profile (*Crossover*, *DSCG*) and (*Crossover*, *ES*), while the contributions of (*Crossover*, *DSCG*) is more evident at later stages of the search. On rotated Rastrigin

TABLE 2 Algorithm parameters setting.

| GENERAL PARAMETERS | |
|---------------------------------------|---|
| ENCODING SCHEME | REAL-CODED |
| POPULATION SIZE | 50 |
| SELECTION SCHEME | ROULETTE WHEEL |
| MERGING SCHEME | ELITISM |
| STOPPING CRITERIA | 300,000 EVALUATIONS |
| INDIVIDUAL LEARNING STRATEGIES | DSCG, DFP AND ES |
| INITIAL INDIVIDUAL LEARNING INTENSITY | 300 EVALUATIONS |
| VARIATION OPERATOR | TWO-POINT CROSSOVER AND GAUSSIAN MUTATION $N(0, 1)$ |

function, however, (*Mutation, ES*) is chosen for most individuals in the early generations of the SE search, before (*Crossover, DSCG*) begins to take effect as the search space is refined. For unimodal landscapes including Rosenbrock and noisy Schwefel functions, the plots in Figures 6(b) and 7(b) showed that decreasing frequencies of usage for symbiotic profiles with Gaussian mutation operator at the later stages of search. This appears to be due to the destructive effect of the Gaussian mutation operator when the search tries to converge to the global optimum with high precision. The observations of no fixed symbiotic configuration working as best throughout the search and across different optimization problems further confirm our motivation for introducing the concept of Symbiotic Evolution.

2. Computational Complexity

Algorithmically, Symbiotic Evolution differs from canonical evolution in that the former introduces a *Statistical Learning of Evolvability* phase that involves two core computations, namely

- Modeling the density distribution $P(\mathbf{y}|P^t, \mathbf{x})$ of stochastic variation for all individuals in the reproduction pool. The computational cost or time complexity of this estimation largely depends on the form of variation method considered. For instance, the costs of modeling the density function of the Gaussian mutation and crossover operators, described in Section IV A, is of order $O\{n_{\text{indivs}}\}$ and $O\{1\}$, respectively, where n_{indivs} denotes the size of reproduction pool.
- Computing weights w_i of the archived solutions for all individuals in the reproduction pool. The computational

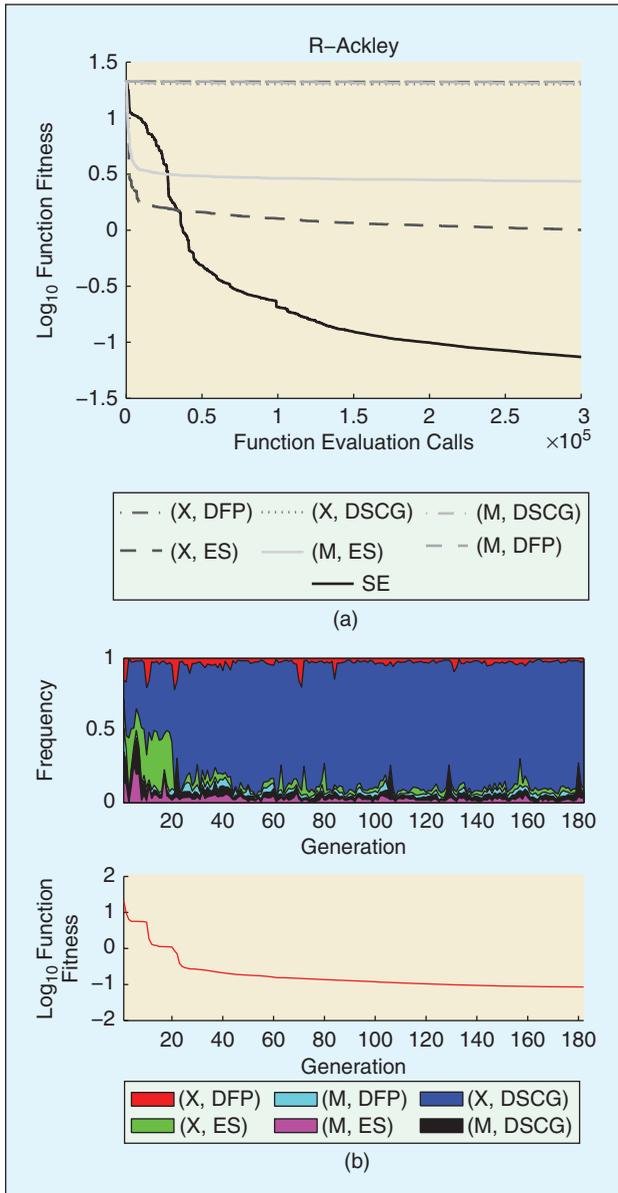


FIGURE 3 Shifted rotated Ackley (30D) function. (a) Convergence trend and (b) Profile frequency.

