QUANTUM COMPUTATION INSPIRED CONSTRAINT HANDLING AND INTELLIGENT LEARNING FOR DATA-DRIVEN COMBINATORIAL OPTIMAL DECISION-MAKING IN OPERATIONS ENGINEERING

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$\|0\rangle$	a basis state of qubit
$\|1\rangle$	a basis state of qubit
$\max_{k=1,\dots,T}\{D_p^k\}$	the highest workforce demand on day *d*
$\|\psi\rangle$	the state of a single qubit
Ω_j	the subset of components in module *j*
$C^n(X)$	multiple qubits controlled NOT gate
D^d	the workforce demand in day *d*
D_k^d	the workforce demand at the *k*th time slot in day *d*
F_1	The value of F_1 measure
I_{2^n}	an $2^n \times 2^n$ identity matrix
$f_c(S)$	the shift operation cost
$f_o(S,D)$	the overstaff cost caused by the unoccupied shift workforce
$f_p(S)$	the penalty for violating the preferences (soft constraints)
$f_u(S,D)$	the understaff cost caused by the uncovered workforce demand
g_l	the granularity of feasible shift lengths
g_{st}	the granularity of feasible starting times
$max_l(d)$	the longest shift length in day *d*
$max_p(d)$	the number of available staffs in day *d*
$max_{st}(d)$	the latest shift starting time in day *d*
$min_l(d)$	the shortest shift length in day *d*
$min_{st}(d)$	the earliest shift starting time in day *d*
p_s	the number of assigned staffs in shift *s*

p_s^d	the number of assigned staffs in a feasible shift *s* in day *d*
t_s	the starting time of shift *s*
t_s^d	the starting time of a feasible shift *s* in day *d*
w_c	the assigned weight for shift operation cost
w_o	the assigned weight for overstaff cost
w_p	the assigned weight for preference violation
w_u	the assigned weight for understaff cost
α_i	the amplitude of qubit *i* in basic state $\|0\rangle$
β_i	the amplitude of qubit *i* in basic state $\|1\rangle$
λ_s	the length of shift *s*
λ_s^d	the length of a feasible shift *s* in day *d*
$\Delta\theta$	rotation angle parameter in QIEA
ASP	airport shift planning
BPNN	backpropagation neural network
CGA	classical genetic algorithm
CNOT	single qubit controlled NOT gate
COP	constrained optimization problem
CSP	Constraint satisfaction problem
D	a set of workforce demand over the planning horizon
d	a day in the planning horizon
Div	dimension-wise population diversity
EA	evolutionary algorithm
EPR	Einstein-Podolsky-Rosen pair (also known as Bell state)
GHZ	Greenberger-Horne-Zeilinger state

H	quantum Hadamard Gate
HQISNN	hybrid quantum inspired neural network
LQIGA	lightweight quantum inspired genetic algorithm
M	the number of modules
$median(x^j)$	the median of dimension j in the population
MRM	material reuse modularity
NSGA-II	non-dominated sorting genetic algorithm II
OE	operations engineering
PSO	particle swarm optimization
QEI-GA	quantum entanglement inspired genetic algorithm
QIEA	quantum inspired evolutionary algorithm
QIGA	quantum inspired genetic algorithm
QINN	quantum inspired neural network
qubit	quantum bit
S	a set of work shifts
s	a shift in the shift set
T	the number of equal-size time slots in a day
TSM	technical system modularity
TU-QIGA	twofold update quantum inspired genetic algorithm
X	quantum NOT gate (also known as Pauli X gate)
Xpl	the percentage of exploration
Xpt	the percentage of exploitation
Γ	a set of objects
Ω	a set of modules
$F(\Omega)$	the overall modularity of module set Ω

$R(\theta)$ simplified single qubit rotation gate

$U(\Delta\theta)$ “update” procedure in QIEA

SUMMARY

Combinatorial optimal decisions are widely observed in operations engineering applications. The emerging field of quantum inspired computation has shown some salient features of quantum information processing that are promised to excel in quantum speedup contributing to solving operational optimization problems of practical relevance more efficiently than conventional paradigms.

This research investigates the potential of quantum inspired optimal decision-making modeling and solutions with the objective of creating mathematical and computational models to advance operations engineering problem solving with respect to three particular technical focuses: (1) Improving computational efficiency through quantum inspired combinatorial optimization; (2) Enhancing domain problem context representation in operations system modeling via quantum entanglement inspired hard constraint handling; and (3) Bolstering data-driven decision making by quantum inspired neural network modeling.

The research proposes and validates a variety of new methods to synthesize a novel quantum inspired decision-making framework, including a twofold update quantum inspired genetic algorithm (TU-QIGA) for computationally efficient combinatorial optimization, a quantum entanglement inspired hard constraint handling approach (QEI-GA) and its variant lightweight quantum inspired genetic algorithm (LQIGA) for optimization with context related hard constraints, and a hybrid quantum inspired semantic neural network (HQISNN) model for learning and supporting data-driven decision making. The accuracy and reliability of the proposed quantum inspired methods and algorithms are

assessed based on computational experiments, along with practical applications of industrial case studies.

CHAPTER 1. INTRODUCTION

1.1 Overview and Motivation

Optimal decisions are widely observed and required in operations engineering (OE) applications (Alcott and Peters, 1996), ranging from modular design (Borissova and Keremedchiev, 2019) to operations planning and scheduling (Gao et al., 2017), and to logistics and supply chain engineering (Vogiatzis and Pardalos, 2013). These decisions essentially entail typical optimization problems that involve planning of an optimal allocation of resources in order to achieve the goal of maximization of some performance metrics (e.g., profit) or minimization of some negative consequence of the operations (e.g., cost) (Curtin, 2005). These combinatorial optimal decision models and solutions are significantly limited by the growing complexity and problem size incurred in practical applications (Ausiello et al., 1999; Neumann and Witt, 2013). Critical research problems that are imperative regarding the complexities of combinatorial optimal decisions in operations engineering problem solving are observed as following:

1.1.1 Computational Efficiency

Combinatorial optimization is proven to be an NP-hard problem, for which computational efficiency is recognized as one classic challenge (Wolsey and Nemhauser, 1999). It is associated with the well-known combinatorial explosion problem due to the inherent enumeration nature of combinatorial optimization (Mukelabai et al., 2018). Exact solutions methods are used to solve small-scale combinatorial optimization problems, but these methods are practically infeasible for large-scale problems due to the modeling

complexities and time constraints. Heuristic methods, on the other hand, are capable of providing near-optimal solutions for large-scale problems due to their characteristics in handling exploration-exploitation tradeoffs. Improvement of computational efficiency remains to be a critical research issue, especially for heuristic methods of combinatorial optimization.

1.1.2 Domain Problem Context Awareness

The conventional wisdom of combinatorial optimization problem solving is consistent with the basic modeling framework of mathematical programming that is based on simplification and approximation to abstract domain problems in the expressions of objective functions and constraints. There are reported ample practical evidence revealing that many types of operational optimization problems are solved by leveraging their particular domain contexts and decision structures (Jouglet and Carlier, 2011). Noticeably, in many engineering scenarios, the domain context information, as well as other problem definition information, can only be specified in a set of constraints on the decision variables (Dagdia and Mirchev, 2020). Thus, the complexity and scale of the constraints can often explicitly decide the complexity of the optimization task. It is important to examine the potential of quantum inspired computation paradigm for discovering new optimization algorithms, especially for applied operational problems.

1.1.3 Data-driven Decision Making

Optimal decision making in practical engineering application scenarios requires not only the optimization capability based on a rigid formulation of the problem domain, but also a data-driven learning ability to proactively respond to the dynamic nature of the real-

world environment. Data-driven machine learning and the decision making based upon has attracted much attention as a paradigm for making better-informed decisions possible (Jin et al., 2019). By exploiting the highly contextualized data, the organization's competitive edge can be harnessed by uncovering patterns, novel insights, and knowledge through data-driven decision making (Zhao et al., 2007). Nonetheless, the effectiveness of learning from actual data with suitable domain knowledge representation applications still lacks practical implementation (Hou and Jiao, 2020). It is of practical significance to examine the essential impact and best form of data-driven domain context-aware learning for decision making in order to embrace the benefits of the data analytics and machine learning paradigms.

1.2 Research Objectives and Technical Roadmap

This research aims to develop a novel quantum inspired optimal decision-making framework. The objective is to create mathematical and computational models to advance operations engineering problem solving with respect to three particular technical focuses:

(1) ***Improving computational efficiency through quantum inspired combinatorial optimization***: The quantum inspired genetic algorithm exploits quantum bit representation to harvest an exponentially higher information density. It operates in accordance with the probability of the initial individual to collapse into the optimal solution, while maintaining the maximum diversity in the population. Quantum inspired probabilistic search to the largest extent augments the exploration capability over the search space to be more thoroughly than conventional deterministic search strategies.

(2) ***Enhancing domain problem context-awareness in operations system modeling via quantum entanglement inspired constraint representation***: In traditional encoding methods, constraints are not built into the solution; but rather they are enforced through supplemental operations. These supplemental operations significantly increase the computational cost, especially for the large-scale and complex problems such as those encountered in practical operations engineering systems. In this regard, quantum entanglement has a unique advantage in that the quantum states of two or more objects have to be described with reference to each other, even though the individual objects may be spatially separated. This leads to the correlations between observable properties of the systems. Therefore, unlike traditional methods, quantum entanglement inspired representation methods enable complex constraints to be represented coherently in the quantum states while mapping back to domain problem contexts.

(3) ***Bolstering data-driven decision making through quantum inspired machine learning***: Due to the ever-increasing consumer demands and industrial needs for efficient operations, future decision making relies more and more on data that packed with uncertainties. Often, the lack of theoretical understanding of underlying input-outcome relationship in the operations leads to errors of predictive modeling accumulated in the final results. The salient advantages of quantum inspired neural network learning models offer great opportunities for empowering domain context representation and domain context-aware learning in supporting data-driven operations decision making.

Based on the aforementioned information, a complete research roadmap regarding the quantum inspired computation for data-driven combinatorial optimal decision-making in operations engineering is illustrated in Figure 1.

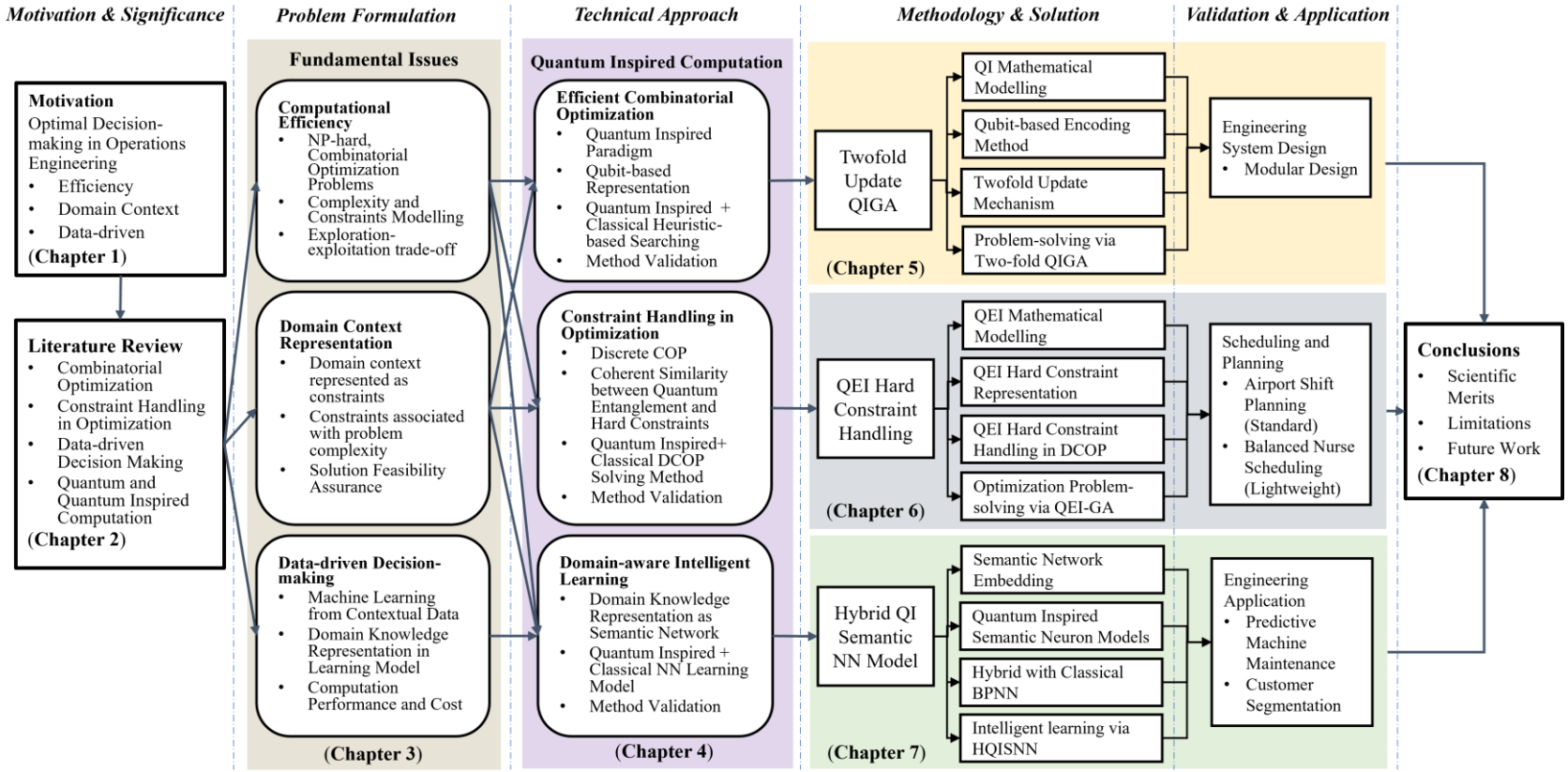


Figure 1. Research Roadmap

1.3 Dissertation Overview

Aligning with the research roadmap in Figure 1, the dissertation is organized as follows:

CHAPTER 1 discusses the motivation and significance of this research topic along with a holistic view of three critical research problems and the corresponding research goals. CHAPTER 2 reviews the literatures of research in the area of optimal combinatorial decision making in operations engineering and the great potentials of the new emerging paradigm of quantum inspired computation.

CHAPTER 3 presents the identification and abstract formulation of the three fundamental research issues, which are computation efficiency, domain context representation and data-driven decision-making, as well as some typical examples of each research issue for the demonstration purpose.

CHAPTER 4 provides the theoretical foundations and technical rationality of the quantum inspired computation paradigm prior to the presentation of each detailed quantum inspired methodologies in the follow-up chapters along with the corresponding solutions and validation case studies.

In CHAPTER 5, a twofold update quantum inspired genetic algorithm (TU-QIGA) is proposed for efficient combinatorial optimization. The detailed mathematical modelling, methodologies and solutions are presented, the effectiveness and efficiency are validated through a case study application to engineering system optimization.

In CHAPTER 6, a quantum entanglement inspired hard constraint handling approach is proposed for constrained combinatorial optimization problem solving. The detailed mathematical modelling and the methodologies of the quantum entanglement inspired constraint representation are presented, as well as two possible solutions depending on the scale of the problem. A standard solution is given with the application of the proposed quantum entanglement inspired genetic algorithm (QEI-GA) to airport shift planning (ASP), and a lightweight solution is provided with the application of the proposed lightweight quantum inspired genetic algorithm (LQIGA) to small scale balanced nurse scheduling.

In CHAPTER 7, a hybrid quantum inspired semantic neural network (HQISNN) is proposed for domain context-aware intelligent learning. The detailed methodologies and solutions are presented, with the corresponding validation and application to predictive machine maintenance and customer segmentation.

CHAPTER 8 concludes the dissertation, along with the discussion of the scientific merits and contributions of this research, as well as the limitations and possible future work.

CHAPTER 2. LITERATURE REVIEW

In this chapter, the literatures in related research fields are reviewed. Aligning with the three research objectives, the literature review focuses on the combinatorial optimization techniques, the mainstream constraint handling approaches for solving discrete constrained combinatorial optimization problems, and the emerging fields of quantum computation and quantum inspired computation, as well as the current research achievements of applying quantum inspired techniques to engineering problem solving.

2.1 Combinatorial Optimization

Combinatorial optimization is the process of searching for optima (i.e., maxima or minima) of an objective function whose domain is a discrete but large configuration space with a finite set of possible solutions. The set of possible solutions is generally defined by a set of restrictions that have to be met for items to be selected into groups, and the configuration space is usually too large for exhaustive search. A considerable number of combinatorial optimization problems, such as the knapsack problem and the Boolean satisfactory problem, are known as NP complete or NP hard. To find the optimal or sufficiently good solutions in practical time, many algorithms have been proposed. In some cases, the problems can be solved exactly using techniques, such as linear programming, dynamic programming, branch-and-bound algorithms (Wolsey and Nemhauser, 1999). These algorithms guarantee that an optimal result to be found if one exists. With the appropriate problem formulation modeling and application of many powerful programs, most of non-large-scale problems can be solved within minutes or even seconds. While in other cases, no exact algorithms are feasible and thus, approximation algorithms must be

employed with no guarantee to find an optimal solution. Polynomial-time approximation algorithms are often desirable due to their guarantees in the computation efficiency, though many real-life problems are inapproximable. Various heuristics for solving combinatorial optimization problems have been proposed by many researchers, since the heuristics methods are often easy to implement and can be tailor-made for particular domain problems. Evolutionary Algorithms (EAs) are heuristic-based algorithms inspired by the principles of natural selection, molecular genetics and biological processes; they provide a general approach to solve complex problems, especially for those that cannot be solved in polynomial time easily, as supplements to conventional optimization methods. Many evolutionary algorithms have been proposed and researched, including Genetic Algorithm (GA), Swarm Algorithms and so on. While the essential feature differences among them are mainly the representation/encoding of chromosomes/individuals, the selection/reproduction strategies, mutation and/or recombination operators (Back, 1996), the core mechanism of EAs computation success is associated with a generic population-based metaheuristic and strategies to handle the exploration-exploitation tradeoff (Črepinšek, 2013) even among the most recent variants of EAs (Faramarzi et al., 2020; Salgotra et al., 2021).

2.2 Constraint Handling in Optimization

A constraint is a logical relation between one or more variables. The goal of the logical relations is to restrict the feasibility each potential solution can assume. Hard constraints must be satisfied by all feasible solutions (Berrada et al., 1996), since they are related to the axioms, postulates, rules, and principles associated with the specific problem domain. The rest of constraints (also known as soft constraints) are more of concerns and

preferences. Conceptually, optimization algorithms for unconstrained and constrained optimization problems are based on the same iterative philosophy. Therefore, in some sense, the constraint handling mechanisms can be discussed and employed as a separate issue from the search algorithms (Mezura-Montes and Coello, 2011).

2.2.1 Mainstream Approaches

Enormous research has been done in the field of constraint handling mechanisms, some eliminate the infeasibility completely, while others may allow a certain amount of tolerance for infeasible solutions during the searching process. The former category usually requires additional manipulations during the generation and update of individuals via special decoders and operators (Koziel and Michalewicz, 1998), however, such methods often involve additional computational cost and the risk of searching diversity decrease. The latter category measures the violation of constraints of each individual by different metrics to guide the searching process with various of strategies. Some mainstream approaches include:

2.2.1.1 Use of Penalty Functions

A COP can be converted to an unconstrained one by using predefined penalty function (Kitayama et al, 2006; Park and Kim, 2015), which is a stationary measurement of the violation of constraints. This type of methods is very popular due to their ease of implementation, and thus commonly being used in operations engineering optimization, especially for the COPs with only soft constraints, however, the suitable setting of penalty function is usually problem-dependent and requires the experience of users.

2.2.1.2 Multi-objective Concepts-based Methods

Constraint handling methods based on multi-objective concepts transform a single-objective COP to multi-objective unconstrained one by creating an additional objective for constraint violation measure (Wang et al., 2007; Segura et al., 2016), besides the original objective function. It allows a proportion of infeasible solutions in order to maintain population diversity, however, this type of methods require the matching algorithm to process multi-objective searching ability and the multi-objective handling strategies can be complicated.

2.2.1.3 Feasibility Rules-based Approaches

Feasibility rules enable COP solving by coupling with a variety of dynamic control mechanisms for adjusting the tolerance of constraint violations (Barkat Ullah et al., 2008; Jiao et al., 2019). The popularity of this category is largely due to its general suitability with various of searching algorithms, however, the proper setting of some parameters can be challenging.

2.2.2 Critical Research Problems

In the particular application domain of operations engineering, optimization problems, such as scheduling and planning tasks, often contain both hard and soft constraints, where the hard constraints are domain associated and static while the soft constraints are more flexible and dynamic. The hard constraint handling abilities of these optimal decision models and solutions are significantly limited by the growing problem size and complexity incurred in practical applications. Critical research problems that are

imperative in regard to the complexities of discrete COPs in operations engineering optimization problem solving are observed as following:

2.2.2.1 Representation of Constraint Relationships

As a first step of hard constraint handling, constraint representation can fundamentally influence the computation difficulty and efficiency, especially when the problem scale and complexity are considerably large. Branch-and-bound, which is one of the most successful algorithms for solving discrete COPs, involves a bounding function for calculating lower bound of cost in a set of candidate solutions, and a branching rule to divide the subset into smaller subsets for later exploration if the no-feasible solution situation occurs. Branch-and-bound method explores subsets of potential solutions and rules out the feasible solutions with costs that are higher than the lowest bound found thus far, to avoid exploring every solution in the search space (Przybylski and Gandibleux, 2017). The set of candidate solutions is represented in the form of rooted tree, and correspondingly constraints are represented as the full routes to the root that satisfy the given conditions. However, with this tree representation of hard constraints, the number of subsets produced by the branching steps can grow exponentially, thus branch-and-bound method is usually only preferred for small scale problems that require global optimal solution. For large scale discrete optimization problems, heuristic-based optimization approaches are commonly used as they are easy to implement and can be customized for problems that do not require an exact solution. As a popular category of heuristic-based methods, evolutionary computation methods, such as particle swarm optimization (PSO) (Breaban et al., 2007; Bidar and Mouhoub, 2019) and genetic algorithm (GA) (Sanabria et al., 2003; Karim and Mouhoub, 2014), have demonstrated a valid way to find near-optimal

solutions of related COP. Constraints, in these methods, are represented using some specific solution encoding manners. Furthermore, some hard constraint handling strategies also include the multi-membered evolution strategy (Mezura-Montes and Coello, 2005), which allows some infeasible solution to remain in the population; the predator-prey model (Paredis, 1994) to explore the boundary of feasible region, which keeps two populations, one for constraint violations and the other for potential solutions; and specially designed genetic operators (Sharma and Sharma, 2012) to differentiate the boundaries of each constraint. Unavoidably, the aforementioned constraint representations and their corresponding constraint handling methods require additional computation efforts as hard constraints are conditions that must be satisfied. Therefore, representing constraint relationships is mathematically more redundant than representing unconstrained variables themselves.

