Pair Swap Strategy in Quantum-Inspired Evolutionary Algorithm

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ABSTRACT

Quantum-inspired Evolutionary Algorithm (QEA) with migration strategy is a coarse-grained parallel algorithm, and involves many parameters that must be adjusted manually. This paper proposes a simple pair-swap method which exchanges good solution information between two individuals, and demonstrates that the method can find good solutions constantly. Our experimental results in Knapsack Problem have shown that the proposed pair-swap strategy could find similar or even better quality solutions than the migration strategy in the QEA.

Categories and Subject Descriptors

I.2 [**Artificial Intelligence**]: Miscellaneous; F.2.2 [**Analysis of Algorithms and Problem Complexity**]: Nonnumerical Algorithms and Problems

General Terms

Algorithms

Keywords

quantum computing, quantum bit, genetic algorithm, pair-swap, knapsack problem

1. INTRODUCTION

Quantum computer[1, 2, 3] is a computation model using quantum mechanical principles such as superposition state, interference effect, and entanglement state. Recently, stochastic combinatorial search algorithms combined with evolutionary algorithm have been recently proposed by incorporating quantum mechanical principles or quantum bits[4, 5, 6, 7].

Narayanan et al.[4] have proposed Interference Crossover (IX) for Classical Genetic Algorithm (CGA) in Traveling Salesman Problem (TSP), and have shown that IX can reduce search cost to 2/3 in CGA with a problem involving 9 cities. We have also shown that the combination of IX and Immune Algorithm (IA) shows better search performance than classical IA in TSP problems involving more than 50 cities[5].

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Table 1: The relationship among CGA, IGA, QEA and QEAPS.

Subpopulations (groups)	Granularity of parallel processing	Genetic representation: definite value	Genetic representation: Quantum bit (Stochastic)
None (1 population)	Fine-grained	CGA	QEAPS
Plural subpopulations	Coarse-grained	IGA	QEA

Han et al.[6, 7] have proposed Quantum-inspired Evolutionary Algorithm (QEA) in which each gene is represented by a quantum bit. QEA can do single-point search and automatically shift from global search to local search like Simulated Annealing (SA)[8, 9]. QEA can also perform multi-point search like CGA in order to solve large-scale optimization problems.

In QEA, there are more than one subpopulations (groups) like Island GA (IGA)[10, 11, 12, 13, 14], and inter- and intra-group migration procedures are performed. Evolution in each group enables coarse-grained parallelization and prevents premature convergence[13, 14, 15, 16], and the migration procedures can control search diversification and intensification. However, the adjustment of a number of parameters is required for the number of group and migration intervals for each problem. In fact, Han et al. [6, 7]had to do vast experiments in order to get guidelines for the parameter adjustment in KP.

In this paper, we propose a simpler algorithm which is referred to as Quantum-inspired Evolutionary Algorithm with Pair-Swap strategy (QEAPS). QEAPS involves just one population and a simple genetic operation which exchanges each best solution information between two individuals chosen randomly. Therefore, QEAPS involves less parameters necessary to be adjusted than QEA.

Table 1 shows the relationship between the proposed QEAPS and conventional QEA in contrast with the relationship between CGA and IGA. QEAPS is the algorithm in which subpopulations and migration procedures are removed from QEA, whereas IGA is the algorithm in which subpopulations and migration procedures are introduced into CGA.

We evaluate the search performance of QEAPS on 0-1 Knapsack Problem (KP), and show that QEAPS can find similar or even highly qualified solutions more efficiently and stably than QEA.

2. EVOLUTIONARY ALGORITHM USING QUANTUM BIT REPRESENTATION

2.1 Quantum Bit Representation of Gene

CGA usually uses the definite value of binary, integer, real number, or character as a gene expression. However, quantum bit (qubit) can be used as a gene in QEA and QEAPS. In general, the qubit is described by two-dimensional column vector in the complex vector space where the inner product is defined. It uses the following standard bases as orthonormal base vectors.

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{1}$$

The qubit can has a stochastic superposition state (vector sum) of the two vectors $|0\rangle$ and $|1\rangle$ with each complex probability amplitude. The superposition state q of the quantum bit can be illustrated by the Bloch sphere and shown as follows,

$$q = \alpha\,|0\rangle + \beta\,|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}, \tag{2}$$

where α, β are the complex probability amplitudes to observe the state of 0 or 1, respectively. They are normalized as $|\alpha|^2 + |\beta|^2 = 1$. $|\alpha|^2$ is the probability that the state of 0 is observed, and $|\beta|^2$ is the probability that the state of 1 is observed.