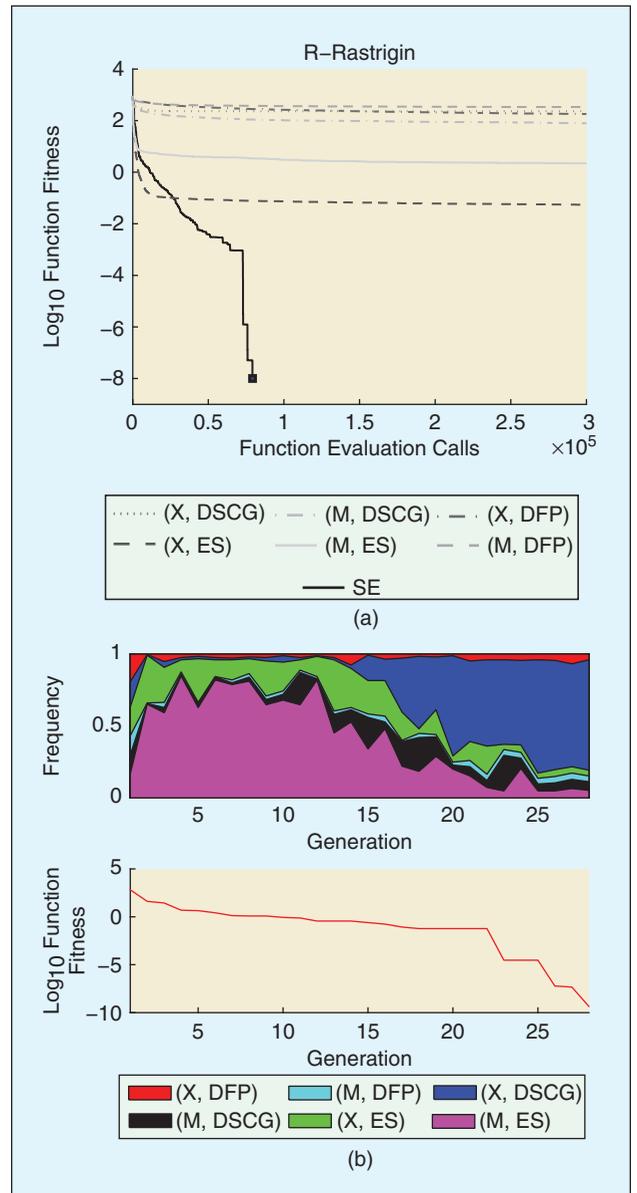


FIGURE 4 Shifted rotated Rastrigin (30D) function. (a) Convergence trend and (b) Profile frequency.

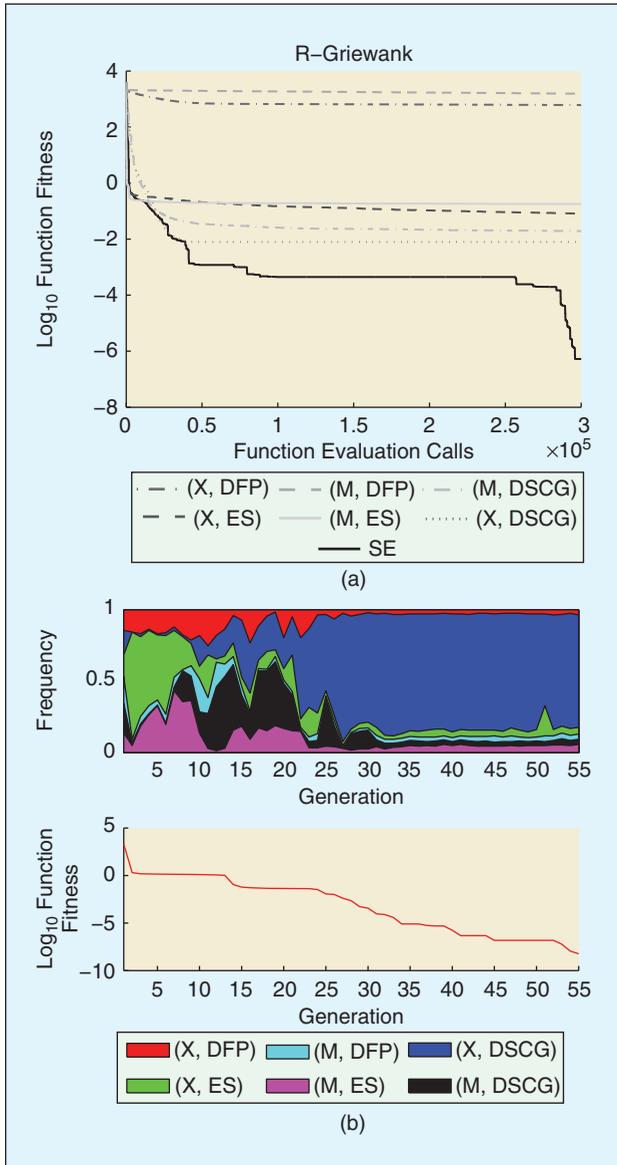


FIGURE 5 Shifted rotated Griewank (30D) function. (a) Convergence trend and (b) Profile frequency.

cost or time complexity involved is of order $O\{n_{\text{indivs}} \times |\Psi| \times |\Phi_{ID}|\}$, with $|\Phi_{ID}|$ denoting the number of archived individuals.

Hence the additional time complexity for one generation of symbiotic evolution is of order $O\{n_{\text{indivs}} \times (|\Psi| \times |\Phi_{ID}| + 1)\}$ in which the number of symbiotic search profiles $|\Psi|$ equals to $n_{IL} \times n_V$, where n_{IL} and n_V denote the number of individual learning and variation methods considered. As the size of reproduction pool n_{indivs} and the size of archived database $|\Phi_{ID}|$ is typically fixed in advance, the time complexity of symbiotic evolution is linearly proportional to the number of search profiles involved. More importantly, since Symbiotic Evolution requires no additional function evaluation calls, the extra cost incurred may be considered to be negligible when dealing with computationally expensive problems [17].

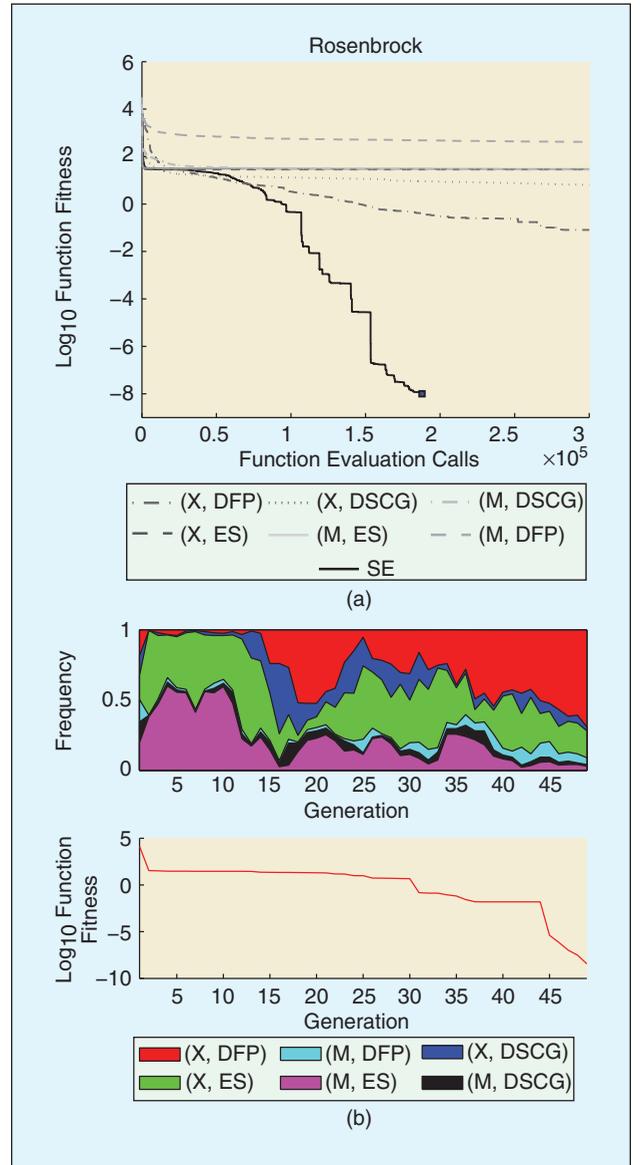


FIGURE 6 Shifted Rosenbrock function. (a) Convergence trend and (b) Profile frequency.

