Quantum Genetic Selection

Using a Quantum Computer to Select Individuals in Genetic Algorithms

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ABSTRACT

This paper proposes an innovative selection operator based on concepts from quantum mechanics. In particular, a quantum state is used to embody genetic individuals and their fitness values, and a quantum algorithm known as amplitude amplification is used to modify this state in order to create a quantum superposition in which the probability to measure an individual is related to its quality. The main peculiarity of this approach is related to the non-zero probability of selecting individuals do not belonging to the current population so as to create new genetic material and reduce the likelihood that genetic evolution will converge to local optima. The suitability of the proposed operator has been proved by an experimental session where a comparison with well-known selection methods has been carried out on a set of benchmark problems.

CCS CONCEPTS

• **Computing methodologies** → **Search methodologies**; • **Computer systems organization** → **Quantum computing**;

KEYWORDS

Genetic selection, quantum genetic algorithms

ACM Reference Format:
Giovanni Acampora, Roberto Schiattarella, and Autilia Vitiello. 2021. Quantum Genetic Selection: Using a Quantum Computer to Select Individuals in Genetic Algorithms. In *2021 Genetic and Evolutionary Computation Conference Companion (GECCO '21 Companion), July 10–14, 2021, Lille, France.* ACM, New York, NY, USA, 2 pages. https://doi.org/10.1145/3449726.3459505

1 INTRODUCTION

The selection mechanism is the procedure that Genetic Algorithms (GAs) use to choose a set of individuals from the current evolutionary population to form a pool of parents from which the next generation will originate. Selection operators play a fundamental role on the performance of GAs in navigating a search space of a specific optimization problem by considering a suitable balance between exploration (i.e. exploring the new areas of search space) and exploitation (i.e. using already detected points to search the optimum) [2]. The aim of this paper is to enrich the literature with an innovative selection operator, denoted as *Quantum Selection Operator* (QSO), which exploits the stochastic nature of quantum computation to perform a suitable selection of individuals in genetic evolution. The key idea behind the design of the proposed selection operator is provided by the jointly usage of two well-known quantum concepts: *quantum state* and *quantum Amplitude Amplification* (QAA) [1]. In quantum mechanics, a state can encode a superposition of all the 2^n possible binary combinations obtainable with n bits. Each classical combination can be obtained with a certain probability measuring the quantum state. On the other hand, QAA is a quantum algorithm aimed at increasing the probabilities of measuring desired classical binary strings. Starting from these concepts, QSO is defined as a selection operator that models genetic individuals and their fitness values by a quantum state $|\psi\rangle$ opportunely generated by the application of a modified version of the QAA. The main peculiarity of QSO is that it allows to select individuals that are not present in the current genetic population with a non-zero probability. This leads to add new genetic material into the population, reducing the likelihood that genetic evolution will converge to local optima. QSO is able to control its effects on population diversity thanks to the opportune choice of its hyper-parameters.

GECCO '21, July 10–14, 2021, Lille, France

ACM ISBN 978-1-4503-8351-6/21/07…$15.00
https://doi.org/10.1145/3449726.3459505

2 QSO: A NEW SELECTION OPERATOR

Let us suppose to run a binary-encoded genetic algorithm equipped with QSO as selection operator. The workflow of QSO is hereafter described:

(1) Let $\mathcal{P}$ be a genetic population of k binary encoded individuals and let $\mathcal{P}' = \{s_{i_0}, s_{i_1}, \ldots, s_{i_{t-1}} | i_j \in \{0, 1, \ldots, 2^n - 1\}\}$ be the ordered set of t individuals of $\mathcal{P}$ with the best fitness values $f_{i_0}, f_{i_1}, \ldots, f_{i_{t-1}}$, where f_{i_m} is a better value than f_{i_n} if $i_m < i_n$. Let $\mathcal{G} = \{s_{l_0}, s_{l_1}, \ldots, s_{l_{2^n-t-1}} | l_j \in \{0, 1, \ldots, 2^n - 1\}\}$ be the complementary set of $\mathcal{P}'$ composed of all the remaining possible binary strings of n binary digits.

(2) Initialize a quantum register $\mathcal{R}$ of n qubits $|\psi_0\rangle = |0\rangle^{\otimes n}$ by applying n Hadamard gates to create a quantum uniform superposition of elements belonging to $\mathcal{P}'$ and $\mathcal{G}$ as described in :

$$
\begin{aligned}
|\psi\rangle = H^{\otimes n} |\psi_0\rangle = \sum_{x=0}^{2^n-1} \frac{1}{\sqrt{2^n}} |s\rangle = \\
= \sum_{j=0}^{t-1} \frac{1}{\sqrt{2^n}} \left|s_{i_j}\right\rangle + \sum_{j=0}^{2^n-t-1} \frac{1}{\sqrt{2^n}} \left|s_{l_j}\right\rangle
\end{aligned}
\tag{1}
$$

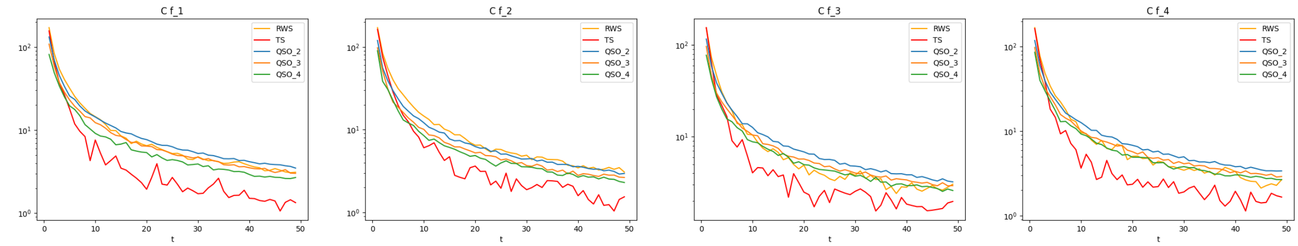

Figure 1: Value of C in logarithmic scale as function of the number of generation t.