As shown in Figure 1, CGA with binary genes uses an individual expression of a binary chromosome, but QEA and QEAPS with qubit genes use an individual expression of a qubit chromosome q_i and the best solution information b_i. The chromosome composed of the genes with the qubit expression is described as a tensor product of the qubits, $q_i = q_{i1} \otimes q_{i2} \otimes \cdots \otimes q_{im}$. If each qubit is quantum-mechanically observed. then binary information of 0 or 1 can be obtained according to the probability amplitude of each qubit in the chromosome. In the same way as CGA, the fitness of the chromosome can be calculated from the binary information. When we repeat the process and change the generation, the chromosome keeps the best solution information (fitness) $b_i = [b_{i1}, b_{i2}, \ldots, b_{im}]$ as Personal Best obtained until the present generation. Here, m is the number of genes or qubits included in an chromosome and i shows the number of chromosomes or individuals when we use multiple chromosomes or individuals.

The chromosome q_i^t of the individual i in the generation t is written by the tensor product of the qubits as follows:

$$q_i^t = \begin{bmatrix} \alpha_{i1}^t \\ \beta_{i1}^t \end{bmatrix} \otimes \begin{bmatrix} \alpha_{i2}^t \\ \beta_{i2}^t \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} \alpha_{im}^t \\ \beta_{im}^t \end{bmatrix}. \tag{3}$$

2.2 Evolution Mechanism for Single-Point Search

Evolutionary algorithm of QEA with the qubit representation can search a solution by using one individual like Stochastic Hill-Climbing or Simulated Annealing (SA). It is noted that QEA has a characteristic of evolving automatically from global search to local search like SA.

We will describe the evolution mechanism by using one individual with the qubit expression as follows. To begin

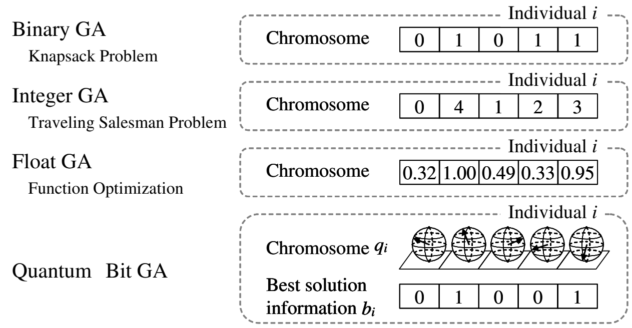


Figure 1: Individual representations in CGA, QEA, and QEAPS.

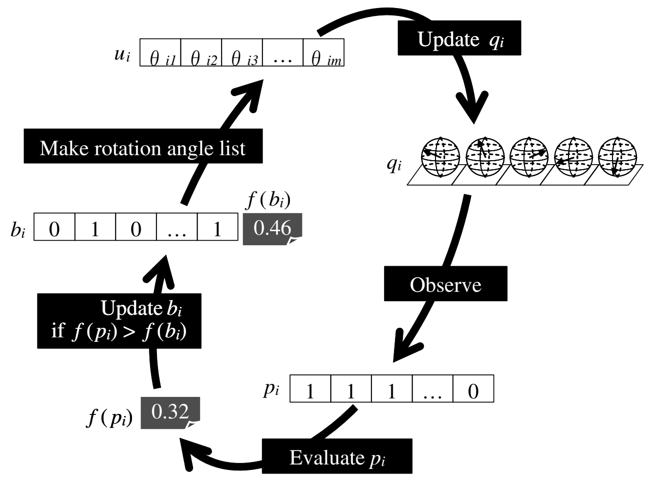


Figure 2: Evaluation of an individual.

with, the initialization is carried out by setting α_{ik} and β_{ik} to $1/\sqrt{2}$ in order to equally observe the states of $|0\rangle$ and $|1\rangle$ in the individual $i(=1)$. This will prepare the equal superposition state of $|0\rangle$ and $|1\rangle$. In this paper, the probability amplitudes of α_{ik} and β_{ik} are supposed to be real number for simplicity. Next, the evolution of an individual with qubits and the exchange of the best solution information in the individual are repeated according to the following procedure, until a given termination condition is satisfied.

The observation for each qubit in an individual is carried out, and then the binary information with 0 or 1 can be obtained depending on the probability amplitude of each qubit in a qubit string as shown in Figure 2. In quantum mechanics, the observation of the qubit results in the contraction of wave packet to the state of 0 or 1. By producing the uniform random number r from 0 to 1, if $r < |\alpha|^2$ then the state will be observed to be 0, and if $r \geq |\alpha|^2$ then the state will be observed to be 1 in QEA and QEAPS. The fitness value $f(p_i)$ of the individual i can be calculated from the binary information p_i like CGA, and then it is used as a fitness of the individual even in QEA and QEAPS.