2.2.2.2 Exploration-Exploitation Balance

One fundamental criterion that can determine the performance of population-based stochastic optimization (Erten et al., 2020), such as evolutionary algorithms, is how to strike a balance between exploration and exploitation. Exploration refers to the discovery of various regions in the search space in order to locate potential better solutions, while exploitation focuses the refinement of existing promising regions, and is associated with conducting through local search (Črepinšek et al., 2013). Thus, exploration and exploitation place essentially conflicting demands on computational resources, trade-offs between exploration and exploitation are unavoidable. Using the diversity of the population to relatively quantify the exploration-exploitation is an intuitive method, since a large diversity would directly imply a large area of the search space being explored, while a

smaller one indicates the exploitation of small promising area in the search space (Olorunda and Engelbrecht, 2008). With various researchers' interest and hard work, improvement of exploitation-exploitation for practical evolutionary optimization methods remains to be a critical research issue.

2.2.2.3 Solution Feasibility Assurance

The optimization effectiveness and efficiency of heuristic-based algorithms often highly relies on local search operators, which sometimes also known as neighbor operator (Kirkpatrick et al., 1983; Glover, 1986) or mutation operator (Beyer, 2001), while a straightforward implementation of local search operator without specific hard constraints handling often results in infeasible solution, which is not acceptable in many real-world scenarios. Furthermore, there exist some problem-specific special encoding and genetic operators for always generating feasible solutions (Zou et al., 2018), and repair strategies that are designed based on additional encoding information to fix an infeasible solution into a nearest feasible one or the one with the smallest hard constraint violation (Pal et al., 2013). However, repair strategies are restricted to a local view, and could eliminate the growth of population diversity, which may deteriorate the optimization performance significantly if the infeasible solutions dominate the search space. Therefore, more generic and robust constraint handling approaches that assure the satisfaction of hard constraints are still in demand.

2.3 Quantum Computation and Quantum Inspired Computation

2.3.1 Quantum Computation

The idea of quantum computation was pioneered by Feynman (Feynman, 1982; Feynman, 1986) and Deutsch (Deutsch, 1985; Deutsch, 1989), who stated that although using a classical computer to simulate the behavior of n-particle systems evolving in accordance with the law of quantum seems perfectly possible but extremely inefficient (takes an amount of time/space that is exponential in *n*). This is because simulating the actual particles with non-quantum classical bits would require the most sophisticated models. If the particles that follow their natural quantum-mechanical behavior can be directly regarded as a "quantum computer", then this "quantum computer" appears to simulate the computation of a quantum system exponentially more efficiently than performing it with a classical computer. Therefore, by carefully engineering the multi-particle systems, their natural quantum behaviors can enable other computations exponentially more efficient. This is the basic idea behind quantum computers; however, the practical execution of quantum computer is still in its very early infancy. So far, the two most spectacular examples of carefully designed quantum system following laws of quantum mechanics are Shor's factoring algorithm (Shor, 1999) and Grover's database search algorithm (Grover, 1996), which show that quantum computer is in some sense more powerful than classical computer at least with respect to solving some specific problems (Narayanan, 1999).

2.3.2 Quantum Inspired Evolutionary Algorithms

Quantum inspired computing has emerged as a novel computational paradigm and is characterized by applying computational method inspired by quantum mechanics principles and concepts while using classical algorithms to evaluate candidate solutions. Quantum inspired computing has shown great potential on the complexity class NP (the

class of exponential search problems), and it does not require to be implemented on an actual quantum computer.

Inheriting most of the above features from EA, Quantum Inspired Evolutionary Algorithms (QIEAs) introduced quantum concepts and principles in the computation, such as qubit, superposition, parallelism and quantum gates, yet only require a classical computer rather than quantum mechanical hardware. QIEA was firstly introduced by Moore and Narayanan (Moore and Narayanan, 1995) in the 90s to solve Travelling Salesman Problem (TSP). Then, Han and Kim (Han and Kim, 2002) came up with practical representation of individuals applied it in 0-1 knapsack problem and the capacity constraint was handled by an additional "Repair" procedure.

Other variants of QIEA also include Genetic Quantum Algorithms (GQAs (Han and Kim, 2000)), Parallel Quantum inspired Genetic Algorithms (PQGAs (Han et al., 2001)), Quantum inspired Multi-objective Evolutionary Algorithms (QMEAs (Kim et al., 2006)), and hybrid QIEA-PSAs (Patvardhan et al., 2015).

Due to the nature of quantum representation, most of the QIEAs create quantum individuals that behave like the classical individuals and uses a probabilistic update operator to obtain better individuals (Xiong et al., 2018), which inevitably limits the application of those algorithms to integer optimization (Samanta, 2017; Wu and Wu, 2017). Commonly seen, the performance experiments were performed on Knapsack problems, which is one well-known binary combinatorial optimization problem. The performances of QIEAs in Knapsack problem solving illustrate that they are efficient alternatives of the traditional genetic algorithm (Arrazola et al., 2019), as they are capable of global search

and obtaining optimal solutions with smaller populations, but usually converge slower than traditional genetic algorithm. More recently, the research effort in QIEA also leads to the possibility of real codification (Talbi and Draa, 2017; Saire and Apaza, 2019) by updating the quantum individuals based on the use of uniform probability density function, which shows the potential of QIEAs in solving numerical optimization problems, however, these techniques are still very limited in solving problems like multimodal optimization (Saire and Singh, 2019). Since the decision making of engineering system optimization are more of a process of selecting the best alternative, the focus of this study lies within the first category of techniques.

Interestingly, many QIEAs, including many variations and applications using so-called QIGA (Konar et al., 2018), only apply the quantum inspired "Update" procedures, which is similar to the concept of "Mutation" operator in CGA, as the only operator to update the population. Another powerful genetic operator "Crossover" in CGA has not been used or explored for its potential in QIEAs.

2.3.3 Quantum Inspired Neural Networks

With the development of the emerging novel computation paradigms associated with quantum computation, quantum neural networks (QNNs) appear with the aim of exploring their promising potentials to surpass the limitations of classical computations (Jeswal and Chakraverty, 2019).

Comparing to classical computation, the quantum version alternative utilizes the concept and principles of quantum mechanics, such as quantum superposition, quantum parallelism and quantum entanglement (Rønnow et al., 2014), which bring the advantages

of exponentially higher information expression and thus enable comprehensive performance enhancements theoretically. However, practically it is very difficult to obtain sufficient computational gain in the current quantum computing environment (Preskill, 2018), and often find it hard to surpass or even reach the performance of classical ANN. Thus, the exploration of potentially promising and more practically feasible alternatives of QNNs has also attracted plenty of research attentions. For instance, hybrid quantum-classical neural networks (HQCNNs), which are hybrid models that combine partial QNN with classical neural network models in order to save on the requirement of computational resources. Some recent developments in this direction include hybrid quantum-classical neural network with deep residual learning (Res-HQCNN) (Liang et al., 2021), the applications of hybrid quantum-classical neural networks on cloud-supported in-vehicle cyberattack detection (Islam et al., 2022) and data classification (Hur et al., 2022).

Further, for those industries that both quantum and classical computation resources are in short supply, another research direction points to quantum inspired neural networks (QINNs), which introduces the mathematical concepts of parameterized quantum circuits into classical backpropagation neural networks and allows the entire algorithm to be applied on classical computers. The recent efforts and achievements in this field include quantum inspired neural network with sequence input (QINNSI) (Li and Xiao, 2014) for breast cancer prediction, and quantum inspired neural network with quantum weights and real weights (Shang, 2015) for the applications on pattern recognition and function approximation. The research work presented in this chapter lies into this category.

Despite the tremendous amount of work current researchers have done and the various of application scenarios, the development of QNN, HQCNN and QINN are still in infant

stage. The potential and possible application scenarios of quantum or quantum inspired neural networks still worth exploration, as well as the suitable knowledge representation during the learning process to tailor the neural network model to be more domain context aware.

CHAPTER 3. PROBLEM FORMULATION

In this chapter, consistent with the research roadmap, the fundamental issues are identified and formulated systematically, with the aim of addressing the respective research problems regarding the computational efficiency, domain problem context representation, and data-driven decision making in operations engineering problem solving.

3.1 Combinatorial Optimization Problems in Operations Engineering

One of the very common methods to model operations engineering optimization problem into combinatorial optimization mathematical form is to use 0-1 variables to represent binary choice. Consider an event i that may or may not occur and suppose that it is part of the problem to decide between the two possibilities, define a binary variable x :

$$x = \begin{cases} 1, & if\ event\ occurs \\ 0, & if\ event\ does\ not\ occur \end{cases} \quad (1)$$

Noticeably, the event itself can be almost anything and the complete problem often consists of multiple events, where the decision on each event is represented by a corresponding binary variable. Thus, the decomposition of the complete problem and appropriate design of the events are highly associated with the specific situation being considered. In the next section, several examples are presented.

3.1.1 The 0-1 Knapsack Problem

As one of the easiest and oldest combinatorial optimization problems that have been studied for more than a century, the 0-1 knapsack problem widely appears in real-world

decision-making processes. Suppose there are *n* projects, each project *i* has a value a_i and and a cost of c_i, also there is a total budget of *b* available for funding the projects. The 0-1 knapsack problem is about choosing a subset of the projects to maximize the sum of the values while not exceeding the budget constraint. The "0-1" indicates that each project can either be chosen or not chosen (it is not allowed to choose a fraction of any project), where the project *i* can be easily interpreted as the event *i*.

$$x_i = \begin{cases} 1, & if\ project\ i\ is\ chosen \\ 0, & if\ project\ i\ is\ not\ chosen \end{cases} \tag{2}$$

The complete problem formulation of 0-1 knapsack problem is:

$$max\ \{\sum_{i=1}^{n} a_i x_i\}$$

- $subject\ to: \sum_{i=1}^{n} c_i x_i \leq b$

3.1.2 The Assignment and Matching Problem

Another classical combinatorial optimization problem concerns the assignment of people to jobs. Suppose there are *n* people and *m* jobs, and $n \geq m$. The cost of person *j* doing job *i* is c_{ij}. This problem is to assign the people to the jobs in order to minimize the total cost of completing all the jobs, while a person can be at most assigned to one job. The binary variable here is then defined as:

$$x_{ij} = \begin{cases} 1, & if\ person\ j\ is\ assigned\ to\ job\ i \\ 0, & if\ person\ j\ is\ not\ assigned\ to\ job\ i \end{cases} \tag{3}$$

The complete problem formulation of this problem is:

$$max\{\sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}x_{ij}\}$$

- $subject\ to: \sum_{j=1}^{n} x_{ij} = 1\ for\ i = 1,..,m$
- $\sum_{i=1}^{m} x_{ij} \leq 1\ for\ j = 1,..,n$

3.1.3 The Set-Covering Problem

Combining the decisions from both the previous problems, a more complex combinatorial optimization problem is set covering problem. Many practical operations engineering problems, such as planning facility locations and assigning workers to shifts, can be formulated as set-covering problems. For instance, suppose there is a set of *n* potential facility locations, denoted as *N*, a set of *m* communities to be covered, denoted as *M*. The cost of building a facility at location i is c_i, and the subset of communities can be covered by the facility at location *i* is M_i. This problem is to pick a subset of *N* so as to minimize the total cost of building facilities with all the communities covered. The binary variable here is similar to the 0-1 knapsack problem:

$$x_i = \begin{cases} 1, & if\ location\ i\ is\ chosen \\ 0, & if\ location\ i\ is\ not\ chosen \end{cases} \quad (4)$$

An additional incidence matrix $A = \{a_{ij}, i = 1, \dots, n; j = 1, \dots, m\}$ is also required here to serve similar purpose as the binary variables in the assignment and matching problem:

$$a_{ij} = \begin{cases} 1, & if\ community\ j \in M_i \\ 0, & if\ community\ j \notin M_i \end{cases} \quad (5)$$

The complete problem formulation of this problem is:

$$min\ \{\sum_{i=1}^{n} c_i x_i\}$$

- $subject\ to: \sum_{i=1}^{n} a_{ij} \geq 1\ for\ j = 1, \ldots, m$

3.2 Discrete Constrained Optimization Problems in Operations Engineering

Numerous operations engineering application problems can be modelled as nonlinear, nonconvex, discrete constrained optimization problems (COPs), whose objective function is usually simple, yet the constraint functions can be tedious and nonlinear. The hard constraints in operation engineering domain often consist of Boolean relation and conditional constraints among variables, and the possible values of variables are discrete. Based on these characteristics, the iterative optimization process can be formed with a solvable constrain satisfaction problem (CSP) defined by the hard constraints and an optimization algorithm to optimize the global objective function. That means, even obtaining feasible solutions in a discrete constrained optimization can be NP-complete or NP-hard.

A typical category of operations engineering optimization problems is operations planning and scheduling. Planning and scheduling are similar mathematical problems with different temporal dimensions. Planning, in general, aims to translate long term goals into short term tasks and objectives, while scheduling focuses more on the near future or even

real-time assignment. Workforce planning, which is a subset of operation engineering problem that involves human as resource, has attracted a surging amount of research attentions, due to the recent public health emergency of international concerns and its associated impact (Maneenop and Kotcharin, 2020), especially to the public transportation systems, such as airlines. In the next section, a case study of airport shift planning is used as an illustrate case about how an operations engineering optimization problem can be formulated into a discrete COP.

3.2.1 Airport Shift Planning (ASP)

The research of shift planning mainly focuses on assigning employees to shifts, determining working length, and many other variations. A typical problem consists of generating a set of work shifts S with the aim of minimizing the deviation of covering pre-specified workforce demands over a planning horizon of h days $H = \{1, \dots, h\}$. Then each day of the planning horizon is further split into T equal-size time slots to adapt to the change of workforce demand, where the workforce demand at the kth time slot is $D_k^d \in D^d$. Each shift $s \in S$ is characterized by the value of the starting time t_s, the number of assigned staffs p_s and the length of the shift λ_s, however, not all starting times are feasible, nor are unlimited number of staff and working lengths allowed, yet some preferences within the allowed region are encouraged. Also, the values of starting time and work length must be practically achievable.

The multiple optimization targets include the minimization of the shift operation cost $f_c(S)$, the understaff cost caused by the uncovered workforce demand $f_u(S, D)$, and the overstaff cost $f_o(S, D)$ caused by unoccupied shift workforce corresponding to the

generated shift set S. The global optimization function is a function that combining the above targets with corresponding importance coefficient values, as well as the penalty function $f_p(S)$ indicating the preferences as soft constraints. Thus, the work shifts optimization problem can be generally described as:

- $Given$: D, definition of individual shift feasibility, preferences.
- $Goal$: $min\, F(f_c(S), f_u(S,D), f_o(S,D), f_p(S); w_c, w_u, w_o, w_p)$
- $subject\ to$: $\forall s \in S, s$ is feasible; total workforce planned in S does not exceed the available amount of workforce.
- $Output$: S

3.2.2 Hard Constraints Modelling

Besides the explicit hard constraints introduced by the definition of shift feasibility, the above problems in real-life also involve implicit hard constraints, such as "a work shift with zero worker implies that this shift does not exist, thus the length of shift is zero", "the number of workers assigned to a shift should never be more than the highest workforce demand", or "each worker should at maximum fulfill one shift in one day".

A feasible shift $(t_s^d, p_s^d, \lambda_s^d)$ on day *d* requires:

- $min_{st}(d) \le t_s^d \le max_{st}(d), t_s^d = min_{st}(d) + g_{st} \cdot b_d, b_d \in \{0,1,\dots,\frac{max_{st}(d)-min_{st}(d)}{g_{st}}\}$;
- If the personnel resource is unlimited, $p_s^d \le \max\limits_{k=1,\dots,T}\{D_p^k\}, p_s^d \in \mathbb{N}$; Else, $\sum p_s^d \le max_p(d)$.
- $\lambda_s^d = \begin{cases} 0, & if\ p_s^d = 0 \\ min_l(d) + g_l \cdot l_d, l_d \in \left\{0,1,\dots,\frac{max_l(d)-min_l(d)}{g_l}\right\}, & otherwise \end{cases}$.

where $min_{st}(d), max_{st}(d)$ are the earliest and latest shift starting time on day d, $min_l(d), max_l(d)$ are the shortest and longest shift length on day d, $\max_{k=1,\dots,T}\{D_p^k\}$ is the highest workforce demand, $max_p(d)$ is the number of available workers on day *d*.

Noticeably, according to this definition, an empty shift at an allowed starting time is also regarded as feasible, since it satisfied all hard constraints and means no shift would be add at that time. The working length of an unemptied shift on day d has $(l_d + 1)$ options.

Each feasible shift can be recognized as a solution to a CSP formed accordingly, which consists of a triple (x, D, R) where:

- x is the set of three variables, $x = \{x_1, x_2, x_3\} = \{t, p, \lambda\}$,
- D is the set of domains, $D = \{D_1, D_2, D_3\}$, $\forall i, 1 \le i \le n, x_i \in D_i = \{v_1^i, \dots, v_{k_i}^i\}$,

$x_1 = t \in D_1 = \{min_{st}(1), min_{st}(1) + g_{st}, \dots max_{st}(1), min_{st}(2), \dots, max_{st}(h)\}$,

$x_2 = p \in D_2 = \{0,1, \dots, \min\{\max_{k=1,\dots,T}\{D_p^k\}, max_p(d)\}\}$,

$x_3 = \lambda \in D_3 = \{0, min_l(1), min_{st}(1) + g_l, \dots max_l(1), min_l(2), \dots, max_l(h)\}$.

- R is the set of constraint relations between two variables, $R = \{R_{ij} | 1 \le i \le 3, 1 \le j \le 3, i \ne j\}$. $R = \{R_{23}\}, R_{23}: (x_2 = 0 \Rightarrow x_3 = 0)\ and\ (x_3 = 0 \Rightarrow x_2 = 0)$. This conditional constraint can also be described using Boolean expression: $(x_2 \wedge x_3) \vee (\neg x_2 \wedge \neg x_3)$.

Complete hard constraints in this formulation include the constraint of value domain and the conditional constraint relations. The regions defined by the domain

constraints is Cartesian product $D_1 \times D_2 \times D_3$. The Boolean expression of the conditional constraint here can also be recognized as a 2-satisficability problem, which has one obvious solution $\forall x_1 \in D_1, x_2 \equiv x_3 \equiv 0$, this solution is feasible but far away from reaching optima for the original optimization problem. Other feasible solutions to this CSP are $D_1 \times ((D_2 - \{0\}) \times (D_3 - \{0\}))$, which is a subset of $D_1 \times D_2 \times D_3$.

3.2.3 Data Structures Implementation

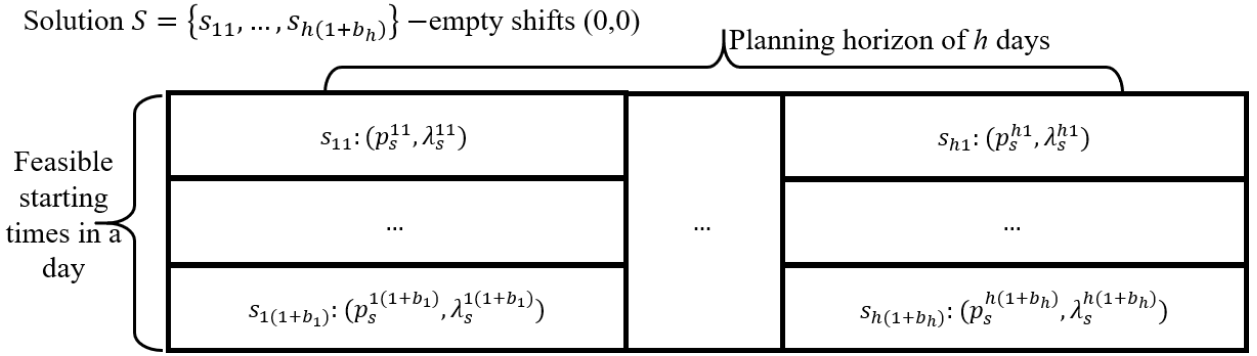
As the carrier of solutions to practical problems, the data structure of a complete solution is always necessary to be implemented whatever constraint handling strategies apply. After solving the CSP of individual shift, a complete solution to the original airport shift planning problem should be a set of multiple feasible shifts. Additionally, if personnel resource limitation also applies to the solution, corresponding data structures for the solution are designed as a complementary constraint handling method.

3.2.3.1 Unlimited Personnel Resource

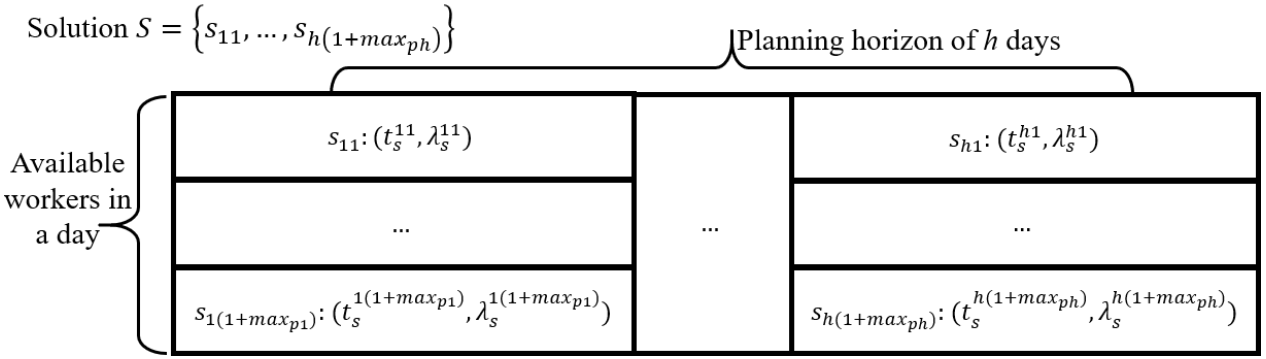
Assuming the personnel resource is unlimited, another hard constraint on the shift set could be that at maximum, only a single shift can be added at any time, i.e., $\forall s_1, s_2 \in S, s_1 \neq s_2, \Rightarrow t_{s1} \neq t_{s1}$. With this additional hard constraint, the maximum number of feasible shifts can be generated on day d is $(b_d + 1)$, and the total number of possible feasible shifts over the entire planning horizon is $\sum_{d \in H}(b_d + 1)$.To handle this hard constraint, the constraint of starting time can be treated as another dimension of the fixed data structure, while the choice of each feasible shift at a feasible starting time is only about the number of workers and the shift length, as shown in Figure 2(a).