V. Symbiotic Evolution: Assessment Against Other Evolutionary and Adaptive Search Approaches

In this section, a detail assessment of Symbiotic Evolution (as described in Section IV-C) against several recent state-of-the-art evolutionary and adaptive approaches on commonly used test suite (see Table 1) is presented to verify the efficacy of the proposed approach.

A. Comparison to Adaptive Algorithms

To see how adapting the symbiotic search profiles affects the performance and efficiency of the search as compared to meme adaptation alone, in this subsection, the performance of Symbiotic Evolution is compared with those of other adaptive mechanisms on the choice of individual learning methods (memes) in EA hybrids or MAs. Researchers use the

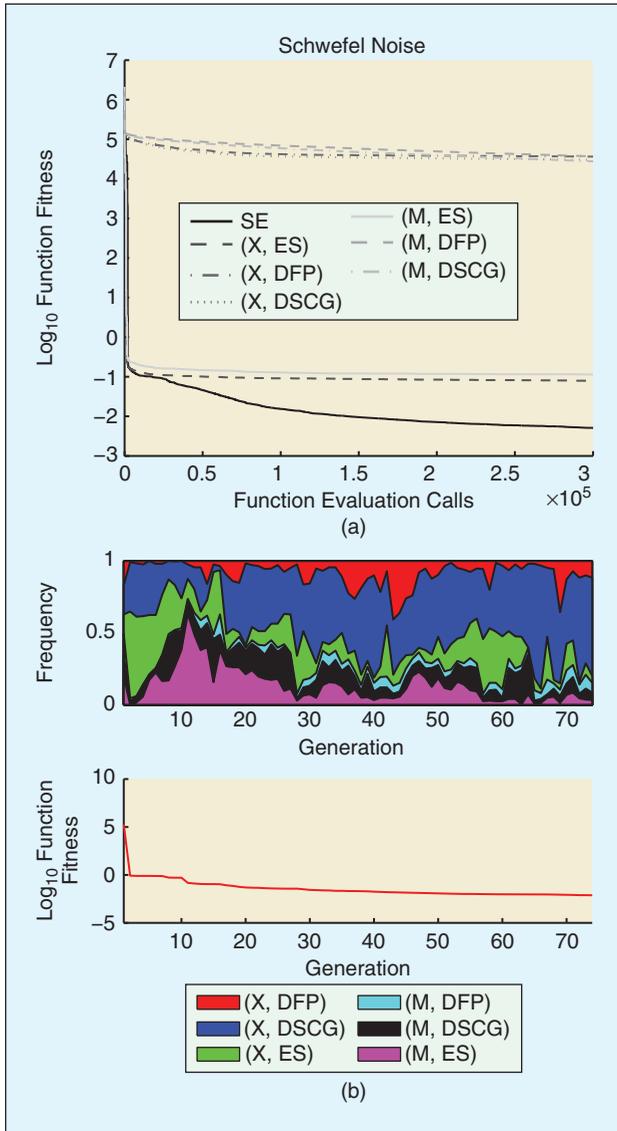


FIGURE 7 Shifted noisy Schwefel (30D) function. (a) Convergence trend and (b) Profile frequency.

TABLE 3 Classification of adaptive MAs.

| ADAPTATION TYPE | |
|------------------|--|
| STATIC | NO FORM OF FEEDBACK (IMPROVEMENT ATTAINED BY THE CHOSEN MEME ON THE CHROMOSOME SEARCH) IS USED DURING THE SEARCH |
| ADAPTIVE | QUALITATIVE OR QUANTITATIVE FEEDBACK INFLUENCES THE CHOICE OF MEMES AT EACH DECISION POINT |
| SELF-ADAPTIVE | THE SELF-ADAPTATION OF MEMES IS IMPLEMENTED IN THE IDEA OF EVOLUTION |
| ADAPTATION LEVEL | |
| EXTERNAL | NO ONLINE KNOWLEDGE ABOUT THE MEMES IS INVOLVED IN THE CHOICE OF MEMES |
| LOCAL | PARTS OF THE HISTORICAL KNOWLEDGE IS INVOLVED IN THE CHOICE OF MEMES |
| GLOBAL | COMPLETE HISTORICAL KNOWLEDGE IS USED TO DECIDE ON THE CHOICE OF MEMES |

TABLE 4 List of memes or individual learning methods considered.

| ABBREVIATIONS | ALGORITHM DESCRIPTION |
|---------------|--|
| BL | BIT CLIMBING ALGORITHM [30] |
| DP | DAVIS, SWAN AND CAMPEY WITH PALMER ORTHOGONALIZATIONAL [27, 31] |
| FB | SCHWEFEL LIBRARY FIBONACCI SEARCH [27] |
| FL | FLETCHER'S 1972 METHOD BY SIDDALL [32] |
| GL | REPEATED ONE-DIMENSIONAL GOLDEN SECTION SEARCH [27] |
| SX | POWELL'S STRATEGY OF CONJUGATE DIRECTIONS [33] |
| PS | A DIRECT SEARCH USING THE CONJUGATE DIRECTION APPROACH WITH QUADRATIC CONVERGENCE [34] |
| SK | A SERIES OF EXPLORATORY MOVES THAT CONSIDER THE BEHAVIOR OF THE OBJECTIVE FUNCTION AT A PATTERN OF POINTS, ALL OF WHICH LIE ON A RATIONAL LATTICE [35] |

terms meta-Lamarckian learning, hyperheuristic and multi-memes arbitrarily when referring to memes adaptation in adaptive EA hybrids or adaptive MAs. In [21], adaptive mechanisms are classified into adaptation types (static, adaptive and self-adaptive rules using qualitative or quantitative feedback) and levels (external, local and global level) as summarized in Table 3. In addition, comparison to eight canonical MAs reported in the literature as listed in Table 4 are made in the present study.