Next, by comparing the current fitness of p_i with the past best fitness of b_i, the rotation angle list $u_i = [\theta_{i1}, \theta_{i2}, \ldots, \theta_{im}]$ can be created by rotating the superposition state of each qubit to the direction of $|0\rangle$ or $|1\rangle$ depending on the large or

Table 2: Lookup table of the rotation angle θ_{ik}

p_{ik}	b_{ik}	$f(p_i) > f(b_i)$	θ_{ik} $\alpha_{ik}\beta_{ik} > 0$	$\alpha_{ik}\beta_{ik} < 0$	$\alpha_{ik} = 0$	$\beta_{ik} = 0$
0	1	false	θ_C	$-\theta_C$	—	$\pm\theta_C$
1	0	false	$-\theta_C$	θ_C	$\pm\theta_C$	—
Otherwise			0	0	0	0

small relation of $f(p_i)$ and $f(b_i)$ for each qubit.

The rotation angle $\theta_{ik}(k = 1, \ldots, m)$ for k-th qubit determines to increase the probability amplitude of observing 0 or 1 by comparing the fitnesses, as shown in Table 2[6, 7]. Unitary transformation can be used to change the ratio of the probability amplitudes α_{ik} and β_{ik} of the superposition state. To do the unitary transformation, the following rotation matrix can be used and the rotation angle θ_{ik} is used in the rotation matrix.

$$\begin{bmatrix} \alpha'_{ik} \\ \beta'_{ik} \end{bmatrix} = \begin{bmatrix} cos(\theta_{ik}) & -sin(\theta_{ik}) \\ sin(\theta_{ik}) & cos(\theta_{ik}) \end{bmatrix} \begin{bmatrix} \alpha_{ik} \\ \beta_{ik} \end{bmatrix}. \tag{4}$$

For example, the probability amplitude β of observing the 1 is supposed to be increased in the case of not renewing the best solution, i.e., $f(p_i) < f(b_i)$ with $p_{ik} = 0$ and $b_{ik} = 1$. When the superposition state with $\alpha = \sqrt{3}/2$ and $\beta = 1/2$ is located in the first quadrant ($\alpha > 0, \beta > 0$) as shown in Figure 3, the rotation angle θ_{ik} is set to θ_C because of rotating the superposition state to the direction $|1\rangle$ in order that the probability $|\beta|^2$ of observing the 1 will be updated to be increased.

If the rotation angle θ_C is bigger, then the global search becomes dominant. If the rotation angle θ_C is smaller, then the local search is carried out. According to the paper [6], θ_C[rad] is experimentally found to be an adequate value ranging from 0.001π to 0.05π.

If the rotation angle θ_C is too big, then the probability amplitudes do not converge and sometime vibrate, or premature convergence to local maximum will occur. If the rotation angle θ_C is too small, then the search efficiency is confirmed to decrease[6]. We have also confirmed the same effect at our experiments for the 0-1 Knapsack Problem.

In order that the probability $|\beta'_{ik}|^2$ becomes to be greater than the previous probability $|\beta_{ik}|^2$, the rotation angle θ_{ik} in the rotation matrix is determined depending on positive, negative, and zero signs of the probability amplitude α_{ik} and β_{ik} as shown in Figure 3. For example, the state vector in the first and second quadrants shown in Figure 3 is rotated to come close to the axis $|1\rangle$, the vector in the third and forth quadrants shown in Figure 3 is inversely rotated to come close to the axis $-|1\rangle$. The vector $\pm|0\rangle$ ($\beta_{ik} = 0$) in the horizontal axis will show the same effect, even if it is rotated to any directions. The vector $\pm|1\rangle$ ($\alpha_{ik} = 0$) in the vertical axis will not need to be rotated and then the rotation angle θ_{ik} should be naught.

Therefore, the rotation angle list u_i will be made by doing the same procedure, and the qubit chromosome q_i is evolved by the unitary transformation of the rotation matrix with the rotation angle list u_i and updated for the next generation. At the same time, if $f(p_i) > f(b_i)$, then the best solution of the new individual is replaced by the currently observed binary information.

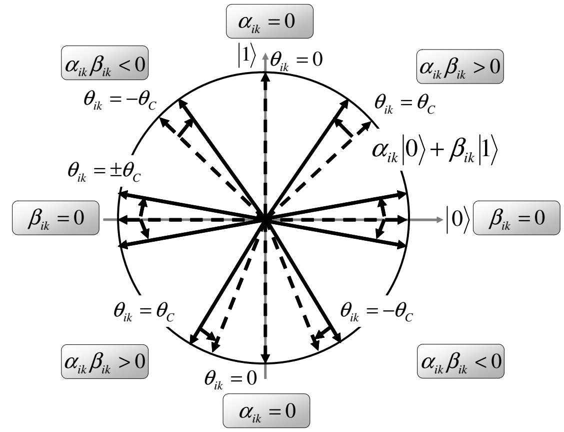


Figure 3: Rotation direction to amplify the observation probability of the state $|1\rangle$.

3. EVOLUTION MECHANISM FOR MULTI-POINT SEARCH

Although evolutionary algorithm with qubits can evolve by using only one individual as the single-point search, it can also evolve by using a population with several individuals as well as multiple-point search algorithms like genetic algorithm or genetic programming in order to solve a major-scale combinatorial optimization problem.