3.2.3.2 Limited Personnel Resource

In some cases that require very professional skill, such as nurses shift planning, the number of workers becomes another commonly seen hard constraint in the problem. With this constraint, the maximum number of shifts can be generated on day d is $\min\{max_p(d), (b_d + 1)\}$, assuming one worker only in each shift. Similarly, this additional hard constraint is handled as another dimension of the fixed data structure for solutions, while the choice of each available worker is only about the starting time and the shift length, as shown in Figure 2(b). Practically, if multiple workers are assigned in the same shift configuration, these shifts can be combined as a multi-worker shift.



(a) Unlimited Personnel Resource, Maximal One Shift at a Time



(b) Limited Personnel Resource, One Worker Maximal One Shift a Day

Figure 2. Data Structure for Solution to Original Problem

3.3 Domain Context-aware Intelligent Learning for Data-driven Decision-making in Operations Engineering

Practical operational problems require the consideration and balancing of complex and dynamic operational conditions and situations. This gives rise to computational problems that are unique in scale, complexity, and richness, leading to combinatorial decision making in highly dynamic and uncertain environments. Operational decision making requires not only the optimization capability based on a rigid formulation of the problem domain, but also the self-adaptability to proactively respond to the dynamic nature of the operational environment. The uncertainties make the process of decision making extremely challenging for decision makers since the decision space expands exponentially, which makes it extremely difficult to arrive at a practically optimal solution within an acceptable time. With the pervasive connectivity and extensive smart sensing technologies deployed in nowadays operations systems, massive operational data and user generated contents can be collected uninterruptedly. Recently data-driven decision making has attracted much attention as an emerging paradigm to make better-informed decisions possible. By exploiting huge, versatile, and highly contextualized operational data, operation engineers can harness their organization's competitive edge by uncovering patterns, novel insights, and domain knowledge through data-driven decision making.

Over the past few decades, artificial neural networks (ANNs) have become one of the most prosperous computational paradigms (Nielsen, 2015) with the consistently high research passion for exploring new architectures and increasingly wide applications in various fields. Many research efforts have been contributed to make adjustments of ANNs based on the researchers' good understanding of the application domain context, which is

one of the key factors to successful engineering decision making problem solving. With the consistent progress in the development of novel neural architectures and efforts of embedding expert knowledge into the models (Pham et al., 2018; Peng et al., 2020), artificial neural network-based machine learning techniques have shown great success in many research and industry applications. As a powerful and popular machine learning technique that is often used for modelling complex tasks, the concept of an artificial neural network is about utilizing a parallel distributed information processor made of identical or highly similar units (neurons), which are capable of storing and query information, in order to learn the underlying relationship between the explanatory and response variables. Over the years, the advances in quantum computing have witnessed exceptional development in potentials of faster computing comparing to classical computing. Traditional artificial neural network with the enhancement enabled by quantum computing gives a new field known as quantum neural network, which is now explored by various of researchers from different research perspectives. Research evidence (Li et al., 2013; Sim and Johnson, 2019) has also shown that even a hybrid neural network model with some classical and quantum or quantum inspired components is of large practical meaning and can achieve better performance than classical neural networks at least on some testing samples. Similar to the fact that artificial neuron is the smallest information processing unit in artificial neural network, quantum inspired neuron is fundamental to quantum inspired neural network and it also needs to highly simulate the biological neuronal mechanism to process information with the aim of improving the approximation and generalization capabilities of the entire neural network model.

As a type of graphic notation methods for representing knowledge in patterns of concept nodes related by directional relationship links, semantic network representation has been believed by many to be one of the most appropriate methods for satisfying the knowledge representation requirements in computational intelligent environment (Peters and Shrobe, 2003; Sowa, 2014). The network structures and connectivity between nodes make it naturally plausible to hybrid with artificial neural network and further the quantum or quantum inspired version of artificial neural network, where the domain information represented by the former can empirically enhance the performance of the latter. While focusing on the domain knowledge representation aspect, the expected models and methods resulted from this task have profound implications for research on intelligent machine learning of optimization mathematical modeling and solution knowledge for operations engineering applications.

CHAPTER 4. THEORETICAL FOUNDATION AND TECHNICAL RATIONALITY OF QUANTUM INSPIRED COMPUTATION

Quantum computation has been foreseen as the future computation paradigm to bring a huge leap in computation efficiency (Duan and Raussendorf, 2005). Nonetheless, there is still a long way to go for quantum computation to be practically ready to run on quantum computers due to limitations of hardware resources and physical infrastructures (Fellous-Asiani et al., 2020). But rather, quantum inspired techniques are suggested to be more feasible and promising, that is, new quantum inspired computational methods can be originated from the basic principles of quantum mechanics to enhance classical algorithms (Arrazola et al., 2019). The foundation of the technical approaches in this research is rooted in the quantum inspired computation paradigm, and thus the theoretical foundation and technical rationality of quantum inspired computation are addressed in this chapter.

4.1 Quantum Bit (Qubit) Representation

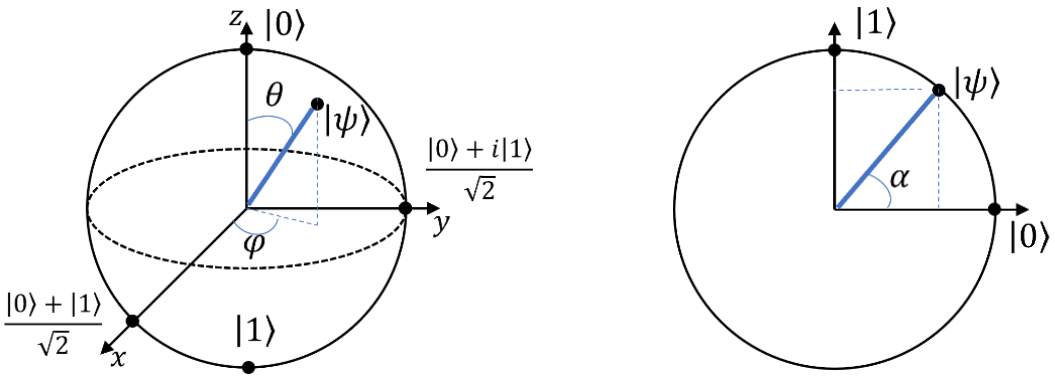
4.1.1 Quantum Bit (Qubit)

Quantum computation manipulates quantum bits (qubits), which are also the smallest information storage units. Based on the theoretical quantum computational modeling, any state of a qubit can be parameterized and described in Hilbert space by a point on a unit sphere (known as Bloch Sphere, shown in Figure 3(a)), written as:

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle,\ 0 \le \theta \le \pi, 0 \le \varphi \le 2\pi \quad (6)$$

For the sake of convenience, another common description of qubit is on a unit circle (shown in Figure 3(b)), especially in the domain of quantum inspired computation, where the imaginary part of a qubit description usually does not play a critical role. This version of qubit description can be written as:

$$|\psi\rangle = \cos\alpha\,|0\rangle + \sin\alpha\,|1\rangle,\ 0 \le \alpha \le 2\pi \quad (7)$$



(a) Description of Qubit on Bloch Sphere (b) Description of Qubit on Unit Circle

Figure 3. Description of a Qubit

In either description, a qubit is represented as a superposition of two basis states, $|0\rangle$ and $|1\rangle$. In this study, the latter description is employed. The vector representation of the single qubit $|\psi\rangle$ is given as $[\cos\alpha \quad \sin\alpha]^T$.

4.1.2 Basic Quantum Gates

In quantum computation, qubits can be manipulated by quantum logic gates, which are the basic building blocks of quantum circuits, in order to perform operations of algorithms. Quantum logic gates are unitary operators, meaning that they are reversible and can be represented by unitary matrices. Under the description of qubit on unit circle, a single qubit rotation gate is defined as:

$$R(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{8}$$

When it applies to a single qubit state $|\psi\rangle$, the result:

$$R(\theta)|\psi\rangle = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\alpha \\ \sin\alpha \end{bmatrix} = \begin{bmatrix} \cos(\theta+\alpha) \\ \sin(\theta+\alpha) \end{bmatrix} \tag{9}$$

Quantum NOT gate (also known as Pauli X), denoted as X, interchanges state $|0\rangle$ and state $|1\rangle$ and can be represented in matrix form $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. When it applies to a single qubit state $|\psi\rangle$, the corresponding output is simply:

$$X|\psi\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cos\alpha \\ \sin\alpha \end{bmatrix} = \begin{bmatrix} \sin\alpha \\ \cos\alpha \end{bmatrix} \tag{10}$$

Quantum Hadamard gate, denoted as H, it creates an equal superposition state if given a computational basis state (i.e. state $|0\rangle$ and state $|1\rangle$) and can be represented in matrix form $H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$. When it applies to a single qubit state $|\psi\rangle$, the corresponding output is:

$$H|\psi\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}\begin{bmatrix}\cos\alpha\\ \sin\alpha\end{bmatrix} = \begin{bmatrix}\frac{1}{\sqrt{2}}\cos\alpha + \frac{1}{\sqrt{2}}\sin\alpha\\ \frac{1}{\sqrt{2}}\cos\alpha - \frac{1}{\sqrt{2}}\sin\alpha\end{bmatrix} \quad (11)$$

4.2 Quantum Inspired Evolutionary Algorithms

The representation and operations of qubit in QIEAs are usually simplified even more:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \alpha\begin{bmatrix}1\\0\end{bmatrix} + \beta\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}\alpha\\ \beta\end{bmatrix} \quad (12)$$

where the amplitude $\alpha, \beta \in \mathbb{C}$, $|\alpha|^2$ gives the probability of the qubit in the state $|0\rangle$, and $|\beta|^2$ the state $|1\rangle$, which naturally leads to $|\alpha|^2 + |\beta|^2 = 1$.

A qubit-based individual is often represented as a string of *n* qubits as below:

$$\left[\begin{array}{c|c|c|c}\alpha_1 & \alpha_2 & \cdots & \alpha_n\\ \beta_1 & \beta_2 & \ldots & \beta_n\end{array}\right] \quad (13)$$

where the amplitude $\alpha_i, \beta_i \in \mathbb{C}, i = 1,2,\ldots,n$, $|\alpha_i|^2$ gives the probability of the qubit *i* in the state $|0\rangle$ and $|\beta_i|^2$ the state $|1\rangle$, $|\alpha_i|^2 + |\beta_i|^2 = 1$.

The advantage of qubit-based individual representation in QIEAs is that the quantum concept of superposition enables *n*-qubit system to contain the information of 2*n* states simultaneously. Thus, under the condition of same population size, the population diversity of qubit-based encoding method is significantly higher than that of the classical methods, and high diversity of a population greatly contributes to better performance (Michalewicz, 2013).

A general form of QIEAs can be described in pseudo code, as shown in Figure 4, where the "Make" procedure corresponds to "Measurement" in quantum physics but with the assumption of no "wave function collapse" which would "destroy" the quantum system, and the "Update" procedure $U(\Delta\theta_i)$ applies the concept of quantum rotation gate $R(\Delta\theta_i)$, which is a unitary matrix. The update of a single qubit aims to adjust the probability of the state in one specific basis state based on the evaluation result, and it follows:

$$U(\Delta\theta_i) = R(\Delta\theta_i) = \begin{bmatrix} \cos(\Delta\theta_i) & -\sin(\Delta\theta_i) \\ \sin(\Delta\theta_i) & \cos(\Delta\theta_i) \end{bmatrix} \tag{14}$$

$$\begin{bmatrix} \alpha_i' \\ \beta_i' \end{bmatrix} = \begin{bmatrix} \cos(\Delta\theta_i) & -\sin(\Delta\theta_i) \\ \sin(\Delta\theta_i) & \cos(\Delta\theta_i) \end{bmatrix} \begin{bmatrix} \alpha_i \\ \beta_i \end{bmatrix} \tag{15}$$

The absolute value of $\Delta\theta_i$ can be 0 or 0.01π (a definable parameter that would have an effect on the convergence speed), and the lookup table helps decide the value and sign of $\Delta\theta_i$ based on the quadrant the qubit located.

Procedure QIEA
BEGIN
$t \leftarrow 0$
i) Initialize $Q(t)$
ii) Make $P(t)$ by observing the states of $Q(t)$
iii) Evaluate $P(t)$
iv) Store the best solutions among $P(t)$ into $B(t)$
WHILE (!termination-condition) DO
BEGIN
$t \leftarrow t + 1$
v) Make P(t) by observing the states of $Q(t\text{-}1)$
vi) Evaluate $P(t)$
vii) Update $Q(t)$ using Q-gates
viii) Store the best solutions among $B(t\text{-}1)$ and $P(t)$ into $B(t)$
ix) Store the best solution b among $B(t)$
x) IF (migration-condition)
THEN migrate b or b_j^t to $B(t)$ globally or locally, respectively
END
END

Procedure Make(x)
BEGIN
$i \leftarrow 0$
WHILE ($i < m$) DO
BEGIN
$i \leftarrow i + 1$
IF *random*[0,1] < $|\beta_i|^2$
THEN $x_i \leftarrow 1$
ELSE $x_i \leftarrow 0$
END
END

Procedure Update (q)
BEGIN
$i \leftarrow 0$
WHILE ($i < m$) DO
BEGIN
$i \leftarrow i + 1$
Determine $\Delta\theta_i$ with the lookup table obtain (α_i', β_i') from the following:
IF (q is located in the first/third quadrant)
THEN $[\alpha_i', \beta_i']^T = U(\Delta\theta_i)[\alpha_i, \beta_i]^T$
ELSE $[\alpha_i', \beta_i']^T = U(-\Delta\theta_i)[\alpha_i, \beta_i]^T$
END
$q \leftarrow q'$
END

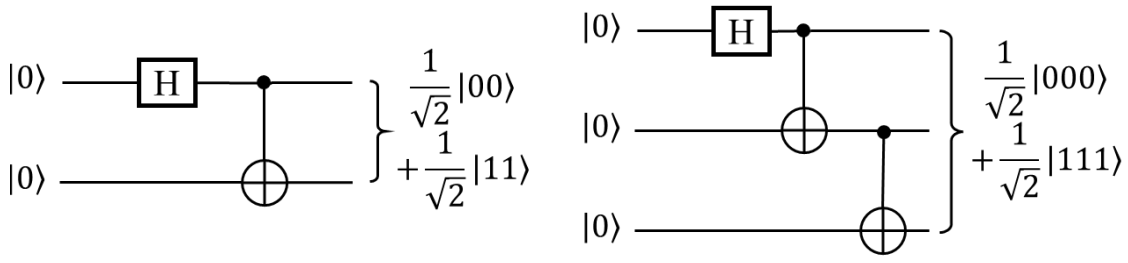
Figure 4. Pseudo Code of General Form of QIEA (Han and Kim, 2002)

4.3 Quantum Entanglement

Quantum entanglement is a unique quantum-mechanical phenomenon in which the quantum state of the entangled system cannot be factored as a product of states of its local constituents, namely, they are not individual particles but an inseparable whole. Entangled particles remain connected so that actions performed on one affect the others instantaneously, even when separated by great distances (Zulehner and Wille, 2020).

Some famous examples include the Einstein-Podolsky-Rosen (EPR) pair (also known as Bell state) $\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$, and the simplest Greenberger-Horne-Zeilinger (GHZ) state $\frac{1}{\sqrt{2}}|000\rangle + \frac{1}{\sqrt{2}}|111\rangle$, where once the measurement of one qubit will assign the

same one of two possible values ($|0\rangle$ or $|1\rangle$) to the other qubits instantly. The entangled state can be created through a well-design series of quantum logic gates, which is also known as quantum circuit, shown in Figure 5.



(a) Generation of the Bell state (b) Generation of the simplest GHZ state

Figure 5. Generation of Entangled States using Quantum Logic Gates

The applications of quantum entanglement feature in quantum and quantum inspired computing have been mainly focused on communication related field (Gao et al., 2005; Ursin et al., 2007). Some recent works also attempt to mimic the dependency characteristics of quantum entanglement in the local searching algorithms, such as tabu search (Kuo and Chou, 2017) and particle swarm optimization (Vaze et al., 2021), to solve high-dependency problems. However, the possibilities of applying quantum entanglement circuit to hard constraint handling for global optimal searching has not been studied.

4.4 Quantum Inspired Neurons

Similar to classical artificial neurons in classical artificial neural networks, quantum inspired neurons, which are parameterized quantum circuits that may not necessarily follow all quantum physical principles strictly, are the elementary information processing

units in quantum inspired neural networks. The quantum inspired neurons receive one or more inputs in the form of qubits and then operate on the inputs to generate output, where various of operation logics can be used. The simplest one is with single input $|\psi\rangle = \cos\alpha\,|0\rangle + \sin\alpha\,|1\rangle$ and operated by a single qubit rotation gate $R(\theta)$ (Figure 6(a)) to get the output:

$$|\psi'\rangle = R(\theta)|\psi\rangle = \cos(\alpha+\theta)\,|0\rangle + \sin(\alpha+\theta)\,|1\rangle \tag{16}$$

Another more complex category of quantum inspired neurons takes multiple qubits as input. In a system of multiple qubits, the state of a single qubit can be affected by the joint control of multiple other qubits. With this concept, in a $(n+1)$ qubits quantum system, when the target qubit is simultaneously controlled by the other n qubits, the behavior of this quantum system can be described by multi-qubits controlled quantum gates $C^n(U)$, which indicates that quantum gate U is applied to the last qubit if the first n qubits are all in state $|1\rangle$, otherwise nothing would be done. A commonly used example is a multi-qubits controlled-NOT gate (Figure 6(b)), denoted by $C^n(X)$.

Suppose $|x_i\rangle = \cos\theta_i\,|0\rangle + \sin\theta_i\,|1\rangle, i = 1,2,\dots,n,$ are the control qubits, and $|\psi\rangle = \cos\alpha\,|0\rangle + \sin\alpha\,|1\rangle$ is the target qubit. The output of the multi-qubit controlled-NOT gate is given by:

$$C^n(X)|x_1x_2\ldots x_n\rangle|\psi\rangle$$

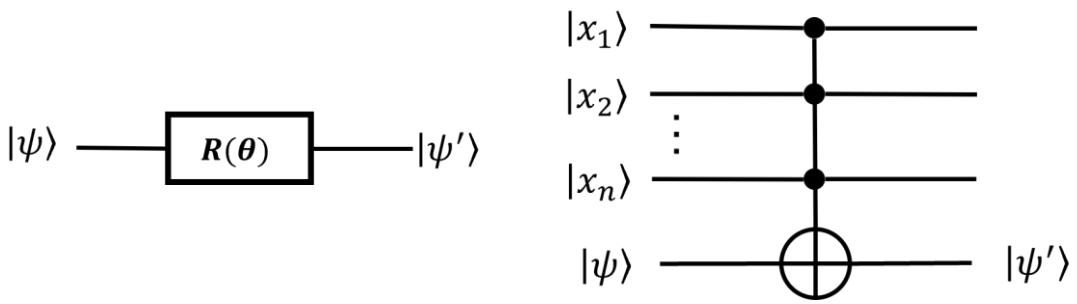
$$\begin{aligned}
&= |x_1\rangle \otimes |x_2\rangle \otimes \ldots \otimes |\psi\rangle - (\prod_{i=1}^{n} \sin\theta_i)\cos\alpha \,|\, \overbrace{11\ldots1}^{n}\, 0\rangle \\
&+ (\prod_{i=1}^{n} \sin\theta_i)\cos\alpha \,|\, \overbrace{11\ldots1}^{n}\, 1\rangle \\
&- (\prod_{i=1}^{n} \sin\theta_i)\sin\alpha \,|\, \overbrace{11\ldots1}^{n}\, 1\rangle \\
&+ (\prod_{i=1}^{n} \sin\theta_i)\sin\alpha \,|\, \overbrace{11\ldots1}^{n}\, 0\rangle
\end{aligned} \tag{17}$$

Namely, after the operation of $C^n(X)$, the probability of the target qubit $|\psi'\rangle$ in state $|1\rangle$:

$$P = (\sin\alpha)^2 - \left[(\prod_{i=1}^{n} \sin\theta_i)\sin\alpha\right]^2 + \left[(\prod_{i=1}^{n} \sin\theta_i)\cos\alpha\right]^2 \tag{18}$$

Thus, qubit $|\psi'\rangle$ can be represented as:

$$|\psi'\rangle = \sqrt{1-P}|0\rangle + \sqrt{P}|1\rangle \tag{19}$$



(a) Single qubit update $R(\theta)$. (b) Multi-qubit controlled-NOT $C^n(X)$.

Figure 6. Two Forms of Quantum Inspired Neuron Operations

After the quantum inspired neuron operations, the state of the target qubit can be determined using the quantum measurement, which is an irreversible operations and ellipses the quantum superposition. The quantum measurement, which logically is similar to a probabilistic thresholding function in the classical artificial neuron, is not always a good alternative for activation function before achieving a classical output since it loses the sensitivity to small changes in the input. In this study, the output of the quantum inspired neuron is defined as the probability amplitude of the target qubit in state $|1\rangle$, which reflects the changes of the inputs on the output value in a finer granularity. Noticeably, the probability amplitude of a qubit cannot be access in real quantum systems, however, since this category of models applied in this study is quantum inspired algorithm running on classic digital computer instead of real quantum algorithms on quantum computer, the quantum physical laws do not have to be strictly followed.

4.5 Theoretical Rationality and Insights of Quantum Inspired Computation in Operations Engineering

Due to the ever-increasing consumer demands and industrial needs for efficient operations, future decision making relies more and more on data that is packed with uncertainties (Feng and Shanthikumar, 2018). The uncertainties will make the process of decision making extremely challenging for decision makers as the decision space increases exponentially, making it extremely difficult to arrive at a feasible solution within a practically acceptable time. Often, the lack of theoretical understanding of underlying input-outcome relationship in the operations leads to errors of predictive modeling accumulated in the final results. Furthermore, conventional optimization techniques are also restricted in their ability to cope with computational complexities due to inefficient exploration processes of the solution space. The salient advantages of quantum inspired modeling offer great opportunities for improving computational efficiency of combinatorial optimization and empowering domain context representation and context-aware learning in data-driven operations decision making:

4.5.1 Exponentially Higher Information Density by Qubit Representation

Quantum mechanics is mathematically formulated in Hilbert space or projective Hilbert space. Unlike traditional computational modeling techniques, quantum computing mechanisms do not use discrete bits to represent potential solutions. Instead, they utilize qubit representation which can be geometrically represented as a Bloch sphere. The pure states of a quantum system correspond to the one-dimensional subspaces of the corresponding Hilbert space (or the "points" of the projective Hilbert space). For a two-

dimensional Hilbert space, the space of all such states is the complex projective line comprising the Bloch sphere (López-Saldívar et al., 2019). The qubit representation exponentially increases the amount of information embedded in each potential solution representation, thus conducive to computational efficiency.