To be consistent, the results presented for Symbiotic Evolution are the average of 50 independent runs. For fair comparison, each run continues until the global optimum was found or a maximum of 40,000 function evaluation calls were reached, which follows the experimental conditions considered in [21]. Using statistical T-test at 95% confidence level, the performance comparison of Symbiotic Evolution to the adaptive MAs on the benchmark test problems are tabulated in Table 5. For the detailed statistical results pertaining to each adaptive method, the reader is referred to Table 6 for the sake of conciseness. In the case where an algorithm manages to locate the global optimum of a benchmark problem, the number of evaluation count presented indicates the effort taken to reach the optimum solution. Otherwise, the best fitness averaged over 50 independent runs is reported.

From Table 5, Symbiotic Evolution is shown to outperform all the canonical EA hybrids and adaptive hybrids significantly, statistically at 95% confidence on all the problems. Note that this is a significant finding, which highlights the benefits of facilitating the self-configuring of emergent productive symbiosis search profiles in evolutionary computation instead of adapting only at the level of lifetime learning, as previously studied in the literature.

B. Assessment Against Other Recent State-of-the-Art Evolutionary Approaches

In this section, we further assess the proposed Symbiotic Evolution against 12 recent state-of-the-art evolutionary

approaches reported in the literature. Table 7 tabulates the list of diverse algorithms, consisting of Memetic Algorithms [16, 37, 36, 41], CMA Evolution Strategy [38, 39], continuous Estimation of Distribution Algorithms [40], Genetic Algorithms [42, 43], Differential Evolution [44], Particle Swarm Optimization [46], Cooperative Co-Evolution [45], considered here for comparisons with a brief description of each algorithm provided. Using a statistical T-test of 95% confidence level, the search performances of each algorithms are pitted against the SE on solving the set of benchmark functions described in Table 1, where the results are tabulated in Table 8. For the sake of conciseness, the detailed statistics of the different algorithms on numerical errors with respect to the global optimum, are provided separately in Table 9. For the sake of fair comparison, note that the accuracy level of convergence ϵ , is configured as $1E-8$, which follows the configuration used by other researchers of earlier studies as a strict guideline.

From the results in Table 8, Symbiotic Evolution is observed to fair competitively or significantly outperform most of the state-of-the-art methods considered, at 95% confidence level on the 30-dimensional benchmark functions, particularly on the noisy and rotated shifted multimodal functions. This highlights the robustness and efficacy attained by taking advantage of the emergent behavior that is resulted from the interactions of stochastic

TABLE 5 Results of t-test at 95% confidence level for SE and other adaptive search algorithms in solving the benchmark problems (Note that s+ or s- indicates that SE is significantly statistically better or not, respectively).

| LEVEL-TYPE | | $F_{\text{GRIEWANK}} (10D)$ | $F_{\text{RASTRIGIN}} (20D)$ | $F_{\text{SPHERE}} (30D)$ | $F_{\text{STEP}} (5D)$ |
|---------------------|--------|-----------------------------|------------------------------|---------------------------|------------------------|
| EXTERNAL-STATIC | S-E | s+ | s+ | s+ | s+ |
| LOCAL-QUALITATIVE | QL1-L | s+ | s+ | s+ | s+ |
| | QL2-L | s+ | s+ | s+ | s+ |
| GLOBAL-QUALITATIVE | QL3-G | s+ | s+ | s+ | s+ |
| GLOBAL-QUANTITATIVE | QN1-G | s+ | s+ | s+ | s+ |
| | QN2-G | s+ | s+ | s+ | s+ |
| LOCAL-QUANTITATIVE | QN3-L | s+ | s+ | s+ | s+ |
| LOCAL SELF-ADAPTIVE | S-L | s+ | s+ | s+ | s+ |
| CANONICAL MAS | GA- <> | s+ | s+ | s+ | s+ |

variations and lifetime learning working in symbiosis, as advocated in the symbiotic evolution.

Further, to access the overall performance quality of these approaches on the representative benchmark functions considered, a non-parametric Wilcoxon's signed-ranks test is also used according to the procedure suggested in [14]. The results in Table 10 show that Symbiotic Evolution statistically exhibits superior performance

TABLE 6 Success measure of the algorithms in solving the benchmark functions. Either average best fitness or average number of evaluation count incurred to locate the global optimum is presented for each function. Bold italic also highlights the best search performance.

| LEVEL-TYPE | | $F_{\text{GRIEWANK}} (10D)$ | $F_{\text{RASTRIGIN}} (20D)$ | $F_{\text{SPHERE}} (30D)$ (EVAL. COUNT) | $F_{\text{STEP}} (5D)$ (EVAL. COUNT) |
|---------------------|-------|-----------------------------|------------------------------|--|---|
| LOCAL-QUANTITATIVE | SE | 0 | 0 | 3,429 | 1552 |
| EXTERNAL-STATIC | S-E | 5.2500e-3 | 16.8760 | 12,593 | 23,433 |
| LOCAL-QUALITATIVE | QL1-L | 5.2537e-1 | 84.9772 | > 40,000 | 19,504 |
| | QL2-L | 1.0610e-2 | 18.6215 | 8,599 | 8,942 |
| GLOBAL-QUALITATIVE | QL3-G | 4.5000e-4 | 18.0530 | 8,599 | 8,056 |
| GLOBAL-QUANTITATIVE | QN1-G | 6.2000e-5 | 9.6078 | 8,193 | 9,653 |
| | QN2-G | 6.1060e-3 | 14.5241 | 9,196 | 14,329 |
| LOCAL-QUANTITATIVE | QN3-L | 5.5800e-4 | 33.4929 | 10,194 | 12,007 |
| LOCAL SELF-ADAPTIVE | S-L | 2.8630e-3 | 14.1689 | 11,792 | 28,100 |
| | GA-BL | 6.1370e-1 | 92.3340 | > 40,000 | 8,588 |
| | GA-DP | 5.1600e-4 | 14.4480 | 9,098 | 8,931 |
| | GA-FB | 1.9096e+1 | 144.2500 | > 40,000 | 25,706 |
| CANONICAL MAS | GA-FL | 7.0700e-3 | 69.8630 | 6,666 | > 40,000 |
| | GA-GL | 2.2646e+1 | 155.1100 | > 40,000 | 25,706 |
| | GA-PS | 3.3780e-3 | 74.1060 | 12,292 | > 40,000 |
| | GA-SK | 3.3862e-1 | 81.1180 | 40,000 | > 40,000 |
| | GA-SX | 7.8610e-1 | 73.7900 | > 40,000 | > 40,000 |

