A quantum simulation algorithm for continuous optimization

Anna Ouskova Leonteva
University of Strasbourg, ICUBE Lab
CNRS UMR 7357 — France

Ulviya Abdulkarimova
University of Strasbourg, ICUBE Lab
CNRS UMR 7357 — France
Azerbaijan State University of Oil and Gas Industry, Baku — Azerbaijan

Tobias M. Wintermantel
University of Strasbourg, ISIS UMR 7006 — France
Universität Heidelberg, Physikalisches Institut — Germany

Anne Jeannin-Girardon
University of Strasbourg, ICUBE Lab
CNRS UMR 7357 — France

Pierre Parrend
University of Strasbourg, ICUBE Lab
CNRS UMR 7357 — France
ECAM Strasbourg Europe — France

Pierre Collet
University of Strasbourg, ICUBE Lab
CNRS UMR 7357 — France

ABSTRACT

This paper presents a novel multi-threaded quantum inspired optimization algorithm targeted at global search in continuous domains. The proposed approach is based on a Diffusion Monte Carlo (DMC) physical model and is characterized by a set of parallel quantum walk processes. The effectiveness of the proposed algorithm is demonstrated by experimental results on the 24 noiseless functions from the Black Box Optimization Benchmark of the Comparing Continuous Optimization benchmarking platform (COCO).

KEYWORDS

Quantum evolution, single objective optimization, black-box optimization

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1 INTRODUCTION

One of the main problems of all global search optimization algorithms is premature convergence into local optima. In order to overcome this problem, quantum theories are introduced into optimization algorithms such as Quantum Particle Swarm Optimization (QPSO) [1] or Quantum Annealing (QA) [2]. QA applies quantum tunneling effects in order to explore the search space towards the best solution. QPSO creates a quantum delta potential well model as the sample function for PSO. These quantum simulation algorithms perform better in global optimization [3] than their classical counterparts (Particle Swarm Optimization, Simulating Annealing), but they also have a very slow convergence rate towards the global optimum.

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This work tries to improve the exploration *versus* exploitation trade-off by proposing a new quantum simulation algorithm, named QAFFE, for Quantum Algorithm For Fast Evolution by:

- adapting the DMC model to the evolutionary optimization process and
- using a multi-threaded algorithm structure, to speed up the optimization process.

The performance of QAFFE is evaluated on 24 test functions [4] and compared with the results of QPSO, BFGS [5] and BIPOP-CMAES [6]. The results demonstrate the effectiveness of the proposed algorithm to find global optima.

2 PROPOSED APPROACH

The Diffusion Monte-Carlo algorithm is well presented in Kosztin *et al.* [7]. It is based on the Feynman Path Integral solution of the imaginary time Schrödinger equation, where the wave function is signified as an integral, evaluated by the Monte Carlo method.

We use the same analogy of seeing the cost function as a potential energy and a particle as an individual in the population. The initial population is small and is equal to the number of CPU threads. All threads launch the quantum evolution process based on three steps of DMC:

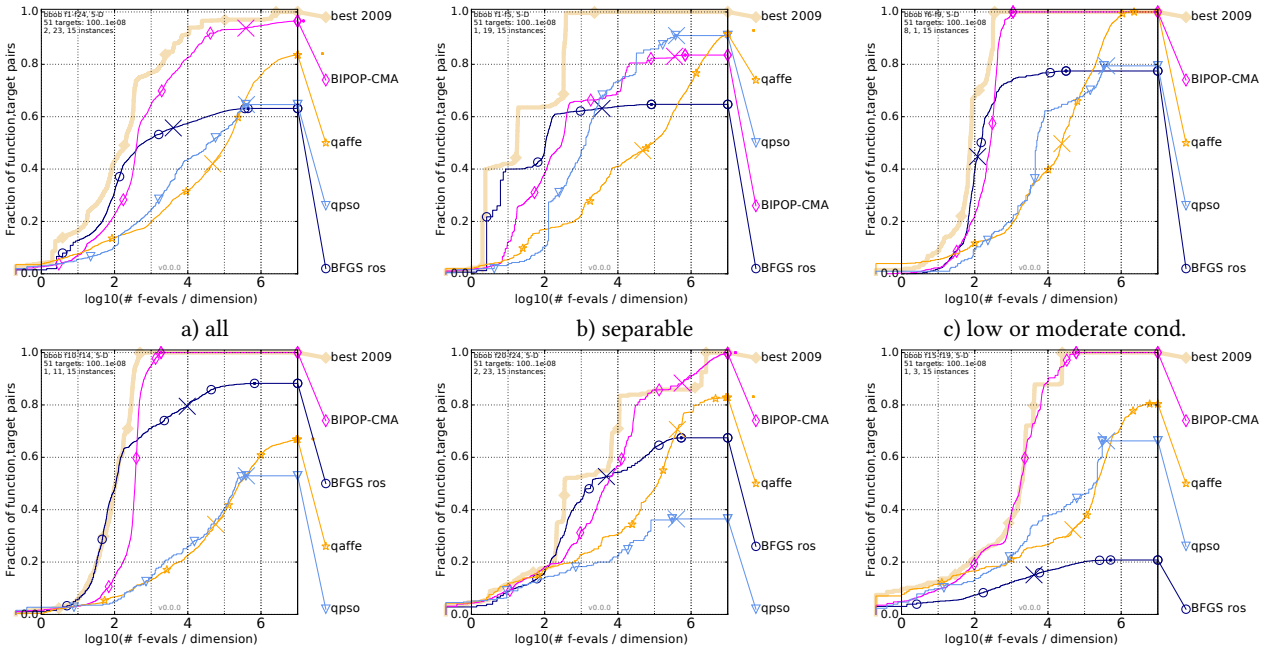
- Diffusive displacement with the Gaussian probability distribution for the local "attractor".
- Branching to achieve better accuracy.
- Adjusting variance to control the convergence rate.

The threads are coupled to each other by their reference energy. During the iterations, the size of population is dynamically adjusted (larger or smaller than previous one) according to the branching step. This technique improves the global search ability.

3 EXPERIMENTAL RESULTS

The main goal of the experiments is to validate the global search capability with a relatively fast convergence rate for various problems in a 5-dimensional space. The performance is measured in terms of Expected Run Time (ERT - the number of evaluations conducted on a given problem until a given target value is hit). The performance of QAFFE is compared with the results obtained by QPSO [1] and of two referenced algorithms: BFGS [5] and BIPOP-CMAES [6].

The test suite consists of the 24 single-objective noiseless functions [4] from the COCO framework [8], which is divided into 5



a) all b) separable c) low or moderate cond.

d) high cond. and uni-modal e) multi-modal adequate glob.struct. f) multi-modal weak glob.stuct.

Figure 1: Runtime distribution summary by function groups

groups: separable, with low or moderate conditioning, with high conditioning and uni-modal, multi-modal with adequate global structure and multi-modal with weak global structure. Figure 1 (a-f) displays the achieved target value precision (y-axis = fraction of function, target pairs) in proportion with the number of needed evaluation functions in logarithmic scale (x-axis = $\log(\frac{f_{\text{eval}}}{\text{dimension}})$) for each group of functions.

Figure 1 (a) represents an integral characteristic in terms of ERT for all groups of functions for each algorithm. QAFFE takes the second place in accuracy after BIPOP-CMA, but QAFFE shows lower convergence rate.

The results for the group of separable functions are demonstrated in Figure 1 (b). QAFFE shows the best accuracy, as well as QPSO, but it has lower convergence rate.

Figure 1 (c) represents the results for functions with low or moderate conditioning. QAFFE has the best convergence rate in the initial stage. But upon reaching the first accuracy threshold, QAFFE shows lower convergence rate than BFGS and BIPOP-CMA. QAFFE achieves the best accuracy, as well as BIPOP-CMA.

The results for the group of uni-modal and functions with high conditioning are shown in Figure 1 (d). QAFFE is inferior in all parameters than BFGA and BIPOP-CMA, but shows better accuracy than QPSO.

Figure 1 (e, f) represents the results for multi-modal functions. QAFFE has the best convergence rate in initial stage for several functions, but upon achieving the first accuracy threshold, QAFFE shows lower convergence rate than BIPOP-CMA. QAFFE takes the second place in accuracy after BIPOP-CMA.

4 CONCLUSION

Analysis of experimental results on the BBOB testbed shows that:

- QAFFE demonstrates better performance than QPSO.
- QAFFE has the second accuracy value in the integral characteristic (in terms of ERT) for all groups of functions.
- The low convergence rate of QAFFE after the initial stage is explained by a deterministic scheme of variance reducing, which is used to sampled candidate solution during diffusive displacement.

The current work in progress aims at eliminating this shortcoming by adding step-size adaptation techniques.

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