4.5.2 Logically Coherent Representation of Constraints by Quantum Entanglement

In traditional encoding methods, constraints are not built in the solution; rather they are enforced through supplemental operations. These supplemental operations significantly increase the computational cost, especially for large-scale and complex problems such as those encountered in practical operations engineering systems. In this regard, quantum entanglement has a unique advantage in that the quantum states of two or more objects have to be described with reference to each other, even though the individual objects may be spatially separated. This leads to correlations between observable properties of the systems (Popescu et al., 2006). Therefore, unlike traditional encoding methods, quantum entanglement-inspired encoding methods enable complex constraints to be represented coherently in the quantum states while embedding domain problem contexts through optimization.

4.5.3 Efficient Function Approximation through Quantum Inspired Neurons

A large class of conventional neural networks uses binary McCulloch-Pitts neurons (Rabinovich et al., 2006) to reduce the complex process of signal transmission in neural cells to the two state “active/resting”. As models or systems that combine features of quantum information with the properties of artificial neural networks (Panella and Martinelli, 2011), quantum inspired neural networks are based on the idea of quantum

inspired neurons that are constructed as two-level quantum systems. The potential of quantum inspired neural networks lies in the exploitation of the double advantages of superposition-based quantum computation and parallel-processed neural computation at the same time.

4.5.4 Insights of Quantum Inspired Computation in Operations Engineering

The new emerging field of quantum inspired computation has shown some salient features of quantum information processing for quantum speedups, which can be utilized to solve certain operational optimization problems of practical relevance exponentially faster than conventional mathematical programming models. Quantum inspired optimization modeling enhances the approximation and generalization abilities of combinatorial optimization problem formulation by incorporating domain problem context awareness in operations engineering problem solving. Thus, the technical rationalities of this research (Figure 7) can be summarized as follows:

- It brings great opportunities for developing novel algorithms to improve computational efficiency of combinatorial optimization. It does so by leverage the power of exponentially higher information density carried by qubit representation.
- It opens a distinguished chance for capacitating complex constrained combinatorial optimization problem solving, which comes from the logically coherent representation of constraints by quantum entanglement.
- It gives the possibility for empowering domain problem context awareness in intelligent learning with efficient function approximation by quantum inspired neurons.

Furthermore, the exploration and efforts of forming the theoretical foundation and problem formulation framework for quantum inspired optimal combinatorial decision-making can be a meaningful attempt to embrace quantum inspired computation paradigm in complex operations and production system. It can have a potential broader impact and shed light on the development of exploration in the broader decision science field and other similar engineering fields.

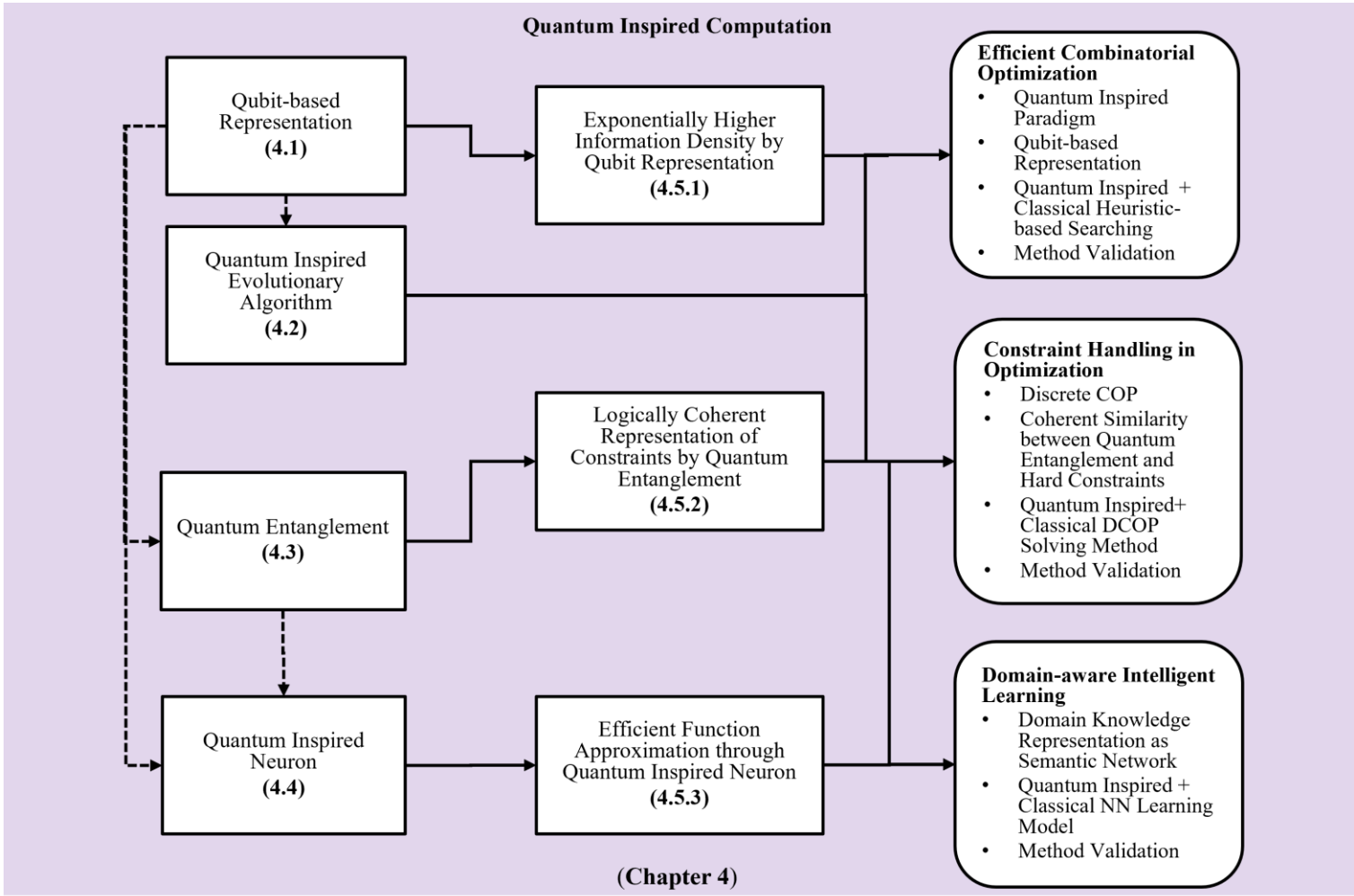


Figure 7. Insights of Quantum Inspired Computation in Operations Engineering

CHAPTER 5. TWOFOLD UPDATE MECHANISM OF QUANTUM INSPIRED GENETIC ALGORITHM FOR EFFICIENT COMBINATORIAL DECISIONS

It is often computationally intensive to solve combinatorial optimization problems due to their large solution space. These problems are also common in the field of engineering design. Traditional techniques are incapable of handling the growing complexity and size of these problems efficiently. This chapter presents a twofold update quantum inspired genetic algorithm, an improved version of quantum inspired evolutionary algorithm, to solve combinatorial optimization problems. First, the mathematical modelling is presented as well as the solution procedure for quantum inspired evolutionary algorithms. Second, the improved quantum inspired genetic algorithm with twofold update mechanism is proposed along with various operators and its application to integer combinatorial optimization. Thirds, the proposed method is applied to solving a real-life engineering system optimization problem, modular design. The obtained results are compared with those obtained using a classical genetic algorithm and a quantum inspired evolutionary algorithm and it is found that the proposed method was more robust and more efficient to solve combinatorial optimization problems than those obtained by the selected other methods.

5.1 Mathematical Modelling

As a typical combinatorial optimization problem, the clustering problem can be defined in the following form: Given a set of N objects Γ that need to be clustered into

several clusters and a fitness function *f*, the problem is to find a splitting strategy in order to maximize the fitness. The splitting strategy includes the number of clusters *M* and the assignment of the objects correspondingly. Theoretically, *M* can be any value between 1 and *N*. The above problem can be represented in the following format:

$$max\ (f(\Omega_1, \Omega_2, \dots, \Omega_M))$$

- $subject\ to\colon \bigcup_{k=1}^{m} \Omega_k = \Gamma$
- $\bigcap_{k=1}^{m} \Omega_k = \emptyset$
- $\forall\ k \in \{1, 2, \dots, M\}, \Omega_k \neq \emptyset$
- $M \in \{1, 2, \dots, N\}, M \in \mathbb{Z}$

5.2 Quantum Inspired Encoding and Measurement

To support the utilization of quantum representation in the optimization, the encoding method, which is the way the chromosome represents the information about solutions, also needs to apply the matching quantum concept and structure. The binary encoding method, in which every chromosome is a string of bits, is the most commonly used for classical genetic algorithms (CGAs), and one intuitive way to modify it into quantum inspired version is to substitute the classical bit with qubit.

For the given problem, the chromosome needs to represent for each object that which cluster it belongs to. The representation of m clusters would require $m = CEIL(log_2 M$ qubits to form one qubit cell, where *CEIL*() is the function to return the smallest integer value that is bigger than or equal to the given number. The k^{th} qubit cell at

t^{th} epoch can be expressed as: $\begin{bmatrix} \alpha_{k1}^{(t)} & \alpha_{k2}^{(t)} & \cdots & \alpha_{kc}^{(t)} \\ \beta_{k1}^{(t)} & \beta_{k2}^{(t)} & \cdots & \beta_{kc}^{(t)} \end{bmatrix}$, where $\left|\alpha_{ki}^{(t)}\right|^2$ indicates the probability of the i^{th} qubit in the k^{th} qubit cell at t^{th} epoch is $|0\rangle$ and the $\left|\beta_{ki}^{(t)}\right|^2$ $|1\rangle$. Each qubit cell indicates the superposition of the states that the object belongs to all the clusters at the same time. The binary string observed after measuring the k^{th} qubit cell indicates the number that the k^{th} object belongs to. A complete quantum inspired chromosome could look like the structure shown in Figure 8.

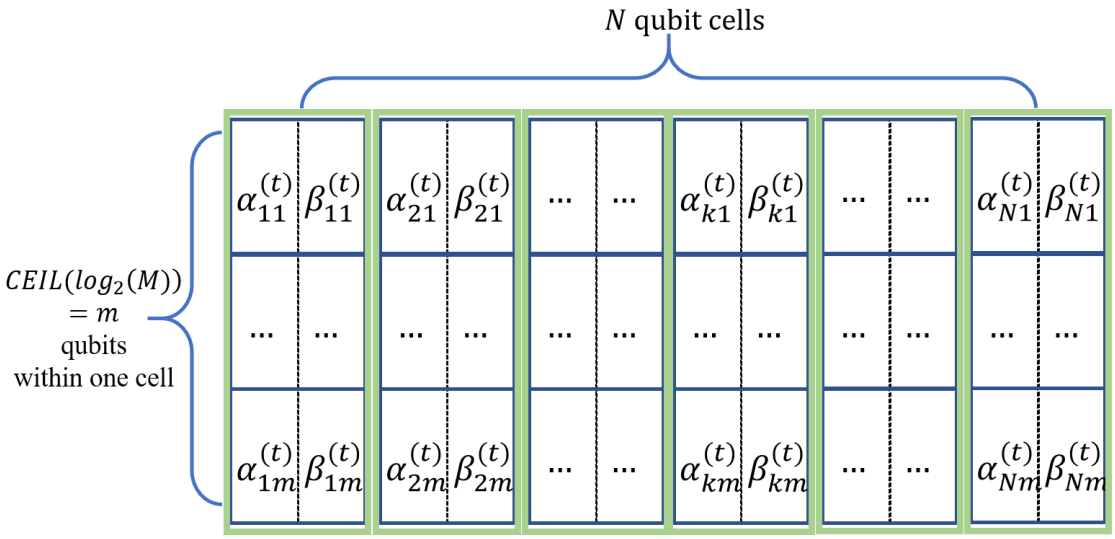


Figure 8. Quantum Inspired Encoding Method

Noticeably, the Qubit-based chromosome cannot directly be evaluated using the fitness function represented in the classical physics. The quantum inspired measurement, or the "Make" function in QIEA, needs to take place before the calculation of fitness. Each qubit $\begin{bmatrix} \alpha_{ki}^{(t)} \\ \beta_{ki}^{(t)} \end{bmatrix}$ in the chromosome will be mapped to either 0 or 1, based on the comparison result of $\left|\beta_{ki}^{(t)}\right|^2$ and a random number between 0 and 1. Namely, if $\left|\beta_{ki}^{(t)}\right|^2 >$

$random[0,1]$, $\begin{bmatrix}\alpha_{ki}^{(t)}\\ \beta_{ki}^{(t)}\end{bmatrix} \rightarrow |1\rangle$, otherwise, $\begin{bmatrix}\alpha_{ki}^{(t)}\\ \beta_{ki}^{(t)}\end{bmatrix} \rightarrow |0\rangle$. The calculation of fitness is then calculated based on the complete binary string obtained from the quantum inspired measurement, while the state of the qubit-based chromosome that is being measured is not altered (shown in Figure 9). This action is probability-based. Multiple quantum inspired measurement actions may map the same qubit-based chromosome into different binary strings, and therefore different solutions. However, the chromosome with higher probabilities in the fitter solutions is still more likely to be evaluated fitter.

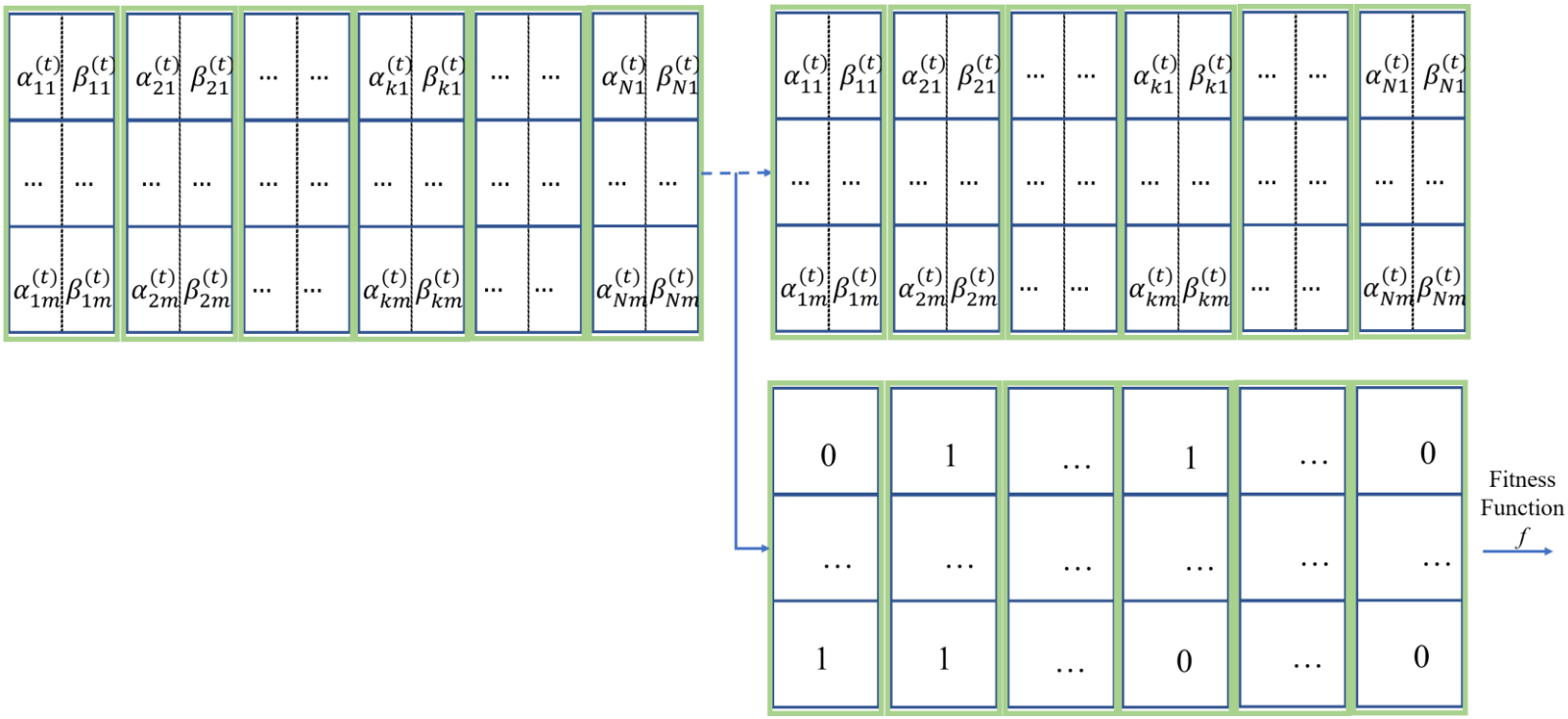


Figure 9. Quantum Inspired Measurement

Additionally, when $m = CEIL(log_2 M) = log_2 M$, the binary string obtained from the measurement would always solidly represent the number of the cluster, therefore automatically satisfies the constraint that each subject has to belong to exactly one cluster. When $m = CEIL(log_2 M) > log_2 M$, the binary string after measurement can possibly point to a non-exist cluster, then the repair operation would fix this scenario by redirecting to the last cluster.

5.3 Twofold Update Quantum Inspired Genetic Algorithm (TU-QIGA)

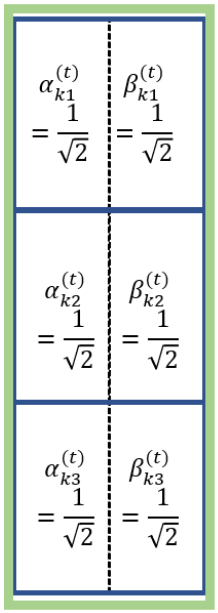
5.3.1 Quantum Inspired Genetic Operators

The evolution process in genetic algorithms starts with the creation of an initial population, then the fitness of individuals is evaluated, which enables the selection operator to identify the fittest candidates. A crossover operator then acts on a couple of parent chromosomes by randomly choosing a locus and exchange their substrings to create offspring, with the aim of mixing useful parts to produce new, better chromosomes (Urso et al., 2018). Crossover alone cannot provide enough diversity to the population if the individuals are too similar to each other, while a mutation operator can alter the current individuals with randomness. To keep these genetic operators in TU-QIGA, they also need to be modified or adjusted in order to fit the quantum inspired concepts and the chromosome encoding method mentioned earlier.

5.3.1.1 Qubit-based Creation Operator

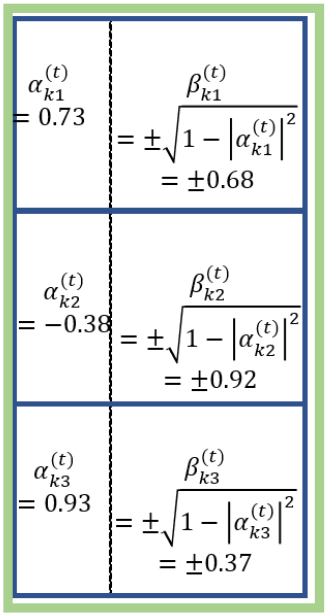
The initial population is filled by the creation operator with the individual chromosomes that encoded by the qubit string with initialized amplitude values of states

$|0\rangle$ and $|1\rangle$. Assuming there are no prior solutions in the creation stage, one direct initialization method is to set all amplitude values to $1/\sqrt{2}$ or $-1/\sqrt{2}$, which indicates the condition that the probabilities of all solutions are equal. For instance, in one qubit cell consists of three qubits, setting all six amplitude values to $1/\sqrt{2}$ is equivalent to that the probability of each possible binary string is $1/8$ (Figure 10(a)). Considering that the population diversity in GAs is usually counted as crucial to continue "fruitful exploration" (Nsakanda et al., 2007), an alternative method is to randomly assign the initial amplitude values in which the probabilities of all solutions are randomly assigned. In the same instance, there are only three degrees of freedom to set the six amplitude values randomly, which introduces randomness in the probability of each possible binary string (Figure 10(b)).



$$Prob(|000\rangle) = \left|\alpha_{k1}^{(t)}\right|^2 \times \left|\alpha_{k2}^{(t)}\right|^2 \times \left|\alpha_{k3}^{(t)}\right|^2 = 1/8$$
$$Prob(|001\rangle) = \left|\alpha_{k1}^{(t)}\right|^2 \times \left|\alpha_{k2}^{(t)}\right|^2 \times \left|\beta_{k3}^{(t)}\right|^2 = 1/8$$
$$Prob(|010\rangle) = \left|\alpha_{k1}^{(t)}\right|^2 \times \left|\beta_{k2}^{(t)}\right|^2 \times \left|\alpha_{k3}^{(t)}\right|^2 = 1/8$$
$$Prob(|011\rangle) = \left|\alpha_{k1}^{(t)}\right|^2 \times \left|\beta_{k2}^{(t)}\right|^2 \times \left|\beta_{k3}^{(t)}\right|^2 = 1/8$$
$$Prob(|100\rangle) = \left|\beta_{k1}^{(t)}\right|^2 \times \left|\alpha_{k2}^{(t)}\right|^2 \times \left|\alpha_{k3}^{(t)}\right|^2 = 1/8$$
$$Prob(|101\rangle) = \left|\beta_{k1}^{(t)}\right|^2 \times \left|\alpha_{k2}^{(t)}\right|^2 \times \left|\beta_{k3}^{(t)}\right|^2 = 1/8$$
$$Prob(|110\rangle) = \left|\beta_{k1}^{(t)}\right|^2 \times \left|\beta_{k2}^{(t)}\right|^2 \times \left|\alpha_{k3}^{(t)}\right|^2 = 1/8$$
$$Prob(|111\rangle) = \left|\beta_{k1}^{(t)}\right|^2 \times \left|\beta_{k2}^{(t)}\right|^2 \times \left|\beta_{k3}^{(t)}\right|^2 = 1/8$$

(a) Equal Probability Initialization



$$Prob(|000\rangle) = \left|\alpha_{k1}^{(t)}\right|^2 \times \left|\alpha_{k2}^{(t)}\right|^2 \times \left|\alpha_{k3}^{(t)}\right|^2 = 0.07$$
$$Prob(|001\rangle) = \left|\alpha_{k1}^{(t)}\right|^2 \times \left|\alpha_{k2}^{(t)}\right|^2 \times \left|\beta_{k3}^{(t)}\right|^2 = 0.01$$
$$Prob(|010\rangle) = \left|\alpha_{k1}^{(t)}\right|^2 \times \left|\beta_{k2}^{(t)}\right|^2 \times \left|\alpha_{k3}^{(t)}\right|^2 = 0.39$$
$$Prob(|011\rangle) = \left|\alpha_{k1}^{(t)}\right|^2 \times \left|\beta_{k2}^{(t)}\right|^2 \times \left|\beta_{k3}^{(t)}\right|^2 = 0.06$$
$$Prob(|100\rangle) = \left|\beta_{k1}^{(t)}\right|^2 \times \left|\alpha_{k2}^{(t)}\right|^2 \times \left|\alpha_{k3}^{(t)}\right|^2 = 0.06$$
$$Prob(|101\rangle) = \left|\beta_{k1}^{(t)}\right|^2 \times \left|\alpha_{k2}^{(t)}\right|^2 \times \left|\beta_{k3}^{(t)}\right|^2 = 0.01$$
$$Prob(|110\rangle) = \left|\beta_{k1}^{(t)}\right|^2 \times \left|\beta_{k2}^{(t)}\right|^2 \times \left|\alpha_{k3}^{(t)}\right|^2 = 0.34$$
$$Prob(|111\rangle) = \left|\beta_{k1}^{(t)}\right|^2 \times \left|\beta_{k2}^{(t)}\right|^2 \times \left|\beta_{k3}^{(t)}\right|^2 = 0.05$$

(b) Random Probability Initialization

Figure 10. Three-qubit Cell Instance using Different Initialization Methods

5.3.1.2 Qubit-based Selection Operator

A selection operator aims to identify the fittest individual and select proper parent individuals to reproduce based on the probability that is positively correlated with the fitness value. The superposition of qubits makes it extremely challenging to evaluate the fitness of qubit-based chromosome directly, but the evaluation of fitness in TU-QIGA can be hinted by the quantum inspired measurement. The ranking method of the individuals can be the same as CGA, and the roulette wheel method is used for the selection purpose, although the ranking of individuals is more of a reference temporarily for that epoch.