TABLE 7 Recent state-of-the-art evolutionary approaches.

| ABBREVIATIONS | ALGORITHM DESCRIPTION |
|--------------------|---|
| <i>APrMF</i> | APPROXIMATE PROBABILISTIC MEMETIC FRAMEWORK BASED ON GA-DSCG [16] |
| <i>MA-LSCH-CMA</i> | MEMETIC ALGORITHM WITH LOCAL SEARCH CHAINING [36] |
| <i>DEAH-CSPX</i> | ACCELERATING DIFFERENTIAL EVOLUTION USING AN ADAPTIVE LOCAL SEARCH [37] |
| <i>LR-CMA-ES</i> | LOCAL RESTART CMA EVOLUTION STRATEGY [38] |
| <i>IPOP-CMA-ES</i> | RESTART CMA EVOLUTION STRATEGY WITH INCREASING POPULATION SIZE [39] |
| <i>EDA</i> | CONTINUOUS ESTIMATION OF DISTRIBUTION ALGORITHMS [40] |
| <i>RCMA</i> | ADAPTIVE LOCAL SEARCH PARAMETERS FOR REAL-CODED MEMETIC ALGORITHM [41] |
| <i>RCCA-FMD</i> | HYBRID REAL-CODED GENETIC ALGORITHM WITH FEMALE AND MALE DIFFERENTIATION [42] |
| <i>SPC-PNX</i> | STEADY-STATE REAL PARAMETER GENETIC ALGORITHM SPC-PNX [43] |
| <i>DE</i> | DIFFERENTIAL EVOLUTION [44] |
| <i>COEVO</i> | REAL-PARAMETER OPTIMIZATION USING THE MUTATION STEP CO-EVOLUTION [45] |
| <i>PS+CMA-ES</i> | PARTICLE SWARM CMA-ES [46] |

TABLE 8 Results of t-test at 95% confidence level, for SE and other recent evolutionary search algorithms in solving the 30D benchmark problems (Note that s+ or s- indicates that SE is significantly statistically better or not, respectively). ≈ is used when both algorithms are able to locate the global optimum at the accuracy level of convergence $1E-8$. N.A indicates that assessment on the function cannot be made, since it was not considered by the authors in their manuscript.

| ALGORITHM | F_{SPHERE} | $F_{\text{SCHWEFEL1.2}}$ | $F_{R\text{-ELLIPTIC}}$ | $F_{\text{SCHWEFEL1.2-NOISE}}$ | $F_{\text{ROSENBRCK}}$ | $F_{R\text{-GRIEWANK}}$ |
|-------------|-----------------------|--------------------------|--------------------------|--------------------------------|--------------------------------|-------------------------|
| APrMF | ≈ | ≈ | s- | s+ | s+ | s+ |
| MA-LSCH-CMA | N.A | N.A | N.A | N.A | s+ | s+ |
| DEAhCSPX | N.A | N.A | N.A | N.A | ≈ | s+ |
| LR-CMA-ES | ≈ | ≈ | s- | s+ | ≈ | ≈ |
| IPOP-CMA-ES | ≈ | ≈ | s- | s+ | ≈ | ≈ |
| EDA | ≈ | ≈ | s- | s- | s+ | ≈ |
| RCMA | ≈ | s+ | s+ | s+ | s+ | s+ |
| RCGA-FMD | ≈ | ≈ | s+ | s+ | s+ | ≈ |
| SPC-PNX | ≈ | s+ | s+ | s- | s+ | s+ |
| DE | ≈ | s+ | s+ | s+ | s+ | s+ |
| COEVO | s+ | s+ | s+ | s+ | s+ | s+ |
| PS+CMA-ES | ≈ | ≈ | s+ | s- | s+ | ≈ |
| ALGORITHM | $F_{R\text{-ACKLEY}}$ | $F_{\text{RASTRIGIN}}$ | $F_{R\text{-RASTRIGIN}}$ | $F_{R\text{-WEIERSTRASS}}$ | $F_{R\text{-EXPANDEDSCAFFER}}$ | F_{GRIEROS} |
| APrMF | s+ | ≈ | s+ | s+ | s+ | s+ |
| MA-LSCH-CMA | s+ | ≈ | s+ | s+ | s+ | s+ |
| DEAhCSPX | s+ | ≈ | s+ | s+ | s+ | s+ |
| LR-CMA-ES | s+ | s+ | s+ | s+ | s+ | s+ |
| IPOP-CMA-ES | s+ | s+ | s+ | s+ | s+ | s+ |
| EDA | s+ | s+ | s+ | s+ | s+ | s+ |
| RCMA | s+ | s+ | s+ | s+ | s+ | s+ |
| RCGA-FMD | s+ | s+ | s+ | s+ | s+ | s+ |
| SPC-PNX | s+ | s+ | s+ | s+ | s+ | s+ |
| DE | s+ | s+ | s+ | s+ | s+ | s+ |
| COEVO | s+ | s+ | s+ | s+ | s+ | s+ |
| PS+CMA-ES | s+ | ≈ | ≈ | s+ | s+ | s+ |

TABLE 9 Numerical Error to global optimal solution, as attained by SE and the other algorithms considered at $30 * 10^4$ function evaluations on the 30D benchmark functions. N.A indicates that assessment on the function cannot be made, since it was not considered by the authors in their manuscript.