3.1 Algorithm Comparison between QEA and QEAPS

QEAPS proposed in this paper is the algorithm which mainly makes the following improvement for QEA of Han et al.[6, 7].

- The groups are made in the population of QEA, while the groups are not made in the population of QEAPS.
- In QEA, local migration in each group and global migration in the whole population are carried out in the given period, while, in QEAPS, we only exchange each best solution information between two randomly-selected individuals in every generations.

The algorithm of QEA proposed by Han et al.[6, 7] is shown in Figure 4, and the algorithm of QEAPS proposed here is shown in Figure 5. The different processes between QEA and QEAPS in Figures 4 and 5 are shown in gray and black colors, respectively.

3.2 Migration strategy of QEA

Migration strategy of QEA involves local migration and global migration as shown in Figure 6. The local migration is a process of distributing the best solution information of an individual with the highest fitness in each group, to all other individuals in each group, and repeated in every generations. The global migration is a process of distributing the best solution information of an individual with the highest fitness in all groups, to all other individuals in all groups, and repeated in every fixed generations.

QEA is carried out by using two kinds of migrations such as the local and global migrations. QEA shows the centralization of the search, but must determine two parameters of the number of groups and the timing of global migration by considering problem characteristics and scale, convergence speed in a group, rotation angle as QEA fundamental parameter[6, 7].

3.3 Pair Swap method of QEAPS

We propose pair swap strategy in the proposed QEAPS which exchanges each best solution information between two randomly-selected individuals instead of the migration strategy as shown in Figure 7. To begin with, two individuals are randomly selected as a pair from all individuals in the whole group. Then, $n/2$ pairs are generated by selecting two individuals from n (even number) individuals with no overlaps in the group. Only each best solution information is exchanged in each pair without carrying out any operation on the qubits in the individual. The pair swap is preceded as follows: The two individuals i and j exchange each best solution information b_i^t and b_j^t in the generation t, respectively. Each new best solution information made by the pair swap will be $b_i^{t+1} = b_j^t$ and $b_j^{t+1} = b_i^t$ for each individual i and j, respectively. Here, we assume that $f(b_i^t) \geq f(b_j^t)$.

The pair swap is expected to cause that the individual j of which the fitness is lower than that of the individual i increases the probability amplitude to come close to the best solution information b_i^t, and then the fitness is expected to be improved. On the other hand, in the individual i which has the best solution information b_i^{t+1} with the fitness lower than that in the generation t, the best solution information b_i^{t+1} will be updated immediately in the generation $(t+1)$ if $f(p_i^{t+1}) > f(b_i^{t+1})$. The better the probability amplitudes α_{ik} and $\beta_{ik}(k = 1, \ldots, m)$ of the individual i converge to 0 or 1, the worse the individual i is unlikely to become. This is because, even if p_i^{t+1} of the binary string like p_i^t or b_i^t (Figure 8(1)) becomes temporarily worse (Figure 8(2))in the case that α_{ik} and β_{ik} converge, p_i^{t+1} will be immediately renewed by the individual with the qubits (Figure 8(3)). If $f(p_i^{t+1}) < f(b_i^{t+1})$, then the best solution information is not renewed and the probability amplitudes will be changed to become closer to b_j^t.

While the migration strategy stimulates the centralization of the search, the pair swap strategy promotes the diversification of the search in the initial stage that the probability amplitudes are not converging, and then it will stimulate the centralization of the search in the final stage that the probability amplitudes are converging. Although the chromosome with the qubits has features of automatically shifting to the local search from the global search[6], the pair swap strategy is regarded as intensifying the features further.

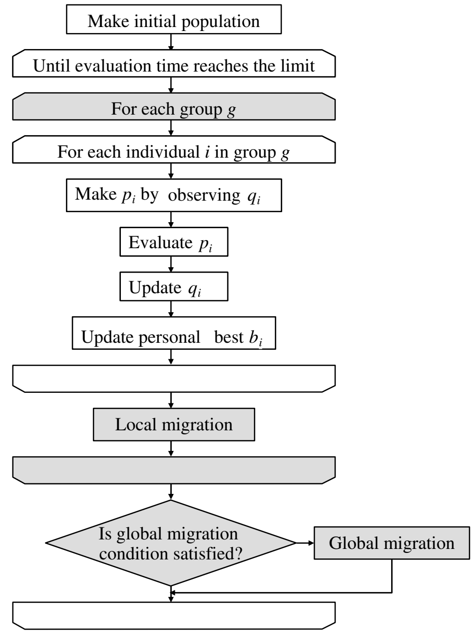


Figure 4: The algorithm of conventional QEA.