5.3.1.3 Qubit-based Crossover Operator

A crossover operator exchanges portion of the selected two parent chromosomes to create two crossover offsprings. This classical method can either be applied to the level of qubit cells or a single qubit (within qubit cell), due to the fact that all qubit cells are equivalent with respect to their representation of the pointed cluster and all qubits are superposed representation of states $|0\rangle$ and $|1\rangle$. Thus, the connective points (Mao, 2010) exist between the qubit-based individuals. Here, the qubit level crossover method is chosen to avoid over-trust in the selection results, due to high stochasticity in the ranking process caused by qubit-based chromosome representation. The crossover process is shown in Figure 11.

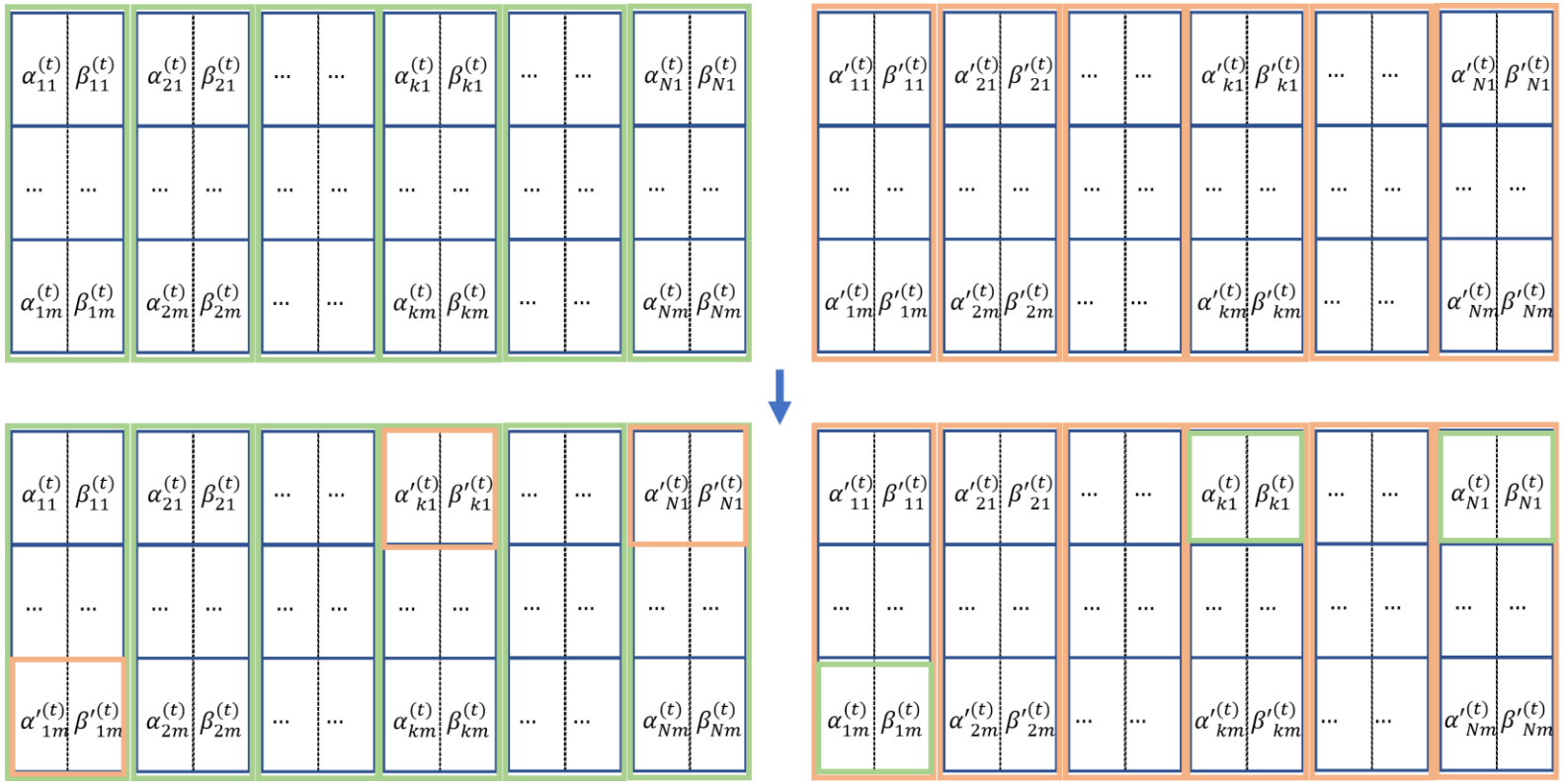


Figure 11. Crossover Operator on the Level of Qubit

5.3.1.4 Qubit-based Mutation Operator

The mutation operator is similar to the "Update" process in QIEA, which applies a quantum gate "Rotation" to a qubit $\begin{bmatrix}\alpha_{ki}^{(t)}\\ \beta_{ki}^{(t)}\end{bmatrix}$ with a chosen angle $\Delta\theta_{ki}^{(t)}$. In QIEA, the value of $\left|\Delta\theta_{ki}^{(t)}\right|$ is chosen based on a lookup table, which either equals to zero or a small non-zero angle and the specific value is chosen case by case. In this study, it is randomly chosen between 0 and a small threshold angle value $\Delta\theta$:

$$\begin{bmatrix}\alpha_{ki}^{(t+1)}\\ \beta_{ki}^{(t+1)}\end{bmatrix} = R\left(\Delta\theta_{ki}^{(t)}\right)\begin{bmatrix}\alpha_{ki}^{(t)}\\ \beta_{ki}^{(t)}\end{bmatrix} = \begin{bmatrix}\cos\left(\Delta\theta_{ki}^{(t)}\right) & -\sin\left(\Delta\theta_{ki}^{(t)}\right)\\ \sin\left(\Delta\theta_{ki}^{(t)}\right) & \cos\left(\Delta\theta_{ki}^{(t)}\right)\end{bmatrix}\begin{bmatrix}\alpha_{ki}^{(t)}\\ \beta_{ki}^{(t)}\end{bmatrix} \tag{20}$$

$$\left|\Delta\theta_{ki}^{(t)}\right| \in Uniform(0, \Delta\theta) \tag{21}$$

$$sign\left(\Delta\theta_{ki}^{(t)}\right) = \begin{cases}+, if\ sign\left(\alpha_{ki}^{(t)}\right) = sign\left(\beta_{ki}^{(t)}\right)\\ -, \qquad\qquad otherwise\end{cases} \tag{22}$$

The mutation operation is always applied to the level of qubits, as shown in Figure 12.

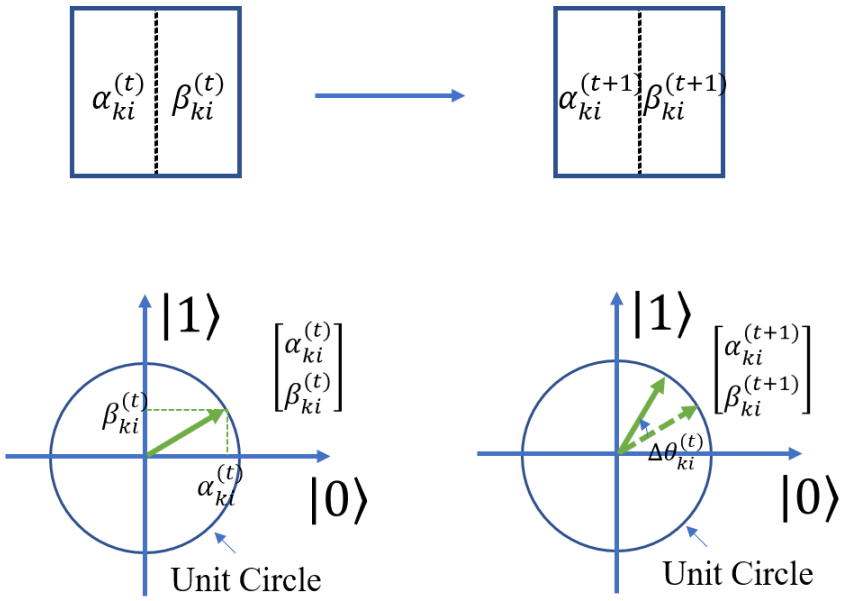


Figure 12. Mutation Operation on a Single Qubit

5.3.2 TU-QIGA Solution

The given combinatorial problem requires the optimization of the best clustering strategy, which includes the number of clusters and the way to assign the objects to. The number of clusters would also change the chromosome size. Therefore, to solve the overall problem, there are two searching loops existing in the proposed method, the outer loop searches for the optimal number of clusters within the given range $[m_s, m_e]$ starting from the given point *m**, while the inner loop looks for the best assignment with the given number of clusters mT provided by its current status in the outer loop. The computation complexity of this solution method is either the multiplication product of the outer loop and inner loop or the joint termination condition, whichever occurs first.

$$
\begin{aligned}
O(TUQIGA) = O\Big(&O(fitness) \\
&\times \big(O(Selection) + O(Crossover) + O(Mutation)\big)\Big) \\
&\times O(m) \\
&\leq O(O(fitness) \times (O(Selection) + O(Crossover) \\
&+ O(Mutation))) \times O(N)
\end{aligned}
\tag{23}
$$

Therefore, TU-QIGA is at the same magnitude of computation complexity as CGA. The solution flow chart is given in Figure 13.

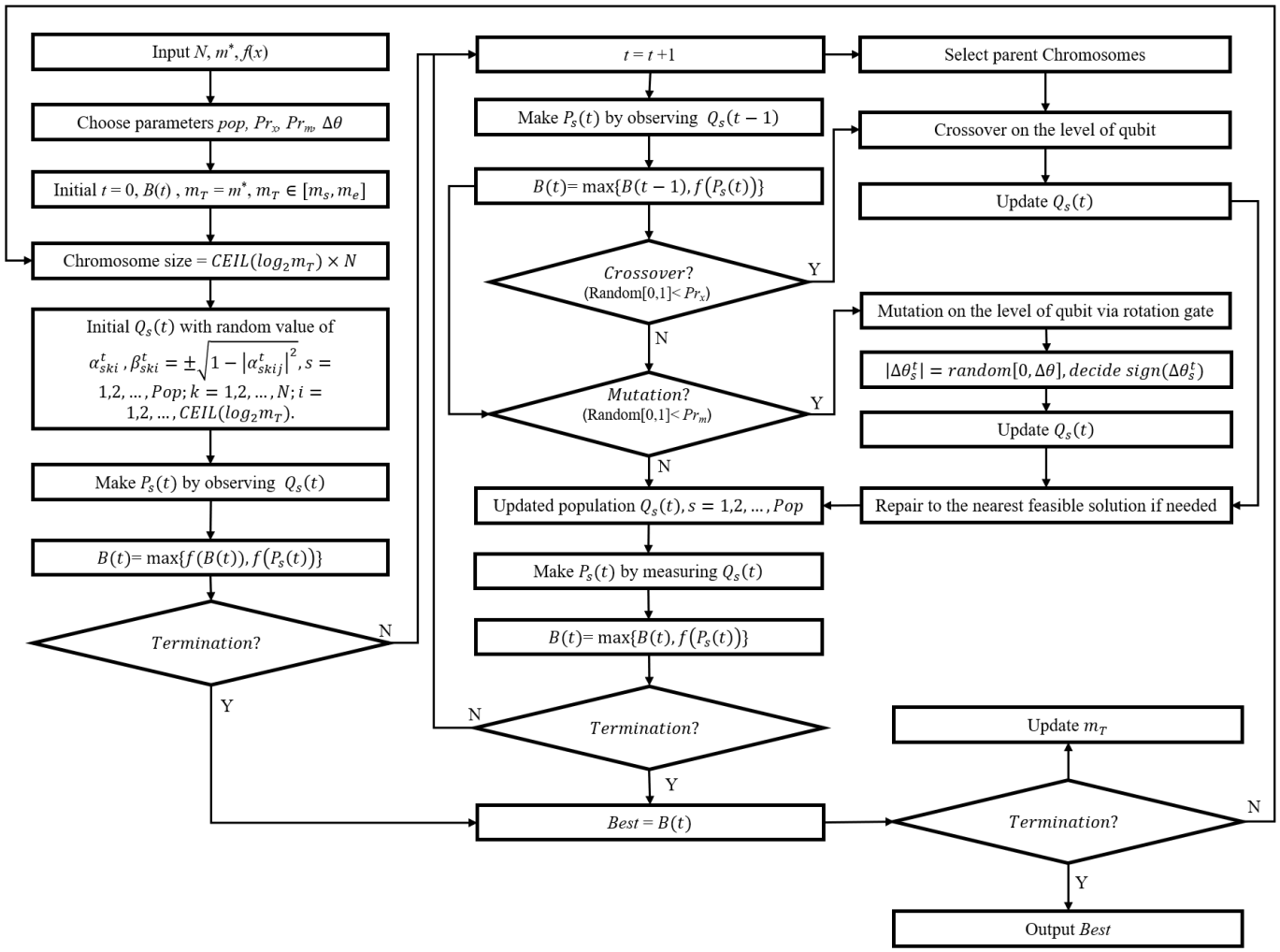


Figure 13. Flow Chart of TU-QIGA Optimization Solution

5.4 Application to Engineering System Optimization

Engineering system optimization is about the technological and managerial decisions at several stages under given domain circumstances with the ultimate goal of minimize the effort required or to maximize the desired benefit (Rao, 2019). As a typical example of engineering system optimization, modular design identifies and group product components into independent modules with the aim of minimizing between-module interactions and maximizing within-module interactions (Ulrich, 1995). Given such an objective, modularization entails rigorous metrics of modularity as measure criteria, interpretable quantification of modularity measures for comparison purpose, and rigorous analysis of granularity tradeoffs. Components used in a modular product must have features that enable them to be grouped together into multiple modules and then form a complex product, following modularity measure criterions. Development of a modular product, which groups components into modules based on modularity matrices, can be classified as an application domain of combinatorial optimization problems. To solve such a domain problem, researchers have utilized, modified, and improved many combinatorial optimization techniques, where GA is one of the most popular ones due to its ease of use and high flexibility (Kamrani and Gonzalez, 2003).

5.4.1 Problem Context

Modular design requires a partitioning of product components into meaningful subgroups, when the number of subgroups and other information about their composition may be unclear, which is a typical clustering analysis problem. To solve this problem, quantum inspired modular design is proposed as a double nesting decision-making model,

where the outer decision layer is a decision model with a single control variable, which is the total number of modules and the inner layers search for the best assignment of the components given a specific granularity.

5.4.2 Problem Solving

Assuming there are *N* total product components to be grouped, denoted as a component set $\Gamma = \{c_i | i = 1,2, \dots, N\}$. The outer decision layer first picks the number of modules m_T first. Given m_T, the *N* components are grouped into m_T modules, the module set can be denoted as $\Omega = \{\Omega_j | j = 1,2, \dots, m_T\}$, where Ω_j is the subset of components in module *j* and it can be expressed in the following form:

$$\Omega_j = \{\delta_{jk} | k = 1,2, \dots, N\} \tag{24}$$

$$\delta_{jk} = \begin{cases} 0, & if\ c_k\ is\ not\ in\ module\ j \\ 1, & if\ c_k\ belongs\ to\ module\ j \end{cases} \tag{25}$$

The objective of modular design is to maximize overall modularity of the product, based on a given modular measure metric, denoted as function *F*. For a module set Ω, its overall modularity is $F(\Omega)$. The constraints in the modular design problem include: 1) each component should belong to one module exactly; 2) the number of modules is usually larger than 1 and smaller than *N*. The above problem can be represented as following combinatorial optimization problem:

$max\big(F(\Omega)\big)$

- $subject\ to: \forall k \in \{1, 2, \dots, N\}, \sum_{j=1}^{m_T} \delta_{jk} = 1$

- $m_T \in [2, N-1], m_T \in \mathbb{Z}$
- $\forall j \in \{1, 2, \dots, m_T\}$,
- $\exists k \in \{1, 2, \dots, N\}, s.t. \delta_{jk} = 0$;
- $\exists l \in \{1, 2, \dots, N\}, s.t. \delta_{jl} = 1$.

The specific modular design case study used here is one with 22 components of a refrigerator (Ji et al., 2013) is used. There are two modularity measure metrics, i.e., Technical System Modularity (TSM) and Material Reuse Modularity (MRM). Here, only TSM is used to simplify the testing case, as TSM is a more widely used modularity metric, which includes both functional similarity and structural similarity. The modular granularity is not considered as the optimization variable of TU-QIGA here, as the evaluation of its fitness can be very computationally expensive. The modularity function *F* is the comprehensive measure given in the original article and used as the fitness function here. Additionally, the searching range of the number of modules can be practically reduced even more according to the empirical knowledge in the field of modular design. The component set $\Gamma = \{c_i | i = 1,2, \dots ,22\}$, and the recommended initial number of modules $m^* = round\left(\sqrt{total\ number\ of\ components}\right) = 5$. The search range of the number of modules used here is set as $[m^* - 2, m^* + 2] = [3,7]$. Since the number of modules is not a variable to be optimized in the main body of the algorithm, the experiment is firstly designed to work with a given number of modules as 5.

Next, the robustness of the algorithm is explored and analyzed. Once the effectiveness of the algorithm working on a given number of modules is verified, the complete

optimization process including the optimization of module numbers and assignment schemes is operated.

5.4.3 Results and Analysis

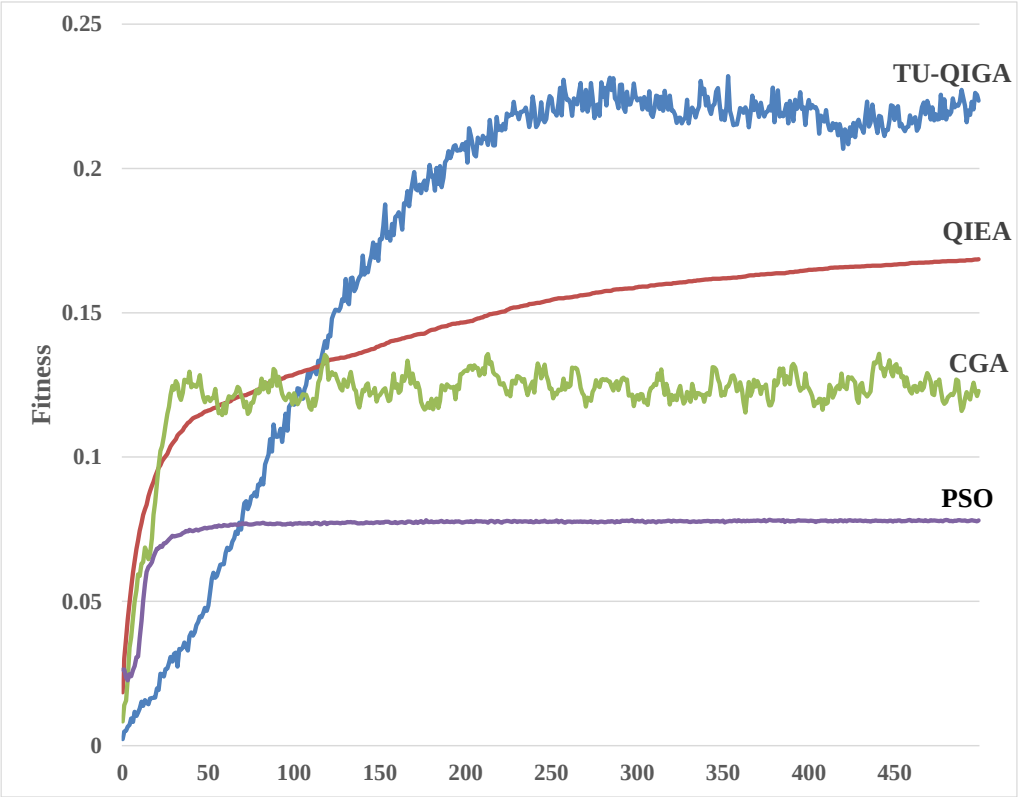
5.4.3.1 Performance Comparison with QIEA, CGA, and PSO

TU-QIGA modular design approach is applied to the given case study, and its performance is compared to that of QIEA, CGA and PSO. Among them, CGA uses binary encoding with similar modeling concepts, TU-QIGA, and QIEA applies the same encoding method. The PSO here is an inertia weight based PSO (Naga Pawan et al., 2020), meaning the main parameters are inertia weight, cognitive and social coefficients (referred as the two learning factors here). The parameter settings for TU-QIGA, QIEA, CGA and PSO are selected based on empirical choices, details are shown in Table 1.