| ALGORITHM | F_{SPHERE} | $F_{\text{SCHWEFEL1.2}}$ | $F_{R\text{-ELLIPTIC}}$ | $F_{\text{SCHWEFEL1.2-NOISE}}$ | $F_{\text{ROSENBRCK}}$ | $F_{R\text{-GRIEWANK}}$ |
|-------------|-----------------------|--------------------------|--------------------------|--------------------------------|--------------------------------|-------------------------|
| SE | 1.815E-26 | 2.901E-10 | 1.319E+00 | 6.040E-03 | 4.186E-09 | 3.480E-07 |
| APrMF | < 1E-8 | < 1E-8 | < 1E-8 | 3.610E+04 | 8.270E+00 | 8.760E-04 |
| MA-LSCH-CMA | N.A | N.A | N.A | N.A | 1.191E+01 | 8.871E-04 |
| DEAhCSPX | N.A | N.A | N.A | N.A | 1.000E-09 | 1.163E-03 |
| LR-CMA-ES | 5.280E-09 | 6.930E-09 | 5.180E-09 | 9.260E+07 | 6.310E-09 | 6.480E-09 |
| IPOP-CMA-ES | 5.420E-09 | 6.220E-09 | 5.550E-09 | 1.110E+04 | 5.900E-09 | 5.310E-09 |
| EDA | 9.095E-15 | 9.095E-15 | 1.776E-12 | 2.260E-12 | 2.110E+01 | 3.865E-14 |
| RCMA | 9.364E-09 | 8.717E-06 | 8.775E+05 | 3.966E+01 | 4.955E+01 | 1.329E-02 |
| RCGA-FMD | 8.878E-09 | 9.835E-09 | 3.112E+03 | 1.684E+01 | 2.598E-07 | 9.073E-09 |
| SPC-PNX | 9.352E-09 | 6.948E-07 | 1.102E+06 | 8.132E-07 | 1.520E+01 | 1.460E-02 |
| DE | 0.000E+00 | 3.330E-02 | 6.920E+05 | 1.520E+01 | 2.510E+01 | 2.960E-03 |
| COEVO | 7.965E-01 | 4.402E-01 | 3.671E+02 | 4.798E+03 | 1.211E+03 | 1.412E-01 |
| PS+CMA-ES | 8.790E-09 | 9.260E-09 | 8.000E+04 | 8.470E-04 | 1.350E+01 | 9.330E-09 |
| ALGORITHM | $F_{R\text{-ACKLEY}}$ | $F_{\text{RASTRIGIN}}$ | $F_{R\text{-RASTRIGIN}}$ | $F_{R\text{-WEIERSTRASS}}$ | $F_{R\text{-EXPANDEDSCAFFER}}$ | F_{GRIEROS} |
| SE | 7.770E-02 | 0 | 8.292E-10 | 4.700E-01 | 2.990E-01 | 1.488E+00 |
| APrMF | 2.060E+01 | < 1E-8 | 2.170E+02 | 2.930E+01 | 5.410E-01 | 7.720E+00 |
| MA-LSCH-CMA | 2.027E+01 | 7.828E-09 | 1.839E+01 | 4.351E+00 | 1.268E+01 | 2.345E+00 |
| DEAhCSPX | 2.095E+01 | 1.000E-09 | 9.450E+01 | 2.922E+01 | 1.279E+01 | 2.366E+00 |
| LR-CMA-ES | 2.000E+01 | 2.910E+02 | 5.630E+02 | 1.520E+01 | 1.400E+01 | 2.320E+00 |
| IPOP-CMA-ES | 2.010E+01 | 9.380E-01 | 1.650E+00 | 5.480E+00 | 1.290E+01 | 2.490E+00 |
| EDA | 2.095E+01 | 1.787E+02 | 1.886E+02 | 3.945E+01 | 1.332E+01 | 1.531E+01 |
| RCMA | 2.071E+01 | 6.806E-01 | 9.058E+01 | 3.114E+01 | 1.256E+01 | 3.963E+00 |
| RCGA-FMD | 2.095E+01 | 1.511E+01 | 3.520E+01 | 2.474E+01 | 1.212E+01 | 5.152E+00 |
| SPC-PNX | 2.093E+01 | 2.393E+01 | 6.030E+01 | 1.126E+01 | 1.313E+01 | 3.588E+01 |
| DE | 2.100E+01 | 1.850E+01 | 9.690E+01 | 3.420E+01 | 1.340E+01 | 3.230E+00 |
| COEVO | 2.090E+01 | 1.314E+02 | 2.324E+02 | 3.770E+01 | 1.325E+01 | 9.020E+00 |
| PS+CMA-ES | 2.100E+01 | 8.850E-09 | 8.980E-09 | 3.910E+00 | 1.29E+01 | 2.110E+00 |

compared to the other evolutionary approaches (the associated R+ values of SE are higher than the corresponding R- values) at 95% confidence level.

VI. OSS2 Potential Modeling for (H₂O)_n Water Clusters

Water clusters play a fundamental role for understanding the enigmatic properties of water. In science, water clusters are heavily studied to characterize the basic molecular interactions, elucidate water's role in biochemical processes and the hydrophobic/ hydrophilic interactions. As opposed to conducting experimental study which is extremely difficult, some scientists have turned to computer simulation studies on the structures, properties and spectra of water, including the potential energy and electrostatic properties. Among the models currently in use are first-principles (*ab initio*) quantum chemical computations and semi-empirical methods. The former possess the benefits of high fidelity but can be extremely computationally expensive, limiting their use to simulations involving only a small numbers of atoms. Advanced empirical water models, which are fitted to experimental data, on the other hand, are computationally more efficient but give a trade-off in terms of model fidelity or accuracy.

Today, the design of computationally cheap advanced empirical water models remains an important and unsolved problem. Here, the parametric design of a potential model, known as OSS2, for describing neutral water clusters (H₂O)_n [47, 48] by means of symbiotic evolution is considered. The benefits of OSS2 potential model include dissociability, polarizability and flexibility, allowing the simulation of different forms of water clusters. It is worth noting that the potential model was originally designed to describe protonated water clusters, H⁺(H₂O)_n, by taking into consideration the interactions between H⁺ and O²⁻ ions, with additional three-body H-O-H interactions terms and self-consistent treatment of the polarizability of the oxygen ions, as described in [47]. In order to adopt the OSS2 potential model for neutral water clusters, (H₂O)_n, 40 variables of the model are generated by fitting to the high level *ab initio* MP2/cc-pVTZ potential energy surface of the H₂O and (H₂O)₂ clusters. The objective is then to minimize the root mean square differences between the cluster potential energies of OSS2 model and those based on high-fidelity *ab initio* MP2 calculations, i.e., $(E_{\text{OSS2}}^k(\mathbf{p}) - E_{\text{MP2}}^k)$, which takes the form of

$$f_{\text{RMS}}(\mathbf{p}) = \sqrt{\frac{1}{M} \sum_{k=1}^M (E_{\text{OSS2}}^k(\mathbf{p}) - E_{\text{MP2}}^k)^2}, \quad (13)$$

where \mathbf{p} is the candidate set of parameters, M is total number of cluster configurations in the fitting data, $E_{\text{OSS2}}^k(\mathbf{p})$ and E_{MP2}^k are the energies of water cluster configuration k obtained by OSS2 and *ab initio* MP2 calculations, respectively.