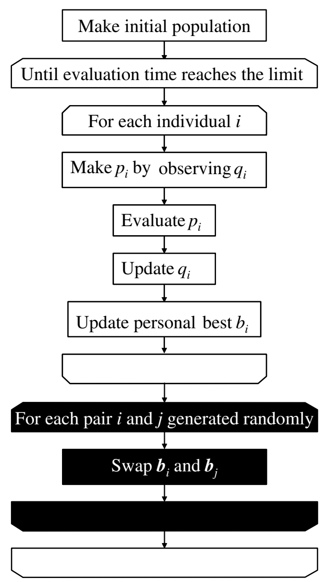


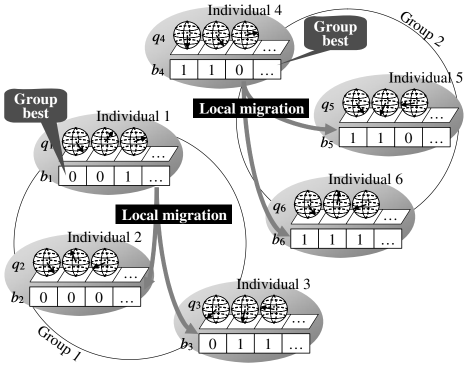
Figure 5: The algorithm of proposed QEAPS.

4. EVALUATION EXPERIMENTS OF PAIR SWAP STRATEGY FOR 0-1 KNAPSACK PROBLEM

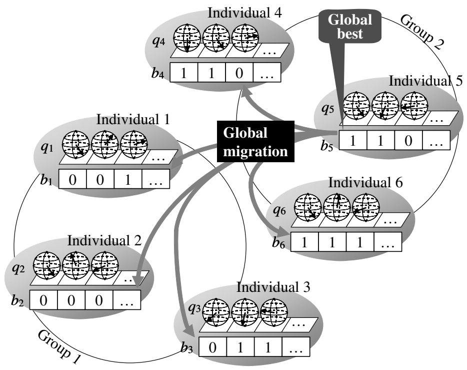
4.1 Preparation for Evaluation Experiments

The 0-1 Knapsack Problem (KP) is used for the evaluation experiments in order to prove the effectiveness of the proposed QEAPS. The KP in the paper [13] is used as a benchmark problem. The number N of items in the KP is used as 100 (the first 100 items are used in the benchmark problem), 250 (the first 250 items are used in the benchmark problem), and 500 (the first 500 items are used in the benchmark problem). The weight limit in the KP is set to be 50% of the total weight of all items. IGA[13] and QEA[7] are used to compare with QEAPS. Parameters such as the population and the number g of groups in IGA and QEA are followed by the previous researches[13, 7], respectively. Parameters used in QEAPS were followed by QEA as shown in Table 3. If the sum weight of selected items happens to exceed the weight limit, then we adjust them by random repair method[6].

The termination condition of search is defined by the evaluation frequency for the individuals in order to compare a few techniques with different experimental conditions of the population. That is to say, the search is finished when



(a) Local migration.



(b) Global migration.

Figure 6: Local and global migration strategy of QEA.

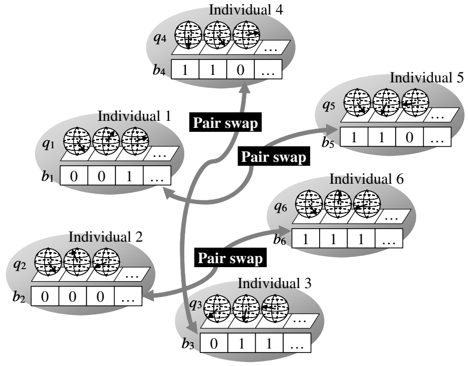


Figure 7: Pair swap strategy in proposed QEAPS.

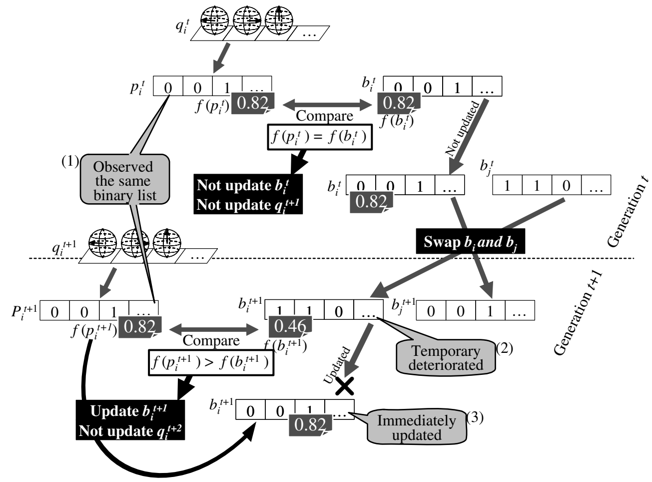


Figure 8: Pair swap example in the case that probability amplitude convergences.

the frequency with which the individual fitness is calculated reaches to a given frequency. We did the same experiments 30 times using each technique for each problem.

Figure 9 shows the evolution of the fitness and the probability amplitudes of 100 qubits of an individual as a function of generations in the KP with $N = 100$ items, where the shading colors show the strengths of the probability amplitude. In the initial stage of the search, the shading colors look gray and blurred which means that the probabilities are near 0.5. In the final stage of the search, the shading colors look black and white which means that the probabilities are near 0 (white) or 1 (black).