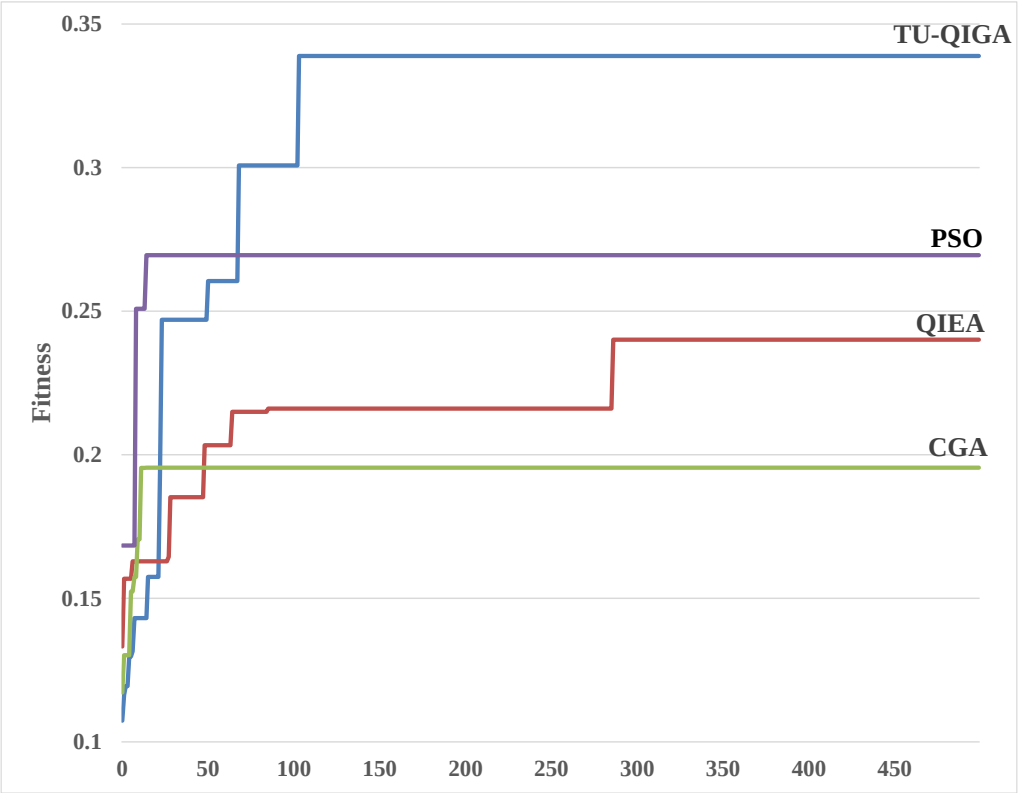
Table 1. Empirical Parameter Settings for TU-QIGA, QIEA, CGA and PSO

Parameter	TU-QIGA	QIEA	CGA	PSO
Population Size	500	500	500	500
Number of Iterations	500	500	500	500
Crossover Probability	0.85	N/A	0.85	N/A
Mutation Probability	0.85	N/A	0.15	N/A
Rotation Angle Threshold	0.01π	0.01π	N/A	N/A
Elite Size	5	N/A	5	N/A
[Inertia weight; Learning factors]	N/A	N/A	N/A	[0.6; (0.2,0.1)]

To track the convergence, all four algorithms are run for 500 iterations, which is considered as more than needed to reach convergence. The average fitness of the entire population and the best fitness are recorded for each iteration, and the corresponding convergence plots are shown in Figure 14.



(a) Convergence Plot of Average Fitness



(b) Convergence Plot of Best Fitness

Figure 14. Comparison on Performance of Convergence without Parameter Tuning

The plots in Figure 14 can be interpreted that, all four algorithms converge before 300 iterations on this problem but to different optimal solutions and fitness values. Noticeably, the two traditional algorithms, CGA and PSO, converge at similar fast pace, while the two quantum inspired algorithms take more iterations to converge. Based on the final fitness value obtained by all four algorithms, the two traditional algorithms may reach some local optimal too fast, possibly due to unsuited parameter settings for CGA and PSO. The same situation happens to QIEA, the parameter setting was reported to be used in 0-1 knapsack problem, which may not be the best parameter setting for this case study. Therefore, to make this performance comparison fair, some trail-and-error based parameter

tuning is done for QIEA, CGA and PSO. The new parameter settings are shown in Table 2. Again, same population size and larger than needed number of iterations are used for comparison purpose. The corresponding performance comparison is shown in Table 3.

Table 2. Parameter Settings for TU-QIGA, QIEA, CGA and PSO after Tuning

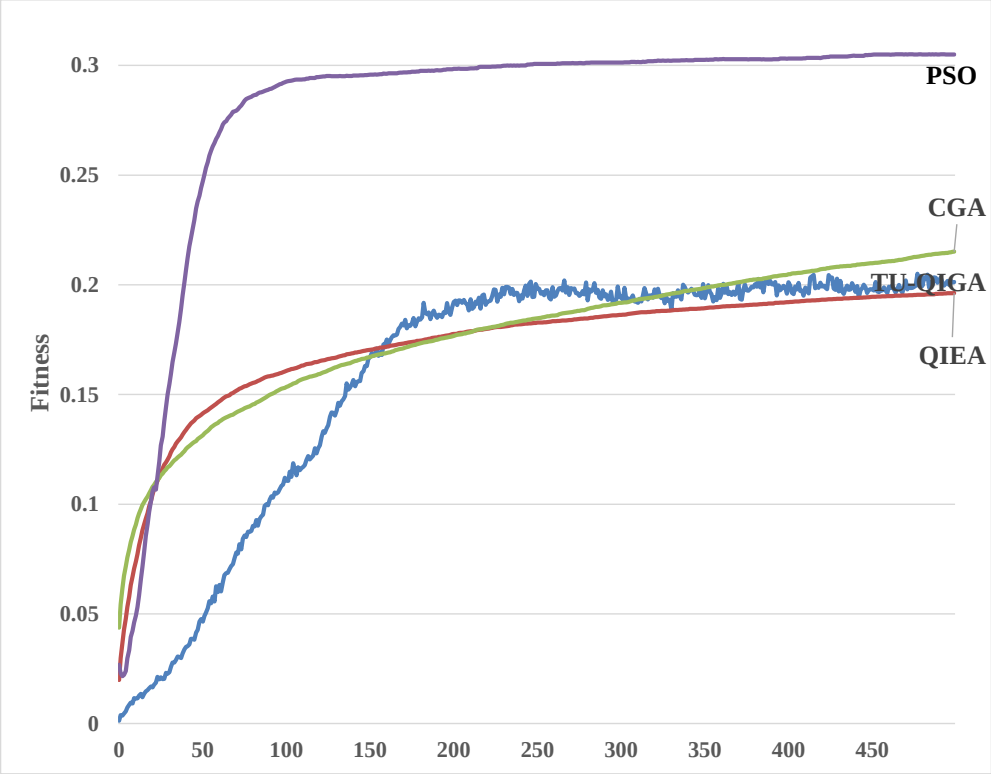
Parameter	TU-QIGA	QIEA	CGA	PSO
Population Size	1000	1000	1000	1000
Number of Iterations	500	500	500	500
Crossover Probability	0.85	N/A	0.85	N/A
Mutation Probability	0.85	N/A	0.10	N/A
Rotation Angle Threshold	0.01π	0.0001π	N/A	N/A
Elite Size	5	N/A	5	N/A
[Inertia weight; Learning factors]	N/A	N/A	N/A	[0.6; (0.3,0.1)]

Table 3. Performance Comparison for TU-QIGA, QIEA, CGA and PSO

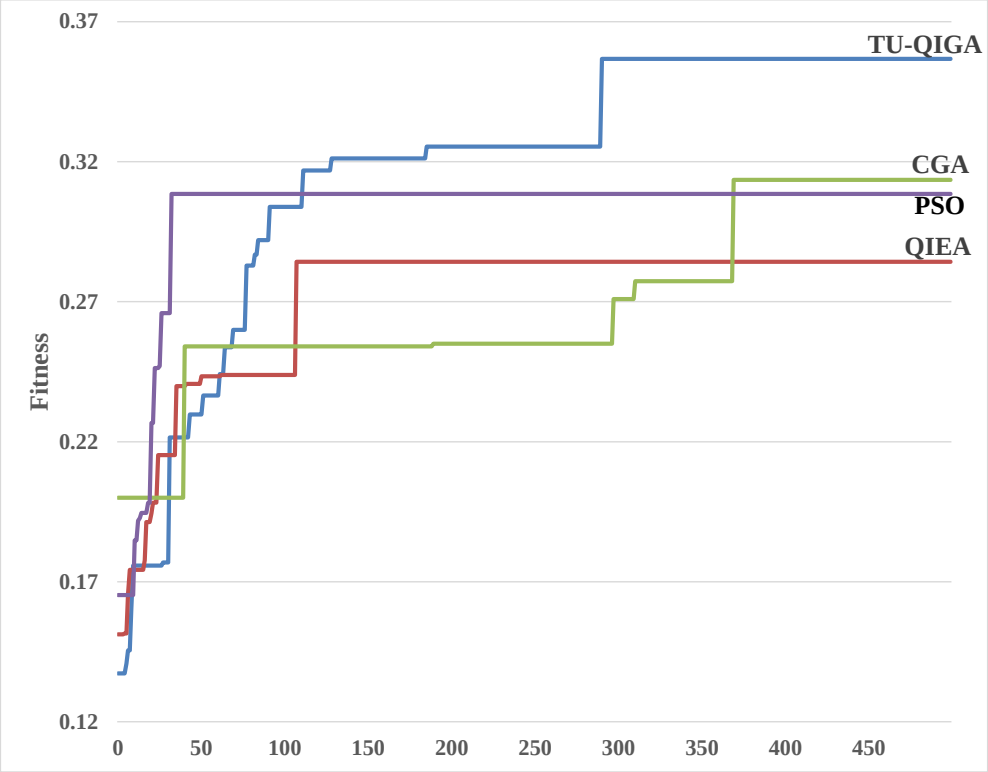
Algorithm	Best Fitness	Required Iterations
TU-QIGA	0.357	290
QIEA	0.284	107
CGA	0.314	369
PSO	0.308	32

The comparison results illustrate that, after the parameter tuning, TU-QIGA still outperforms the other three algorithms in terms of finding the best solution in this testing scenario, while PSO requires the least number of iterations to obtain the best fitness. All three EA-based algorithms, TU-QIGA, QIEA and CGA, end up having similar average fitness, which is much lower than each of the best fitness they obtained, indicating the relative high diversity in the EA population even towards the convergence (necessary for high "exploration"). However, the swarm strategy-based algorithm PSO converge to an average fitness near its best fitness, indicating the high reliance on the "exploitation" part towards convergence. Noticeably, CGA converges to the result very close to the original presented result (obtained by a bi-level GA optimization), which indicates it represents a fair performance of CGA. However, the best modularity obtained by the TU-QIGA is higher than the best result from the original paper. This indicates that TU-QIGA is capable of exploring the solution space more thoroughly.

As for the performance of convergence velocity, it can be seen from Figure 15(a) that PSO converge the fastest, QIEA and CGA almost converge at the same pace, while TU-QIGA has a slowest convergence speed indicating the higher diversity in the population. Figure 15(b) shows that TU-QIGA can search for a better solution continuously within the first 100 iterations, and start outperforming all others around 67^{th} iterations, possibly because the stochasticity introduced by the twofold update mechanism allows larger exploration from the early stage.



(a) Convergence Plot of Average Fitness



(b) Convergence Plot of Best Fitness

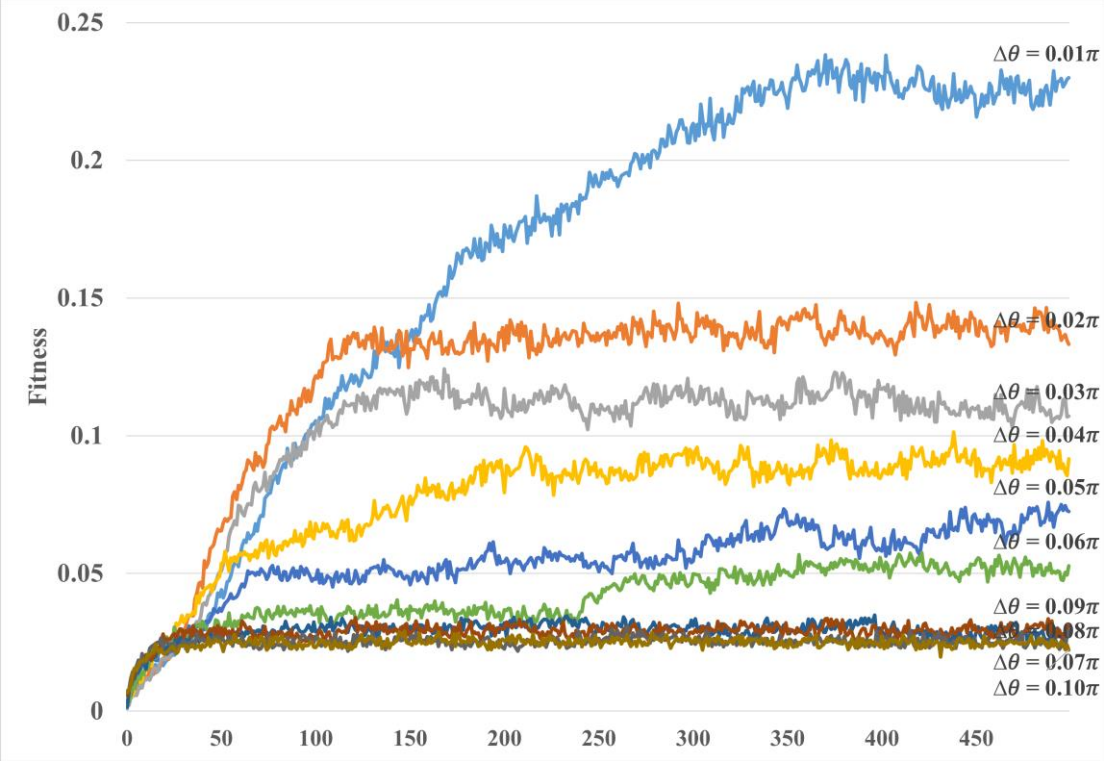
Figure 15. Comparison on Performance of Convergence with Tuned Parameters

5.4.3.2 Robustness Analysis

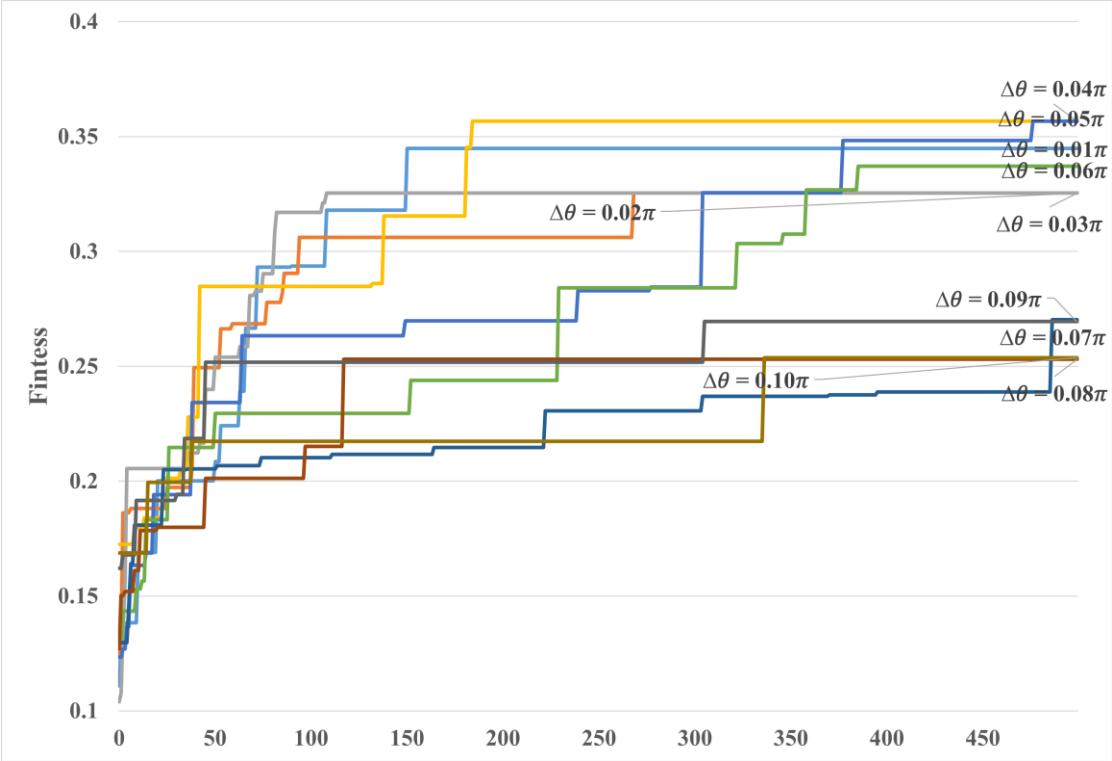
To analyze the robustness of the TU-QIGA, the influence of the rotation angle threshold on the performance of the algorithm was tested. The rotation angle threshold $\Delta\theta$ is chosen as the control parameter here, as the rotation angle has been recognized as a parameter that needs to be determined case by case in order to achieve the best performance in other quantum inspired algorithms. The designed experiments and the corresponding best fitness obtained are shown in Table 4. The convergence plots are shown in Figure 16.

Table 4. Best Fitness Gained by TU-QIGA with Different Values of Control Parameter

$\Delta\theta$	0.01π	0.02π	0.03π	0.04π	0.05π	0.06π	0.07π	0.08π	0.09π	0.1π
Best Fitness	0.345	0.325	0.325	0.357	0.357	0.337	0.345	0.345	0.345	0.345



(a) The convergence Plot of Average Fitness



(b) The convergence Plot of Best Fitness

Figure 16. The Influence of the Control Parameter $\Delta\theta$ on Convergence Performance

According to the results from Table 4, the best result shows up when $\Delta\theta$ equals to 0.04π or 0.05π. Within the range of $[0.01\pi, 0.06\pi]$, $\Delta\theta$ has a relatively small impact on the best result obtained, which might be caused by random errors. However, when $\Delta\theta$ becomes large, the performance becomes deteriorated. Figure 16 illustrates that the algorithm always converges regardless of the value of $\Delta\theta$. While it is larger than 0.06π , it might cause the early convergence problem. Therefore, the TU-QIGA is robust enough and insensitive to the value of $\Delta\theta$ within the range of $[0.01\pi, 0.06\pi]$.

5.4.3.3 Complete Optimization Performance

With the performance of the TU-QIGA on a given number of modules verified, it is then tested for the complete optimization process of modular design, where both the number of modules and the modular assignment schemes are included in the optimization. Smaller values of population size and number of iterations are selected, since a larger population size does not increase the performance of TU-QIGA significantly and using a larger than needed iteration number is no longer a proper stopping criterion. The adjusted parameter settings used for the complete optimization process is shown in Table 5. This testing case is repeated for twenty times, in order to collect enough data for statistical result analysis.

Table 5. Parameter Settings for TU-QIGA in the Complete Optimization

Parameter	Population Size	No. Iterations	Crossover Probability	Mutation Probability	Rotation threshold	Elite Size
Value	500	200	0.85	0.85	0.04π	10

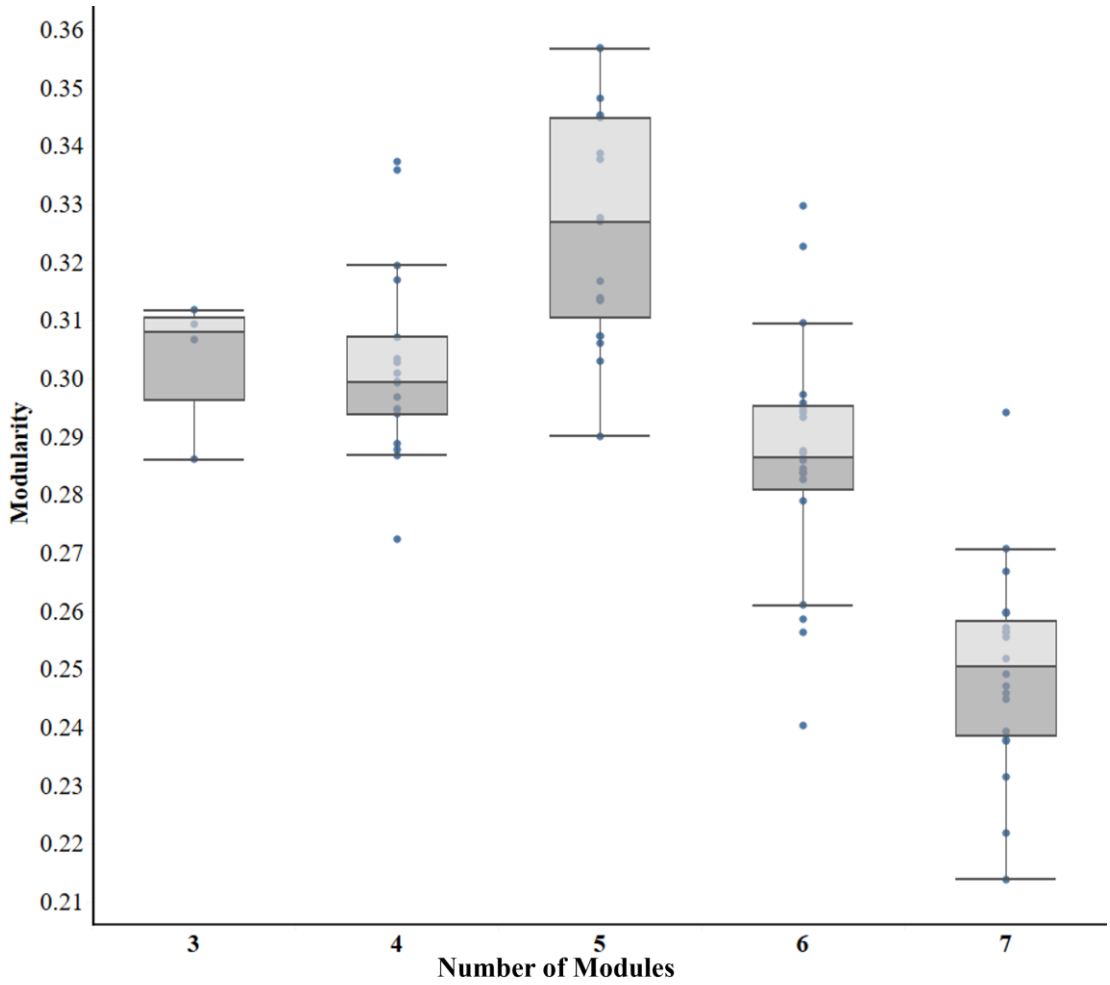


Figure 17. Distribution of Best Results with Given Number of Modules Over Twenty Run

Figure 17 shows the distribution of the best modularity that obtained with each number of modules in the form of box-and-whisker plot. For this particular case study, the plot indicates the near-optimal numbers of modules are 4, 5, and 6, which matches the conclusion from the original research paper (Ji et al., 2013). The results also illustrate that TU-QIGA can perform stably enough over multiple runs, as the standard deviation of results obtained from 20 runs is still relatively small.

5.5 Chapter Summary

Quantum inspired techniques utilize the concepts and principles of quantum physics to explore more solution space within limited amount of computation resources and time, which point to a new and promising direction for combinatorial optimization problem solving. The proposed twofold update quantum inspired genetic algorithm (TU-QIGA) leverages the stochasticity introduced by the twofold update mechanism, which includes the updates of qubit-encoded individuals by applying quantum mechanical phenomena-based quantum operators and hybridized population based genetic operators, with the aim of achieving better exploration-exploitation tradeoff embedded in the combinatorial optimization problem. To obtain feasible solution efficiently, each qubit-based chromosome is encoded to satisfy with the clustering constraints with the repair operator if necessary. The twofold update process is enabled by applying the quantum rotation gate with a randomly chosen small rotation angle as one update operator and hybridized crossover operator as a second update operator to mix and reuse promising segments.