TABLE 10 Results of Wilcoxon's test at 95% confidence level.

| ALGORITHM (SE) | R+ | R- | CRITICAL VALUE (P = .05) | SIGNIFICANT DIFFERENCES? |
|----------------|------|------|--------------------------|--------------------------|
| APRMF | 72.0 | 6.0 | 14.0 | YES |
| MA-LSCH-CMA | 36.0 | 0.0 | 4.0 | YES |
| DEAHCSPX | 34.0 | 2.0 | 4.0 | YES |
| LR-CMA-ES | 68.0 | 10.0 | 14.0 | YES |
| IPOP-CMA-ES | 67.0 | 11.0 | 14.0 | YES |
| EDA | 64.0 | 14.0 | 14.0 | YES |
| RCMA | 78.0 | 0.0 | 14.0 | YES |
| RCGA-FMD | 74.0 | 4.0 | 14.0 | YES |
| SPC-PNX | 75.0 | 3.0 | 14.0 | YES |
| DE | 77.0 | 1.0 | 14.0 | YES |
| COEVO | 78.0 | 0.0 | 14.0 | YES |
| PS+CMA-ES | 67.0 | 11.0 | 14.0 | YES |

On this potential model design problem, the worst and best canonical MA with single search profile were found to be MA-ES and MA-DFP, respectively. Under the computational budget of 300, 000 evaluations, the resultant optimized f_{RMS} on the 40-dimensional problem from each algorithm are MA-DFP (0.298 kJ.mol⁻¹), MA-DSCG (0.436 kJ.mol⁻¹) and MA-ES (2.36 kJ.mol⁻¹). Symbiotic evolution with six search profiles (as described in Section IV-C), on the other hand, generated a low numerical error of 0.222 kJ.mol⁻¹, which outperforms the best canonical MA on this real world problem. It also worth noting

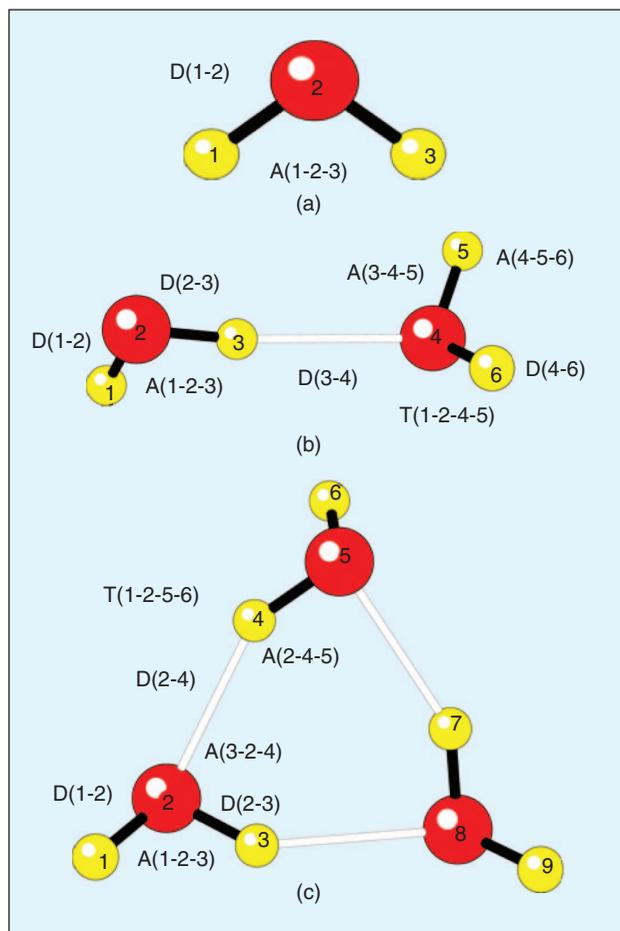


FIGURE 8 Structures of water clusters [(H₂O)_n, n = 1-3].

TABLE 11 Optimized structures of water clusters.

| [(H ₂ O) _n] CLUSTERS | MP2 BONDING INFORMATION | ORIGINAL OSS2 MODEL | MA-DFP | MA-DSCG | MA-ES | SE | UNIT |
|---|-------------------------|---------------------|--------|---------|--------|-------|------|
| N = 1 | | | | | | | |
| D(1-2) | 0.966 | 0.958 | 0.965 | 0.972 | 0.958 | 0.967 | Å |
| A(1-2-3) | 103.9 | 109.2 | 103.9 | 102.1 | 108 | 103.9 | ° |
| N = 2 | | | | | | | |
| D(1-2) | 0.965 | 0.953 | 0.98 | 0.955 | 0.955 | 0.963 | Å |
| D(2-3) | 0.973 | 0.982 | 0.98 | 1.194 | 0.982 | 1.000 | Å |
| A(1-2-3) | 104.3 | 109.7 | 97.8 | 87.1 | 108.1 | 102.3 | ° |
| D(3-4) | 1.952 | 1.932 | 2.109 | 1.309 | 1.935 | 1.899 | Å |
| A(3-4-5) | 104.2 | 113.7 | 126.2 | 80.2 | 114.3 | 114.6 | ° |
| D(4-6) | 0.967 | 0.966 | 0.972 | 0.957 | 0.967 | 0.976 | Å |
| A(4-5-6) | 104.2 | 109.2 | 101.9 | 104.2 | 107.9 | 104.6 | ° |
| T(1-2-4-5) | 123.3 | 116.7 | -90 | 124.9 | 116.8 | 118.8 | ° |
| N = 3 | | | | | | | |
| D(1-2) | 0.965 | 0.96 | 0.968 | 0.975 | 0.963 | 0.967 | Å |
| D(2-3) | 0.979 | 1.008 | 1.027 | 1.209 | 1.007 | 1.046 | Å |
| A(1-2-3) | 105.2 | 111.8 | 104.1 | 75.7 | 109.6 | 106.2 | ° |
| A(3-2-4) | 89.3 | 90.0 | 90.4 | 83.0 | 90.0 | 88.0 | ° |
| D(2-4) | 1.925 | 1.893 | 1.836 | 1.264 | 1.906 | 1.798 | Å |
| A(2-4-5) | 148.4 | 146.2 | 144.7 | 154.9 | 150 | 151.4 | ° |
| T(1-2-5-6) | -21.2 | -2.8 | -24.5 | -176 | -129.5 | -22.2 | ° |