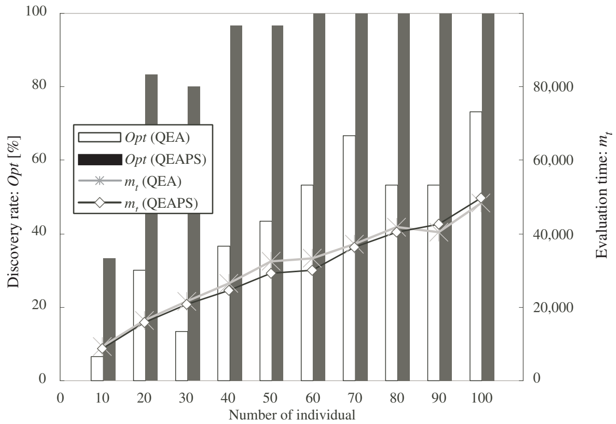
4.2 Comparison between IGA and QEAPS

The proposed QEAPS is compared with IGA. Since IGA avoids the premature convergence at the initial stage in CGA, and carries out the search while keeping a diversity of the group. it is an algorithm for discovering the solution with the quality better than CGA. The experimental results of IGA were taken from our paper [13]. The population is 50 in QEAPS, and the upper limit of the evaluation frequency is 250,000 time in order to use the same experimental conditions with the paper [13]. The number N of items is 500. The averages m_f of the fitness of the best solution as a function of evaluation frequency in QEAPS and IGA are shown in Figure 10. As seen in Figure 10, IGA improved the quality of the discovered best solution by increasing the island number, but the fitness is lower than the optimum solution. However, it should be noted that QEAPS can discover the solution of the quality which is optimum solution or is equivalent to optimum solution. The qubits in QEAPS are considered to discover the solution with the good quality in order to accumulate the information of good items with high values for the weights on continuing the search. As well as Ant Colony Optimization [17, 18] which accumulates pheromone in effective partial routes, the affirmative feedback on the good partial solution is considered to contribute to the improvement on the search performance even in QEAPS.

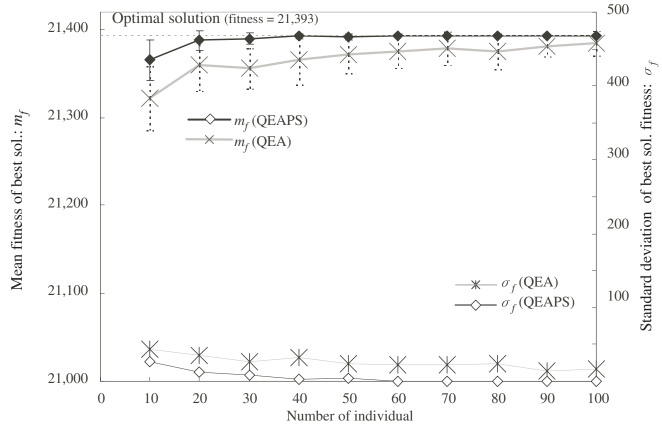
4.3 Comparison between QEA and QEAPS

The proposed QEAPS is compared with QEA in the search performance. Regarding evaluation criteria, we focus on the discovery rate $Opt[\%]$ of the optimum solution per trial number, the average fitness m_f and standard deviation σ_f of the best solution obtained in each trial, and the average m_t of evaluation frequency which discovered the optimum solution in each trial. The upper limit of evaluation frequency is set to $N \times 10^3$ as a termination condition of the search.

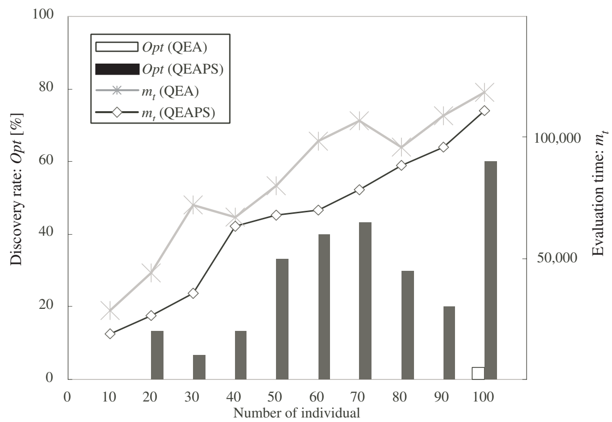
As a function of the individual total numbers, Opt, m_f, σ_f, and m_t are shown in Figure 11. The error bars shown in Figure 11(b), (d) and (f) are the confidence interval with the degree of reliability 95%. According to the discovery rates Opt seen in Figure 11(a), (c) and (e), QEAPS can show a