Results and analysis of a modular design case study show that TU-QIGA can obtain the best fitness value comparing to QIEA, CGA and PSO, with the convergence speed slower than PSO and QIEA but faster than CGA. Noticeably, the mechanism of PSO traverses the search space covering the spaces between like birds flocking, which is not a common requirement considering the characteristics of the combinatorial optimization problems in engineering system design. The application of PSO in such problem can lead to a more exploitation type of search strategy. TU-QIGA, QIEA and CGA are all EA based methods that focus on the operation and selection of randomized candidate solutions, which is the more commonly used type of approach in this application domain despite the slower

convergence speed. Robustness analysis results also demonstrate that TU-QIGA is robust within a certain value range of rotation angle threshold.

CHAPTER 6. QUANTUM ENTANGLMENT INSPIRED HARD CONSTRAINT HANDLING FOR OPERATIONS ENGINEERING OPTIMIZATION

Constraint handling, especially hard constraint handling, is a critical issue for discrete constrained optimization problem solving in operations engineering. The performance of conventional constraint handling techniques, such as penalty functions and repair operators, are susceptible to problem complexity and scale. The recent dawning of quantum computation has been recognized as a very promising direction in the paradigm of optimization. This chapter presents a quantum entanglement inspired hard constraint handling approach, to efficiently solve discrete constrained optimization problems. A quantum entanglement inspired representation method of hard constraints is first proposed, which uses a series of qubits and quantum circuit to coherently represent the hard constraints in the posterior quantum states.

As a standard usage of the proposed quantum entanglement inspired representation method, a quantum entanglement inspired genetic algorithm (QEI-GA) is then proposed by embedding the quantum entanglement inspired representation into classical genetic algorithm optimization strategy. The proposed method is applied to solve a real-world airport workforce shift planning problem to validate the algorithm's effectiveness and robustness. The results of the case study show that the proposed method can consistently reach better solutions for the discrete constrained optimization problem, even with a much smaller population size, compared to the conventional genetic algorithms with penalty function based and multi-objective concept-based strategies.

A lightweight example of the proposed quantum entanglement inspired representation method is also presented. This chapter presents a lightweight quantum inspired genetic algorithm (LQIGA), a variant of quantum inspired evolutionary algorithm (QIEA) with a novel lightweight qubit encoding approach, which can enhance single dimension qubit-encoded chromosome to be sufficiently able to represent complex problem constraint information with the support of quantum circuit. The proposed approach aims to provide effective decision support for small scale personnel scheduling scenarios in a lightweight manner. A mathematical formulation of the personnel scheduling optimization task and corresponding classical qubit encoding method for QIEA is first presented. Next, the lightweight quantum inspired genetic algorithm is proposed along with its design of lightweight qubit encoding approach and its application to balanced nurse scheduling problem. Finally, it is employed to solve a bunch of benchmark balanced nurse scheduling cases for verification and validation purpose. The analysis of the results show that the proposed algorithm is robust in obtaining optimal or near-optimal results in solving the constrained combinatorial optimization problem in personnel scheduling.

6.1 Quantum Entanglement Inspired Mathematical Modelling

Despite many other quantum physical properties, the principles of entanglement coherently match with the underlying nature of hard constraints, that is, the variables connected by hard constraints should be considered as a whole. Together with the concept of quantum superposition, the quantum state of a potential solution to a COP could be considered as a superposition of all feasible solutions, until the optimization process leads the quantum state to collapse into the optimal solution. Qubit-based encoding method has been widely used in many quantum inspired techniques, since its representation of

superposition carries a higher density of information comparing to conventional encoding methods. The searching process with qubit-based encoding is essentially the process of adjusting the probability distribution among all feasible solutions, so that the quantum superposition tends to collapse on the solution with the highest probability without losing population diversity ever. Therefore, with a carefully designed quantum circuit and corresponding qubit-based encoding method, the output is a set of all the possible posterior states following probability distribution that is determined by the circuit parameters. Each posterior state corresponds to a binary string that is encoded to represent one feasible solution. In this regard, this chapter proposes a quantum entanglement inspired hard constraint handling approach in order to leverage the uniqueness of quantum entanglement phenomenon in solving discrete COP. The main challenges of this new paradigm lie in achieving effective qubit-based representation encoding, sufficient flexibility to manipulate quantum superposition probability amplitudes, and the design of quantum entanglement circuit to exclude infeasible solutions.

Aligning with the quantum principles, the probabilities of all feasible solutions sum up to be 1, and the adjustment of the probability distribution of each feasible solution can be done by multiple quantum gates. The optimization process requires sufficient flexibility to manipulate the probability distribution towards the optimal solution, which can be mimic by the parameter tunning of the phase change quantum gates but not Hadamard.

To entangle multiple qubits, it is critical to appropriately use controlled quantum gates, which act on n qubits ($n \geq 2$) and use up to $n-1$ qubits as control points. The controlled operations are only performed when every control qubit is $|1\rangle$, which is a good simulation for conditional constraints. For instance, the controlled NOT gate, often denoted as CNOT

or CX, works on two qubits and performs the NOT operation on the second qubit if and only if first qubit is $|1\rangle$. Correspondingly, its matrix form is $= \begin{bmatrix} I & 0 \\ 0 & X \end{bmatrix}$, where $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. Similarly, controlled-power n-X gate C^nX, which acts on $n+1$ qubits and uses the first n qubits as control points, only performs NOT operation on the last qubit when all first n qubits are in $|1\rangle$. It has the matrix form $C^nX = \begin{bmatrix} I_{2^n} & 0 \\ 0 & X \end{bmatrix}$, where I_{2^n} is an $2^n \times 2^n$ identity matrix. Another group of controlled gates needed in the proposed approach is to add one or more controls to R_x gate, where the simplest single controlled gate $CR_x(\theta) = \begin{bmatrix} I & 0 \\ 0 & R_x(\theta) \end{bmatrix}$.

The core idea of the proposed quantum entanglement inspired hard constraint handling approach in this study is to design and assembly quantum circuit using the above quantum gates, with the aim of assuring the output of the circuit to be a parametric-defined probability distribution among all feasible encoded solutions.

6.2 Quantum Entanglement Inspired Hard Constraints Representation

According to the problem formulated earlier, complete hard constraints in this formulation include the constraint of value domain and the conditional constraint relations, and they cannot be handled identically using quantum entanglement inspired approach. Also, continuous domain constraints cannot be handled by the proposed approach but can be handled in conventional way before the determination of final encoding. A general workflow of this approach is given in Figure 18.

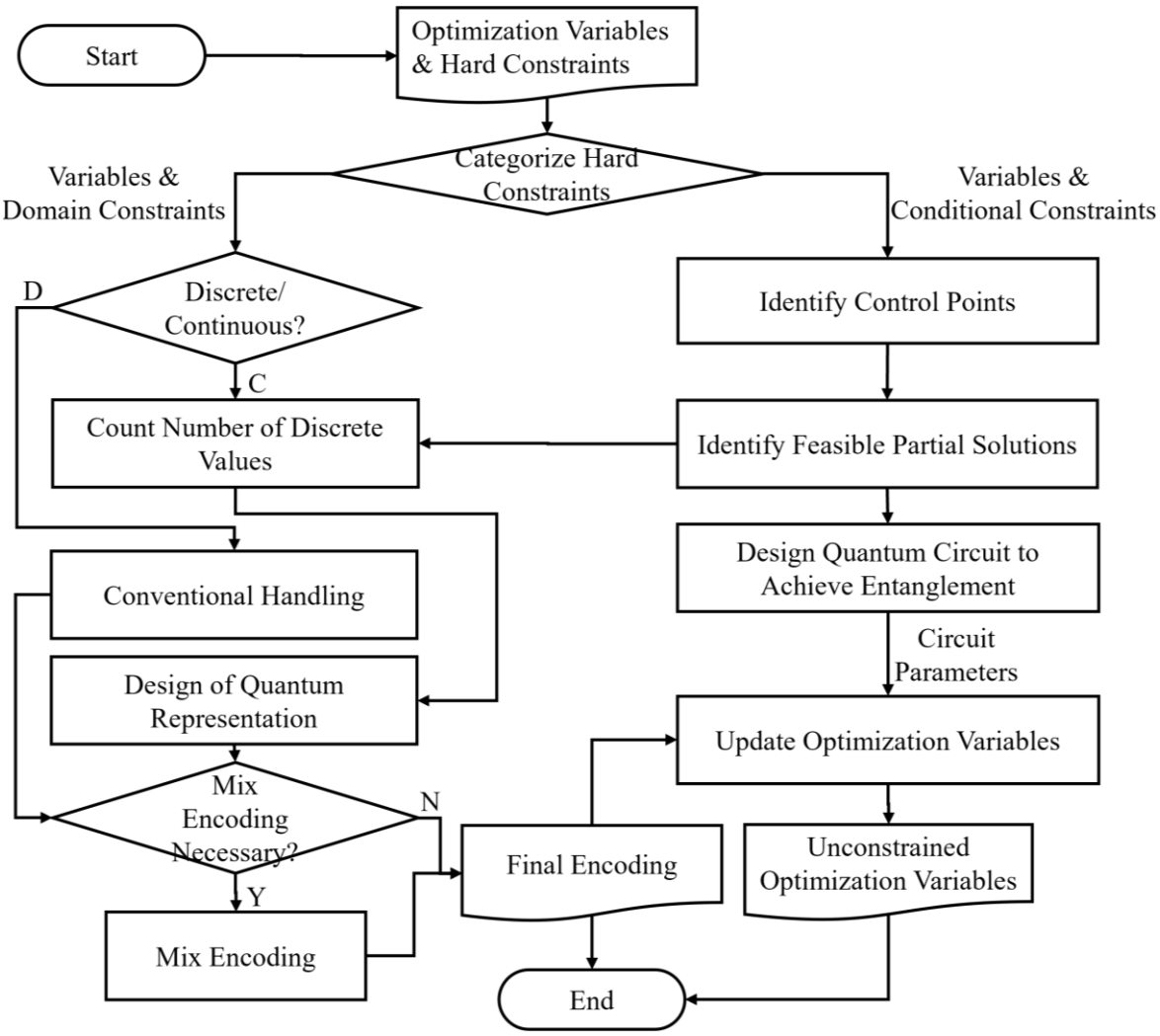
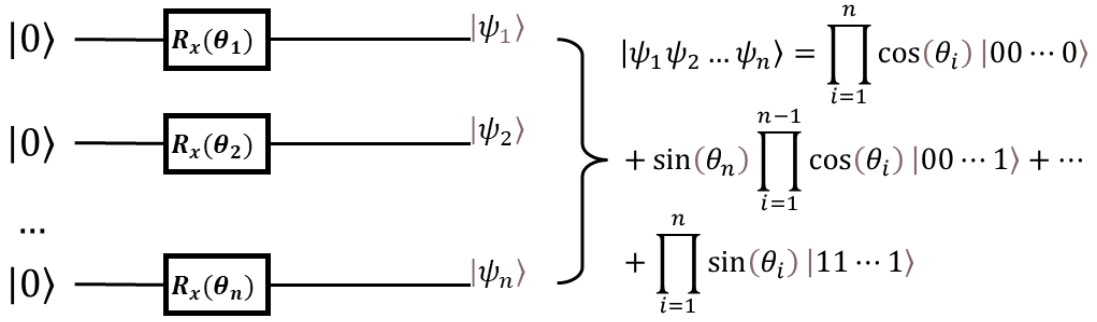


Figure 18. Flow Chart of Quantum Entanglement Inspired Hard Constraint Handling

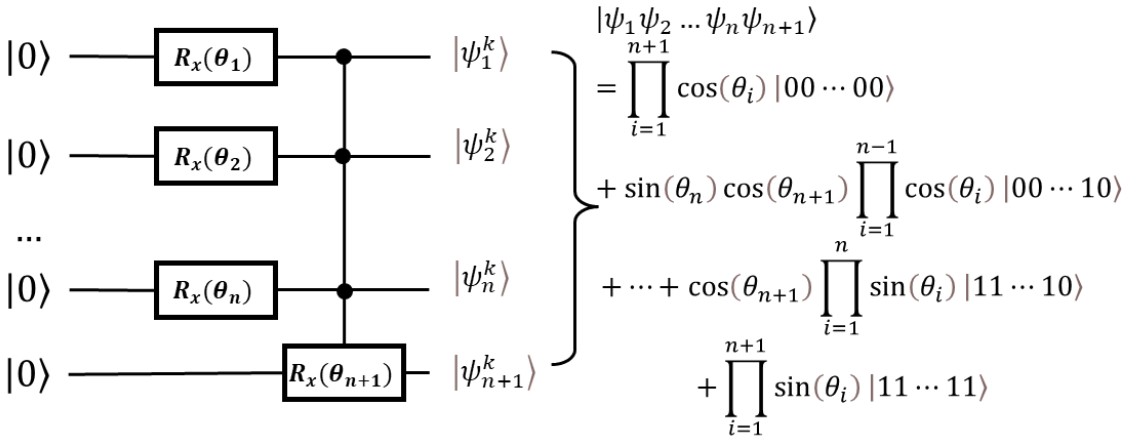
6.2.1 Quantum Representation of Discrete Domain Value Constraints

The constraints of value domain are relatively independent, yet the challenge exists since the number of discrete values in the domain may not be exactly represented by the binary-like manner of qubit representation. To guarantee the purity of feasibility in the encoding method, the output qubit string must be a superposition of all feasible encoded representations exclusively, and the number of possible posterior states has to be equivalent

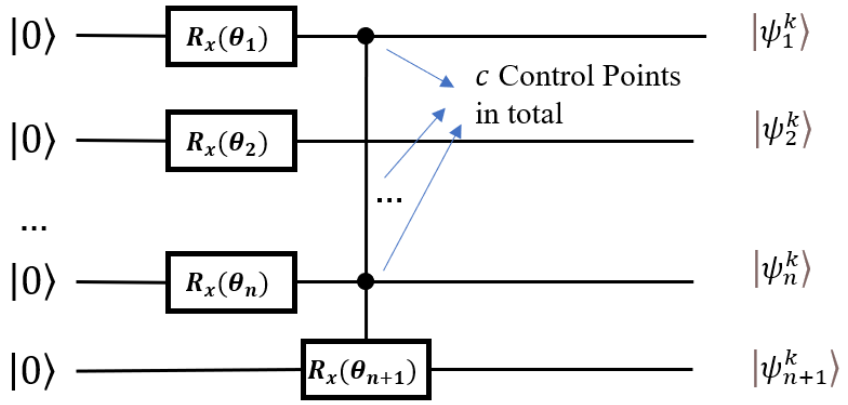
to the number of feasible values to allow one-to-one encoding mapping. One or more quantum control gates $C^m R_x(\theta)$ are used to achieve this form of entanglement, where m is the total number of control points. Several instances with different number of discrete values in the domain are shown in Figure 19.



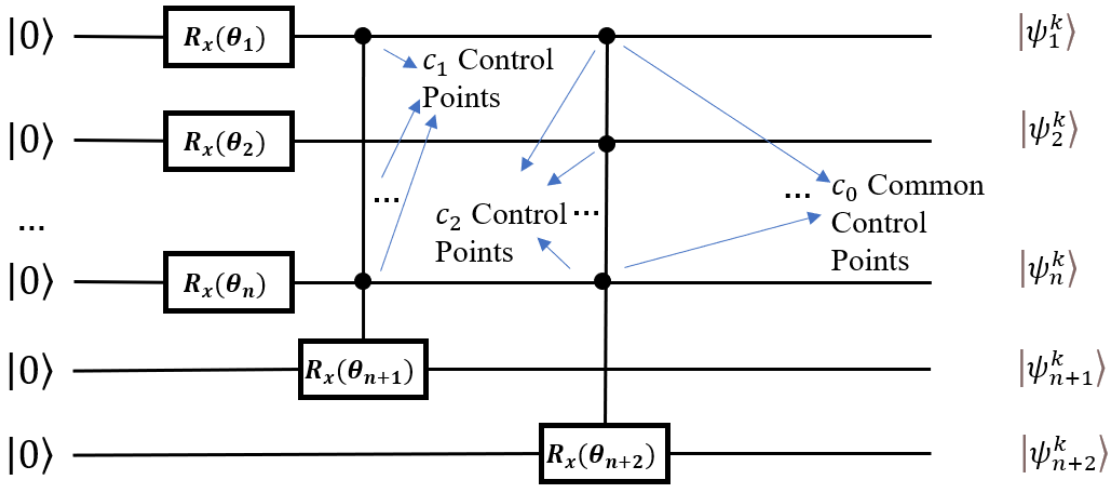
(a) Exact 2^n Discrete Values in the Domain (No Control Gate Needed)



(b) $(2^n + 1)$ Discrete Values in the Domain (One Control Gate Power to n)



(c) $(2^n + 2^{n-c})$ Discrete Values in the Domain (One Control Gate Power to $c, 1 \leq c \leq n$)



(d) $(2^n + 2^{n-c_1} + 2^{n+1-c_2} - 2^{c_o})$ Discrete Values in the Domain (Two Control Gates Powers to $c_1, c_2, 1 \leq c_1 \leq n, 1 \leq c_2 \leq n+1$, c_o is the number of common control points)

Figure 19. Constraints of Value Domain Represented in Quantum Circuits

6.2.2 Quantum Representation of Conditional Constraints

The conditional constraint is defined on two variables, changing the value of one can consequently reflects on that of the other and domain constraints are usually also

embedded. For a conditional constraint, the first step of handling it is the identification of control, and the corresponding changes different condition could cause.

Next, the embedded domain constraints of variables can be represented. For instance, assuming two variables $x_1 \in D_1, x_2 \in D_2$, the conditional constraint: $A = False \Rightarrow x_2 = v_0$; $A = True \Rightarrow x_2 \in D_2 - \{v_0\}, |D_2| = 2^n + 1$, where the control event A is a Boolean expression involving x_1. The corresponding quantum representation is shown in Figure 20, where the $2^n + 1$ discrete values in D_2 can be represented using $n + 1$ qubits and the first qubit also serves as control qubit. Referring to the domain constraint representation mentioned earlier, similar design of circuits can be done if the number of discrete values is different.

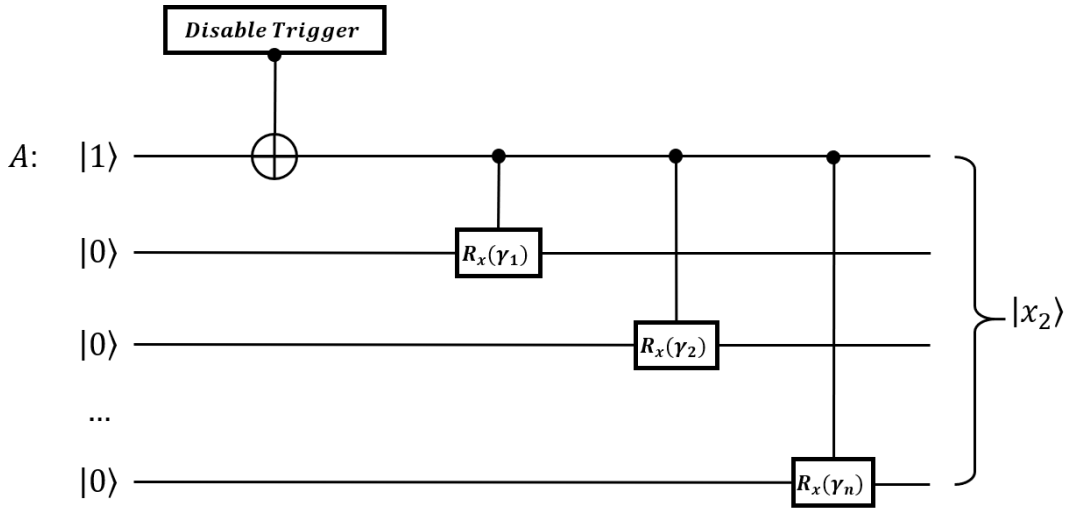
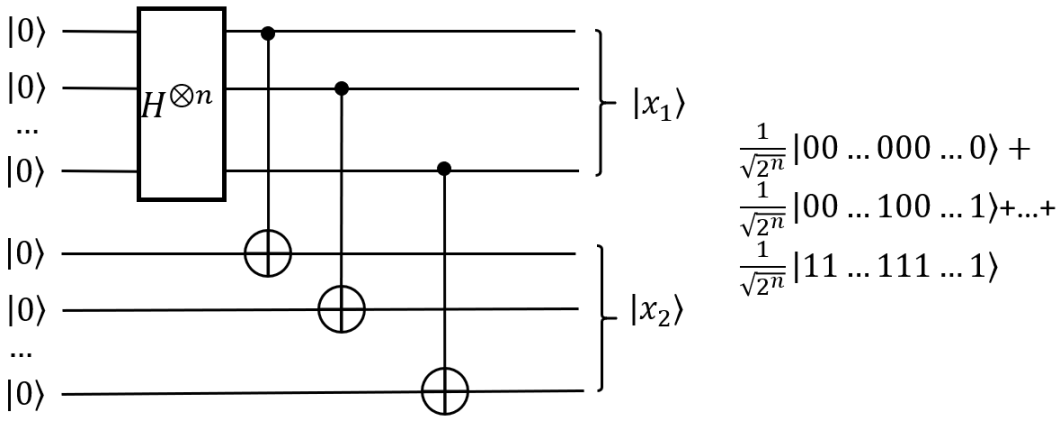


Figure 20. Conditional Constraint Relation Represented in Quantum Circuits

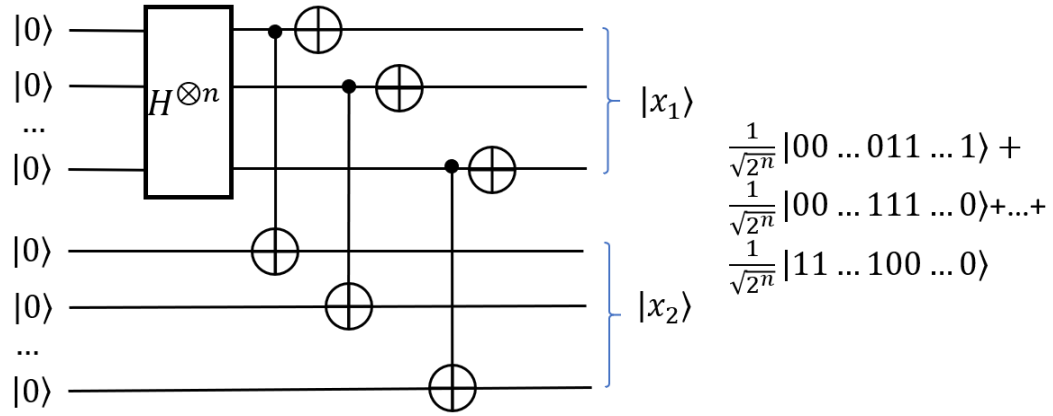
6.2.3 Quantum Representation of Other Constraints Relations

There are also some other constraint relations, which are not mentioned in the problem formation of workforce planning. However, these constraints still exist in some

particular application scenarios and can be expressed in quantum circuit. Some examples are shown in Figure 21.