TABLE 12 Normalized errors on the optimized structures of water clusters.

| [(H ₂ O) _n] CLUSTERS | ORIGINAL OSS2 MODEL | MA-DFP | MA-DSCG | MA-ES | SE |
|---|---------------------|-------------|-------------|-------------|-------------|
| N = 1 | | | | | |
| D(1-2) | 0.33 | 0.04 | 0.25 | 0.33 | 0.04 |
| A(1-2-3) | 0.47 | 0.00 | 0.16 | 0.37 | 0.00 |
| N = 2 | | | | | |
| D(1-2) | 0.24 | 0.31 | 0.20 | 0.20 | 0.04 |
| D(2-3) | 0.03 | 0.03 | 0.81 | 0.03 | 0.10 |
| A(1-2-3) | 0.15 | 0.19 | 0.49 | 0.11 | 0.06 |
| D(3-4) | 0.02 | 0.18 | 0.72 | 0.02 | 0.06 |
| A(3-4-5) | 0.13 | 0.29 | 0.32 | 0.13 | 0.14 |
| D(4-6) | 0.04 | 0.20 | 0.40 | 0.00 | 0.36 |
| A(4-5-6) | 0.44 | 0.20 | 0.00 | 0.32 | 0.04 |
| T(1-2-4-5) | 0.03 | 0.92 | 0.01 | 0.03 | 0.02 |
| N = 3 | | | | | |
| D(1-2) | 0.23 | 0.14 | 0.45 | 0.09 | 0.09 |
| D(2-3) | 0.07 | 0.12 | 0.57 | 0.07 | 0.17 |
| A(1-2-3) | 0.15 | 0.03 | 0.69 | 0.10 | 0.02 |
| A(3-2-4) | 0.07 | 0.11 | 0.62 | 0.07 | 0.13 |
| D(2-4) | 0.03 | 0.10 | 0.71 | 0.02 | 0.14 |
| A(2-4-5) | 0.13 | 0.22 | 0.38 | 0.09 | 0.18 |
| T(1-2-5-6) | 0.06 | 0.01 | 0.54 | 0.38 | 0.00 |
| TOTAL | 2.65 | 3.06 | 7.34 | 2.38 | 1.58 |

distances (D), angles (A) and torsion angles (T) between atoms are shown in the figure.

The stable geometry structures of water clusters with lowest potential energy are first obtained by conducting a structural optimization procedure on the OSS2 potential energy surface with the original and optimized parameters obtained by the algorithms. The bonding information of the optimized [(H₂O)_n, n = 1–3] clusters is then assessed by taking the *ab initio* MP2 calculations as baseline for investigating the quality of the freshly designed OSS2 potential model. The numerical results as reported in Table 11 include, from left to right, the MP2 bonding information and those calculated using the original [47] and optimized OSS2 models obtained by the MAs and symbiotic evolution (SE). The bond information errors of the optimized structures with respect to the *ab initio* MP2 calculations are normalized and reported in Table 12. Summation of the normalized errors for each algorithm on the (H₂O)_n

clusters is subsequently used as an error index for comparison. From the table, SE exhibits the lowest error index, thus indicating that the potential model derived by symbiotic evolution reproduces well not only the *ab initio* potential energies but also the geometrical structures of water clusters that agree favorably with those obtained by means of *ab initio* calculations. Such results confirmed our motivation for formalizing the symbiosis of gene and meme in adaptive search, thus encouraging the use of symbiotic evolution model, rather than relying simply on one fixed, and possibly poor choice of search profile that may not lead to truly optimized designs. Symbiotic evolution clearly offers

that to the best of our knowledge, the f_{RMS} solution attained by SE is much lower than that of the original OSS2 parameters reported in the literature [47], which stands at 2.58 kJ.mol⁻¹. Aside from the ability of the OSS2 potential model in reproducing *ab initio* MP2 energy calculation, it is also desirable for the potential model to be capable of accurately describing the stable geometry structures of (H₂O)_n clusters. Figure 8 illustrates the geometry structures of water clusters [(H₂O)_n, n = 1–3] in which red balls represent the oxygen atoms whereas the yellow ones represent hydrogen atoms. Due to the symmetry of the clusters' structures, only representative bond information of the

a high quality and robust approach for continuous parametric design problems, regardless of whether a *a priori* knowledge of the most suitable search profile on the problem is available.

VII. Conclusion

The general practice on manual crafting of dedicated search solvers in computational intelligence community has evolved into the emerging field of adaptive search algorithms. Adaptation of parameters and operators in search now represents one of the most important, promising and challenging areas of research in the field computational intelligence.

In this article, we have presented the modeling of adaptive search as a *symbiosis* of genetic (through its stochastic variation) and memetic mechanisms (through lifetime learning) in evolutionary search, working in sync on solving a given problem in hand. The potential of each symbiotic search profile composing of stochastic variation and lifetime learning in creating good individuals is then quantified formally using the concept of *evolvability*. To demonstrate how the methodology introduced can be put into practice for solving complex problems, Symbiotic Evolution (SE) as a realization of the proposed theory is then proposed. SE performed a statistical learning of *evolvability* at runtime to infer the respective productive symbiotic search profile for each individual, leading to the self-configuration of solver that searches effectively on a given problem in hand. Numerical study of the SE with assessment made against several recent state-of-the-art modern evolutionary methods, adaptive and hybrid approaches on representative benchmark problems and the design of a real-world OSS2 potential model for $(H_2O)_n$ water clusters confirmed our motivation for formalizing the symbiosis of gene and meme in adaptive search.

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