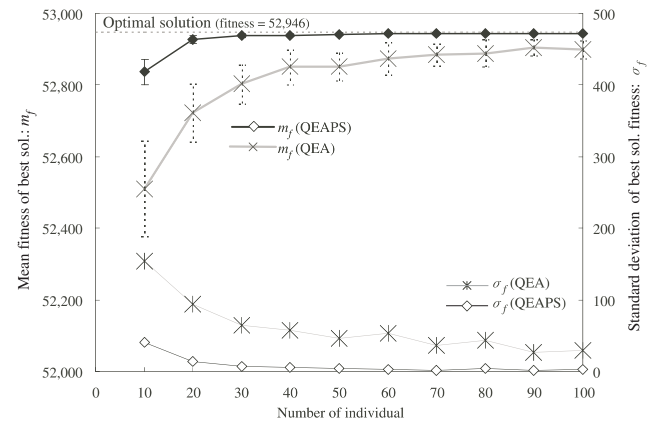
(a) Discovery rate and evaluation time ($N = 100$).



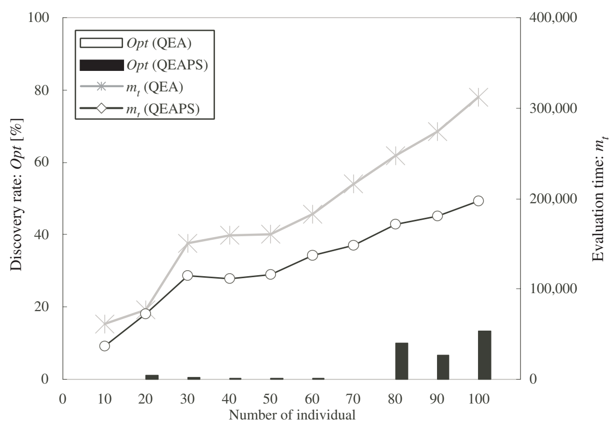
(b) Fitness of best solutions ($N = 100$).



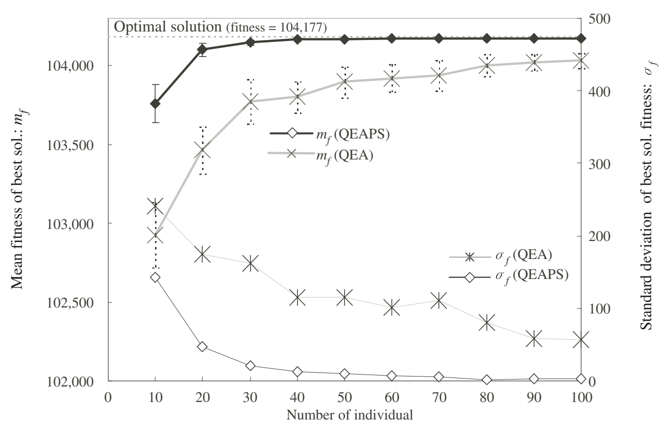
(c) Discovery rate and evaluation time ($N = 250$).



(d) Fitness of best solutions ($N = 250$).



(e) Discovery rate and evaluation time ($N = 500$).



(f) Fitness of best solutions ($N = 500$).

Figure 11: Comparison between QEA and QEAPS

drastically better improvement in the optimum solution discovery rate than QEA, although the overall discovery rates decrease with increasing the number of the items in both of QEA and QEAPS. Moreover, according to Figure 11(b), (d) and (f), QEAPS can significantly improve the discovery rate of the optimum solution which is higher than that obtained by QEA. We have confirmed the significant difference of the average fitnesses m_f in QEA and QEAPS by t-verification with the significant level of 5%. In this experiment, we have examined the average fitnesses m_f by increasing the number of individuals to 100. As a result, the more the number of individuals, the higher the average fitnesses m_f in QEA. This is because QEA uses several groups. On the other hand, the average fitnesses m_f in QEAPS is almost the optimum solution if we use the number of individuals more than 60 even in the problem of $N = 500$ where the discovery rates *Opt* is deteriorated. Regarding the standard deviation σ_f of the best solution, QEAPS shows a significantly smaller standard deviation than QEA, constantly produces the stable good solution, and has a high robustness.

Table 3: Parameter configurations.

Parameter names	Values used IGA	QEA	QEAPS
Number of individuals	500	10, 20, 30, ..., 100	
Number of subpopulations (groups) (g)	5, 10, 30	5	–
Number of individuals in a subpopulation	$\frac{500}{g}$	2, 4,..., 20	–
Rotation angle (θ_C)	–	0.01π	0.01π
Number of observations	–	1	1
Interval of global migration	1 (every generation)	100	–
Crossover rate	$1 - \frac{3\times g}{500}$	–	–
Mutation rate	$\frac{g}{2.5\times 10^5}$	–	–