(3) Define a quantum circuit using the register $\mathcal{R}$ and perform QAA for the states related to individuals in $\mathcal{P}'$ as follows:
- Define a Boolean function $\chi : \{0, \ldots, 2^n - 1\} \longrightarrow \{0, 1\}$:

$$\begin{cases} \chi(s) = 1 & \text{if } s \in \mathcal{P}' \\ \chi(s) = 0 & \text{if } s \notin \mathcal{P}' \end{cases} \tag{2}$$

- Execute the flip phase operation $\mathcal{FP}$, marking the quantum states $|s_{z_j}\rangle$ as follows:

$$|s_{z_j}\rangle \rightarrow \begin{cases} e^{i(\pi - j\beta)}\,|s_{z_j}\rangle & \text{if } \chi(s_{z_j}) = 1 \\ |s_{z_j}\rangle & \text{if } \chi(s_{z_j}) = 0 \end{cases} \tag{3}$$

where $\beta \in \left[0, \frac{\pi}{t+1}\right]$ and i is the imaginary unit.
- Execute the mirror operation $\mathcal{MP}$ and iterate the $\mathcal{FP}$ and $\mathcal{MP}$ for a selected number of iterations N_G, obtaining the final quantum state $|\psi_f\rangle$:

$$|\psi_f\rangle = \sum_{j=0}^{t-1} c_{s_{i_j}}\,|s_{i_j}\rangle + \bar{c} \sum_{j=0}^{2^n - t - 1} |s_{l_j}\rangle \tag{4}$$

such that

$$|c_{s_{i_0}}|^2 > |c_{s_{i_1}}|^2 > \cdots > |c_{s_{i_{t-1}}}|^2 > |\bar{c}|^2 \tag{5}$$

where $\sum_{j=0}^{t-1} |c_{s_{i_j}}|^2 + |\bar{c}|^2 \times (2^n - t) = 1$.

(4) Measure $|\psi_f\rangle$ to obtain one of the 2^n binary strings.
(5) Repeat k times the steps from (2) to (4) to obtain the mating pool from which the next generation will originate.

The selection probabilities of individuals given by the QSO can be tuned by means of three hyper-parameters t, β, N_G.

- The hyper-parameter t sets the size of the sub-population $\mathcal{P}'$ of individuals with the best fitness values in $\mathcal{P}$. In order to ensure the good behaviour of the amplitude amplification algorithm $t << 2^n$.
- The hyper-parameter β sets the angle for the progressive rotation of the phase for the states $|s_{i_j}\rangle_{j \in [0, t-1]}$. The upper limit for β is defined by the number of states to mark t. If β is set equal to zero, the probability to measure one of desired individuals is uniform.
- The hyper-parameter N_G sets the number of iterations of QAA.

3 EXPERIMENTS AND RESULTS

The performance of QSO have been assessed in an experimental session involving a set of benchmark functions reported in Table 1 and properly discretized. The benefits of QSO are shown in a comparison with well-known selection operators such as the Roulette Wheel Selection (RWS) and the Tournament Selection (TS). In particular, three configurations for QSO are investigated: QSO_2 with $t = 3$, $\beta = \frac{\pi}{4}$, $N_G = 2$; QSO_3 with $t = 3$, $\beta = \frac{\pi}{4}$, $N_G = 3$; and QSO_4 with $t = 3$, $\beta = \frac{\pi}{4}$, $N_G = 4$. As for the compared selection operators, we consider the tournament selection size set to 3.

Table 1: Properties of the discretized benchmark functions

Test function	Bounds
$f_1(x) = \sin(x) + \sin\left(\frac{10}{3}x\right)$	$x_l = 2.7, x_u = 7.5$
$f_2(x) = -e^{-x}\sin(2\pi x)$	$x_l = 0.0, x_u = 4.0$
$f_3(x) = \frac{x^2 - 5x + 6}{x^2 + 1}$	$x_l = -5.0, x_u = 5.0$
$f_4(x) = -x\sin(x)$	$x_l = 0.0, x_u = 13$

To evaluate the quality of the compared selection operators the metric C introduced in [3] has been used. Formally,

$$C(t) = \frac{1}{t}\bar{D}(t) + \frac{t-1}{t}\bar{Q}(t) \tag{6}$$

where $\bar{D}(t)$ and $\bar{Q}(t)$ refer respectively to diversity and quality of individuals in the t-th generation of genetic population. The higher the C value is, the better the performance of the considered selection operator is. The experiments are run by using a quantum simulator, namely *QASM Simulator*[1], provided by Qiskit, an open source library for working with the IBM Q quantum processors.

The plots in Figure 1 show the values of the metric C against the number of generations for all considered benchmark functions. As it is possible to see, the value of metric C for the three configuration of QSO is generally greater than or comparable to that of RWS and TS for all considered benchmark functions.

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