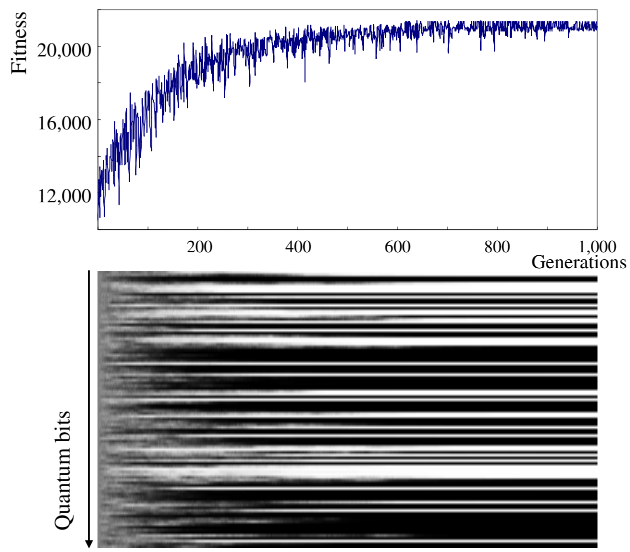


Figure 9: Evolution of probability amplitudes of qubits as a function of generations where the shading colors show the strengths of the probability.

Moreover, QEAPS can efficiently discover the solution of the equivalent or better quality than QEA. In the problem of $N = 100$, the average fitnesses m_f in QEA is 21,385 at maximum in the case of 100 individuals, on the other hand, the average fitnesses m_f in QEAPS is 21,388 in the case of 20 individuals. Regarding the average evaluation frequency m_t shown in Figure 11(a), m_t in QEA with 100 individuals is 48,357, and m_t in QEAPS with 20 individuals is 15,811. Therefore, QEAPS can discover the solution of the equivalent quality in one-third smaller search time than QEA. In the same way, QEAPS can discover the solution of the equivalent quality in one-forth smaller search time than QEA, in the problem of $N = 500$.

4.4 Considerations

The IGA with gene expression having the definite value of integers or bits makes it possible to keep in low communication frequency, to run in a parallel process with coarse

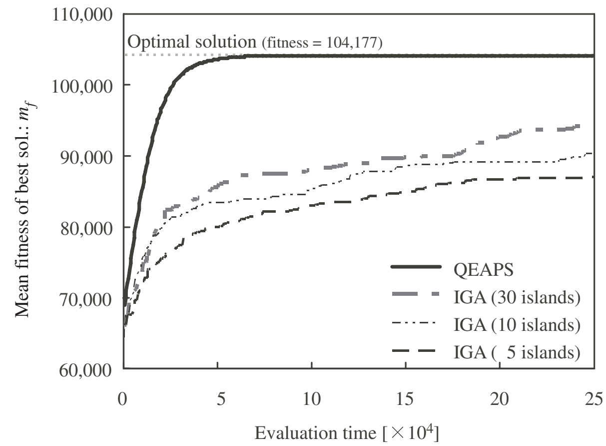


Figure 10: Fitness transitions in QEAPS and IGA ($N = 500$).

grain, and to avoid the premature convergence [13, 14] in the initial search. Since QEA with gene expression of the qubits uses local migrations for each group in every generations, it is necessary to adjust the number of groups and the timing of the global migration in order to avoid the convergence to the local solution.

On the other hand, the pair swap strategy used in QEAPS makes the degree of the centralization in the search region lower than the migration, and can be expected to maintain the diversity in the group, even if several groups are not set up.

In the problem of $N = 500$, the overall optimum solution discovery rate was low even in QEAPS. This is because the diversity in the group gets low in the final stage of the search. It is necessary to use more individuals in a larger scale of problem or to use another mechanism for maintaining the diversity in the group. This paper has just shown the basic effectiveness of the pair swap method, and then the detailed examination must be carried out for the maintenance method of the diversity in the large-scale problem in future.

5. CONCLUSION

We have discussed about the combinatorial optimization using the gene expression of the qubits, and have proposed the combinatorial optimization algorithm QEAPS with the pair swap strategy. The introduction of the pair swap in QEAPS which exchanges each best solution information between two individuals makes it unnecessary to adjust the number of groups and the migration timing necessary for the conventional QEA. The pair swap strategy promotes the global search in the initial stage of the search, and stimulates the local search in the final stage of the search where the probability amplitude is converging. Moreover, the pair swap strategy intensifies the features that the gene expression of the qubits works to automatically shift from the global search to the local search .

It is confirmed that QEAPS obtains the solution of the higher quality than IGA by the evaluation experiment using 0-1 Knapsack Problem. Moreover, it is confirmed that

QEAPS can discover the optimum solution at the higher probability than QEA, that the dispersion of the quality of solution obtained by QEAPS is smaller, and that the solutions with the equivalent quality can be discovered in 1/3 to 1/4 of the search time of QEA.

In the future, the verification and improvement of the search performance in the larger-scale problem should be carried out and the application to the other combinatorial optimization problems should be examined, and the characteristics of the problem where QEAPS is effective should be made clear.

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