(a) $x_1 = x_2, x_1, x_2 \in D, |D| = 2^n$



(b) $x_1 + x_2 = \max(D), x_1, x_2 \in D, |D| = 2^n$

Figure 21. Other Constraint Relation Represented in Quantum Circuits

After determining the minimal number of qubits required in the quantum circuits to represent all the hard constraints, the encoding method can also be finalized. As the number of possible posterior states in the output qubit string is identical to the number of feasible

solutions to the CSP, the final encoding method can apply a prefect one-to-one mapping between coded representations and feasible solutions. Additionally, the proposed hard constraint handling method updates the original optimization variables into the circuit parameters, which is more advantageous since whatever changes in the circuit parameters would not change the posterior states but only the probability distribution among them.

6.3 An Illustrative Example of Airport Shift Planning

To better demonstrate the formulation from problem context to quantum entanglement inspired representation, a real-world case of shift planning in an international airport is given here. Due to the existence of large number of tasks, which are associated with the arrivals and departures of aircrafts and influenced by flight schedules adjustment, the optimal shift planning decision is crucial for the good performance of an airport as a system. The definition of the feasible shift types is given in Table 6.

Table 6. Definition of Feasible Shift Types

Shift Type	min_{st}	max_{st}	min_l	max_l	$g_{st}\ (= g_l)$
AM (Morning)	04:00	08:00	9 hours	11 hours	30 mins
PM (Afternoon)	14:00	18:00	9 hours	11 hours	30 mins

The associated hard constraints include:

- Shift starting time $t \in D_1 =$ $\{04{:}\,00, 04{:}\,30, 05{:}\,00, 05{:}\,30, 06{:}\,00, 06{:}\,30, 07{:}\,00, 07{:}\,30, 08{:}\,00\} \cup$ $\{14{:}\,00, 14{:}\,30, 15{:}\,00, 15{:}\,30, 16{:}\,00, 16{:}\,30, 17{:}\,00, 17{:}\,30, 18{:}\,00\}$, $|D_1| = 9 + 9 = 18$.
- Unlimited personnel resource, the number of workers assigned to a feasible shift $p \in D_2 = \left\{0,1, \dots, \max_{k=1,\dots,T}\{D_p^k\}\right\}$, $|D_2| = \max_{k=1,\dots,T}\{D_p^k\} + 1$.
- Length of a shift $\lambda \in D_3 = \{0,9,9.5,10,10.5,11\}$, $|D_3| = 6$.
- At any shift s, if $p_s = 0$, then $\lambda_s = 0$; if $p_s \neq 0$, then $\lambda_s \neq 0$.
- At any time, there is at maximum one shift that can start.

To demonstrate the design of quantum entanglement, let say in one given scenario, the highest workforce demand $max_p = 15$, $|D_2| = 16 = 2^4$, 4 qubits are required to cover all the feasible options for number of staffs, as shown in Figure 22.

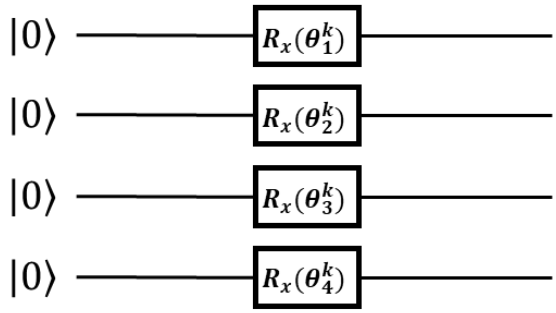


Figure 22. Quantum Circuit for Representation Number of Staffs

With the initial input of qubit string $|0000\rangle$, this part of quantum circuit guaranteed the output quantum state to be a superposition of only feasible solutions. The probability

of each feasible solution is determined by the angle of *n* rotation gates, while the probability of infeasible permutation is zero regardless of parameters variability.

At the k^{th} iteration, as for each of the first 4 qubits that is initialized as $|0\rangle$, a rotation gate $R_x(\theta_i^k)$ would be applied on the i^{th} qubit and achieve:

$$\begin{aligned} |\psi_i^k\rangle = R_x(\theta_i^k)|0\rangle &= \begin{bmatrix} \cos(\theta_i^k) & -\sin(\theta_i^k) \\ \sin(\theta_i^k) & \cos(\theta_i^k) \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos(\theta_i^k) \\ \sin(\theta_i^k) \end{bmatrix} \\ &= \cos(\theta_i^k)\,|0\rangle + \sin(\theta_i^k)\,|1\rangle \end{aligned} \tag{26}$$

The tensor product of the first 4 qubits after the rotation gates:

$$\begin{aligned} &|\psi_1^k\rangle \otimes |\psi_2^k\rangle \otimes |\psi_3^k\rangle \otimes |\psi_4^k\rangle \\ &= \prod_{i=1}^{4} \cos(\theta_i^k)\,|0000\rangle + \sin(\theta_4^k) \prod_{i=1}^{3} \cos(\theta_i^k)\,|0001\rangle \\ &+ \cdots + \prod_{i=1}^{4} \sin(\theta_i^k)\,|1111\rangle \end{aligned} \tag{27}$$

The representation of the conditional constraint between number of staff and length of shift, namely, 1) zero staff in the shift must link with zero shift length; 2) non-zero number of staffs must be linked to one of the five possible shift length. To entangle the above constraints in to encoding presentation, an additional qubit is needed to serve as a control switch to bridge this part with the last part. Noticeably, this qubit requires no rotation gate for probability amplitude tuning. This qubit is added to update the first part of quantum circuit, as shown in Figure 23.

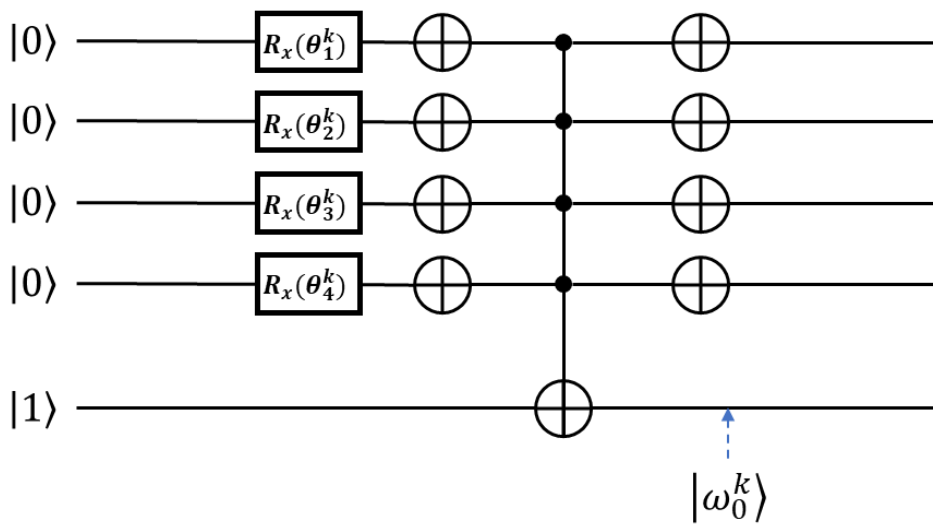


Figure 23. Quantum Circuit for Entangling Number of Staffs with Legal Shift Length

With the help of this qubit $|\omega_0^k\rangle$, a second part of quantum circuit is shown in Figure 24, with 3 more additional qubits used to represent the 5 possible shift lengths.

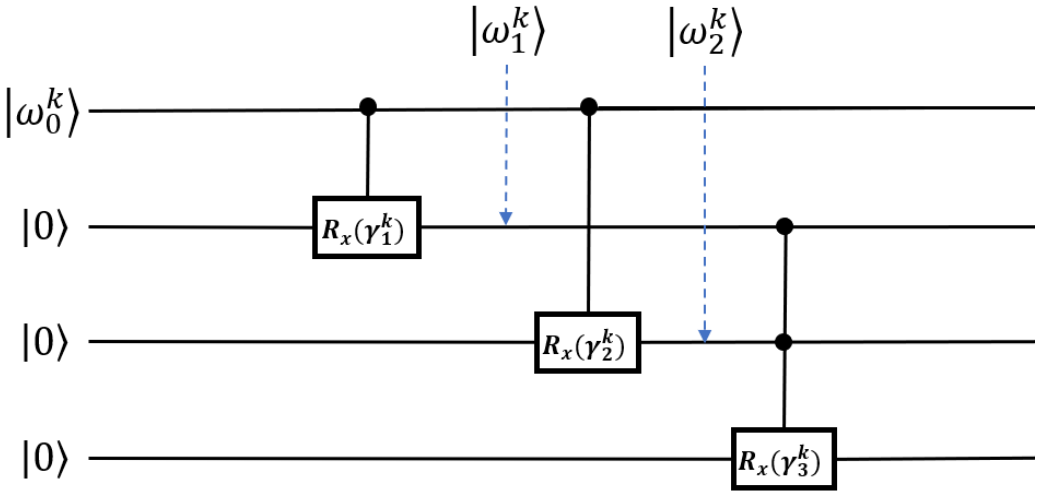


Figure 24. Quantum Circuit for Entangling Number of Staffs with Five Possible Shift Lengths

Firstly, the controlled-rotation gate $CR_x(\gamma_1^k)$ is applied to 5th qubit $|\omega_0^k\rangle$ and the 6th qubit $|0\rangle$ and obtain:

$$
\begin{aligned}
& CR_x(\gamma_1^k)\left(|\omega_0^k\rangle \otimes |0\rangle\right) \\
& = CR_x(\gamma_1^k)\left(\prod_{i=1}^{4}\cos(\theta_i^k)\,|00\rangle + \sqrt{1-\left(\prod_{i=1}^{4}\cos(\theta_i^k)\right)^2}\,|10\rangle\right) \\
& = \prod_{i=1}^{4}\cos(\theta_i^k)\,|00\rangle + \cos(\gamma_1^k)\sqrt{1-\left(\prod_{i=1}^{4}\cos(\theta_i^k)\right)^2}\,|10\rangle \\
& \quad + \sin(\gamma_1^k)\sqrt{1-\left(\prod_{i=1}^{4}\cos(\theta_i^k)\right)^2}\,|11\rangle
\end{aligned}
\tag{28}
$$

where $CR_x(\theta) = \begin{bmatrix} I_2 & 0 \\ 0 & R_x(\theta) \end{bmatrix}, 0 \le \theta \le \frac{\pi}{2}$.

Thus, the state of the 6th qubit after applying $CR_x(\gamma_1^k)$can be expressed as:

$$\left|\omega_1^k\right\rangle = \left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right) + \cos\left(\gamma_1^k\right)\sqrt{1-\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)\right)^2}\right)|0\rangle + \sin\left(\gamma_1^k\right)\sqrt{1-\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)\right)^2}|1\rangle \tag{29}$$

Similarly, the controlled-rotation gate $CR_x\left(\gamma_2^k\right)$ is applied to 5th qubit $\left|\omega_0^k\right\rangle$ and the 7th qubit $|0\rangle$ and obtain:

$$\begin{aligned} & CR_x\left(\gamma_2^k\right)\left(\left|\omega_0^k\right\rangle \otimes |0\rangle\right) \\ & = CR_x\left(\gamma_2^k\right)\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)|00\rangle + \sqrt{1-\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)\right)^2}\,|10\rangle\right) \\ & = \prod_{i=1}^{4}\cos\left(\theta_i^k\right)|00\rangle + \cos\left(\gamma_2^k\right)\sqrt{1-\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)\right)^2}\,|10\rangle + \sin\left(\gamma_2^k\right)\sqrt{1-\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)\right)^2}\,|11\rangle \end{aligned} \tag{30}$$

Thus, the state of the 7th qubit after applying $CR_x\left(\gamma_2^k\right)$can be expressed as:

$$\left|\omega_2^k\right\rangle = \left(\prod_{i=1}^{4} \cos\left(\theta_i^k\right) + \cos\left(\gamma_2^k\right) \sqrt{1 - \left(\prod_{i=1}^{4} \cos\left(\theta_i^k\right) \right)^2} \right) |0\rangle + \sin\left(\gamma_2^k\right) \sqrt{1 - \left(\prod_{i=1}^{4} \cos\left(\theta_i^k\right) \right)^2} \, |1\rangle \tag{31}$$

Lastly, the controlled-controlled-rotation gate $CCR_x\left(\gamma_3^k\right)$ is applied to $\left|\omega_1^k\right\rangle$ and $\left|\omega_2^k\right\rangle$ complete the entanglement:

$$
\begin{aligned}
&\left|\omega_0^k\right\rangle \otimes CCR_x\left(\gamma_3^k\right)\left(\left|\omega_1^k\right\rangle \otimes \left|\omega_2^k\right\rangle \otimes |0\rangle\right) \\
&\quad = \prod_{i=1}^{4} \cos\left(\theta_i^k\right) |0000\rangle \\
&\quad + \cos\left(\gamma_1^k\right)\cos\left(\gamma_2^k\right)\sqrt{1-\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)\right)^2}\,|1000\rangle \\
&\quad + \cos\left(\gamma_1^k\right)\sin\left(\gamma_2^k\right)\sqrt{1-\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)\right)^2}\,|1010\rangle \\
&\quad + \sin\left(\gamma_1^k\right)\cos\left(\gamma_2^k\right)\sqrt{1-\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)\right)^2}\,|1100\rangle \\
&\quad + \sin\left(\gamma_1^k\right)\sin\left(\gamma_2^k\right)\cos\left(\gamma_3^k\right)\sqrt{1-\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)\right)^2}\,|1110\rangle \\
&\quad + \sin\left(\gamma_1^k\right)\sin\left(\gamma_2^k\right)\sin\left(\gamma_3^k\right)\sqrt{1-\left(\prod_{i=1}^{4}\cos\left(\theta_i^k\right)\right)^2}\,|1111\rangle
\end{aligned}
\tag{32}
$$

where $CCR_x(\theta) = \begin{bmatrix} I_4 & 0 \\ 0 & R_x(\theta) \end{bmatrix}, 0 \le \theta \le \frac{\pi}{2}$.

After the development of the two partial quantum circuits, the complete quantum circuit for the encoding of each shift at a feasible starting time can be presented. The entire quantum circuit with the corresponding rotation angles set $\{\theta_1^k, \theta_2^k, \theta_3^k, \theta_4^k, \gamma_1^k, \gamma_2^k, \gamma_3^k\}$ specified in the k^{th} iteration is denoted as U^k.

The corresponding assembled quantum circuit is given in Figure 25. In the tested scenario, at a feasible starting time of a day, at maximum one shift can be added, the configuration of this shift has $1 + (|D_2| - 1) \times (|D_3| - 1) = 76$ options including empty shift. The circuit in Figure 25 guarantees the output state is a quantum superposition of 76 feasible states, where each feasible state maps to one feasible shift setting represented by an eight-bit long binary string. The first four bits of this binary string indicate the number of staffs in this shift, which indicates that the number of staffs can be any integer between 0 and 15. The last four bits represent the length of the shift, where the 5th bit indicates if the length is at minimum 9 hours long, the 6th bit indicates another one hour on top of the minimum shift length, and the 7th and 8th bits both indicate another half hour on top of the minimum shift length. For instance, the last four bits being $|1100\rangle$ maps to a total shift length of $9 \times 1 + 1 \times 1 + 0 \times 0.5 + 0 \times 0.5 = 10\ (hr)$.

Given the value of circuit parameters, the probability distribution among the feasible states is also calculatable.

$$
\begin{aligned}
&U_s^k(\theta_{s1}^k, \theta_{s2}^k, \theta_{s3}^k, \theta_{s4}^k, \gamma_{s1}^k, \gamma_{s2}^k, \gamma_{s3}^k)(|00001000\rangle) = \textstyle\sum_{j=1}^{76} A_{sj}^k |v_j\rangle = \\
&\textstyle\prod_{i=1}^{4} \cos(\theta_{si}^k)\, |00000000\rangle + \\
&\cos(\gamma_{s1}^k) \cos(\gamma_{s2}^k) \sin(\theta_{s4}^k) \textstyle\prod_{i=1}^{3} \cos(\theta_{si}^k)\, |00011000\rangle + \\
&\cos(\gamma_{s1}^k) \sin(\gamma_{s2}^k) \sin(\theta_{s4}^k) \textstyle\prod_{i=1}^{3} \cos(\theta_{si}^k)\, |00011010\rangle + \\
&\sin(\gamma_{s1}^k) \cos(\gamma_{s2}^k) \sin(\theta_{s4}^k) \textstyle\prod_{i=1}^{3} \cos(\theta_{si}^k)\, |00011100\rangle + \\
&\sin(\gamma_{s1}^k) \sin(\gamma_{s2}^k) \cos(\gamma_{s3}^k) \sin(\theta_{s4}^k) \textstyle\prod_{i=1}^{3} \cos(\theta_{si}^k)\, |00011110\rangle + \\
&\sin(\gamma_{s1}^k) \sin(\gamma_{s2}^k) \sin(\gamma_{s3}^k) \sin(\theta_{s4}^k) \textstyle\prod_{i=1}^{3} \cos(\theta_{si}^k)\, |00011111\rangle + \cdots +
\end{aligned}
\tag{33}
$$

$\cos(\gamma_{s1}^k)\cos(\gamma_{s2}^k)\prod_{i=1}^{4}\sin(\theta_{si}^k)\,|11111000\rangle + \cdots +$

$\sin(\gamma_{s1}^k)\sin(\gamma_{s2}^k)\sin(\gamma_{s3}^k)\prod_{i=1}^{4}\sin(\theta_{si}^k)\,|11111111\rangle$

$$\text{Prob}(|v_j\rangle) = |A_{sj}^k|^2, \sum_{j=1}^{76}\text{Prob}(|v_j\rangle) = \sum_{j=1}^{76}|A_{sj}^k|^2 = 1 \quad (34)$$

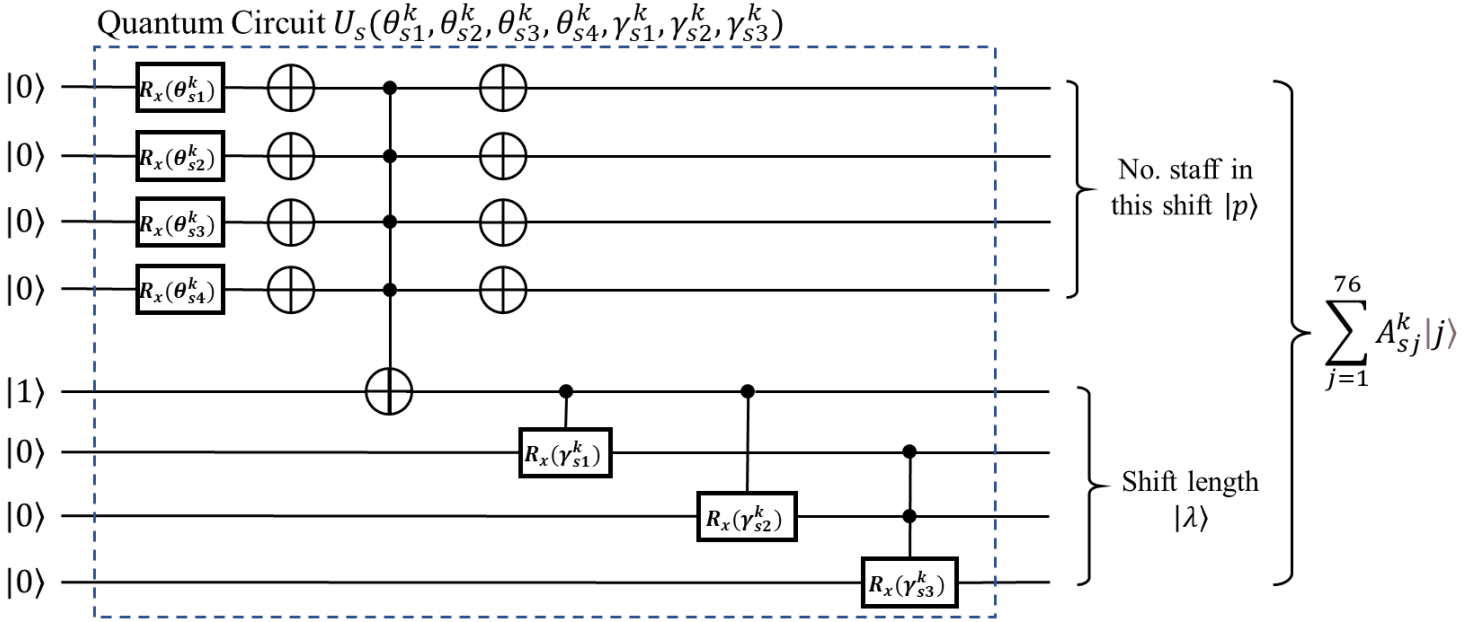


Figure 25. Quantum Circuit for Feasible Shift Design at One Feasible Starting time of a Day

6.4 Quantum Entanglement Inspired Genetic Algorithm (QEI-GA)

To leverage the hard constraint handling strength of quantum entanglement for optimization, the quantum entanglement inspired hard constraint handling needs to be assembled with some effective searching techniques. In this case example, the proposed approach is embedded in genetic algorithm (GA) due to its ease of use and flexibility. Additionally, a recent review article (Nguyen et al., 2014) also reveals the fact that GA is the most frequently applied optimization technique in solving engineering problems.

6.4.1 Standard QEI-GA

Once the problem is formulated, the original optimization variables and associated hard constraints are sent thru the quantum entanglement inspired hard constraint handling approach as shown in Figure 26, while the optimization objectives and soft constraints are combined to generate the global objective function. The quantum entanglement inspired hard constraint handling approach outputs the final qubit encoding scheme, as well as the quantum entanglement circuit parameters and the other variables that cannot be fully handled by this approach, which compose the new unconstrained optimization variables for the initialization of GA. Those new optimization variables are encoded into GA chromosome, and the random initial population of GA can be generated accordingly. Next, GA evaluates the fitness value of each individual in the initial population, where the information carried in each chromosome corresponds to a quantum circuit with given parameter values that define the probability distribution of all feasible states. A feasible state is chosen stochastically using the probability-based Roulette selection method after which the feasible state is deciphered into feasible solution in order to allow fitness

evaluation. The population update process in GA only changes the quantum circuit parameters, which would never influence the components of feasible state space of the circuit but only the probability distribution. The evaluation to one exact same chromosome can lead to different fitness values due to the nature of quantum superposition, which enables a high population diversity. The optimization process continues to run until a termination condition is met and outputs the best result found thus far. The flow chart of this quantum entanglement inspired GA (QEI-GA) is shown in Figure 26.

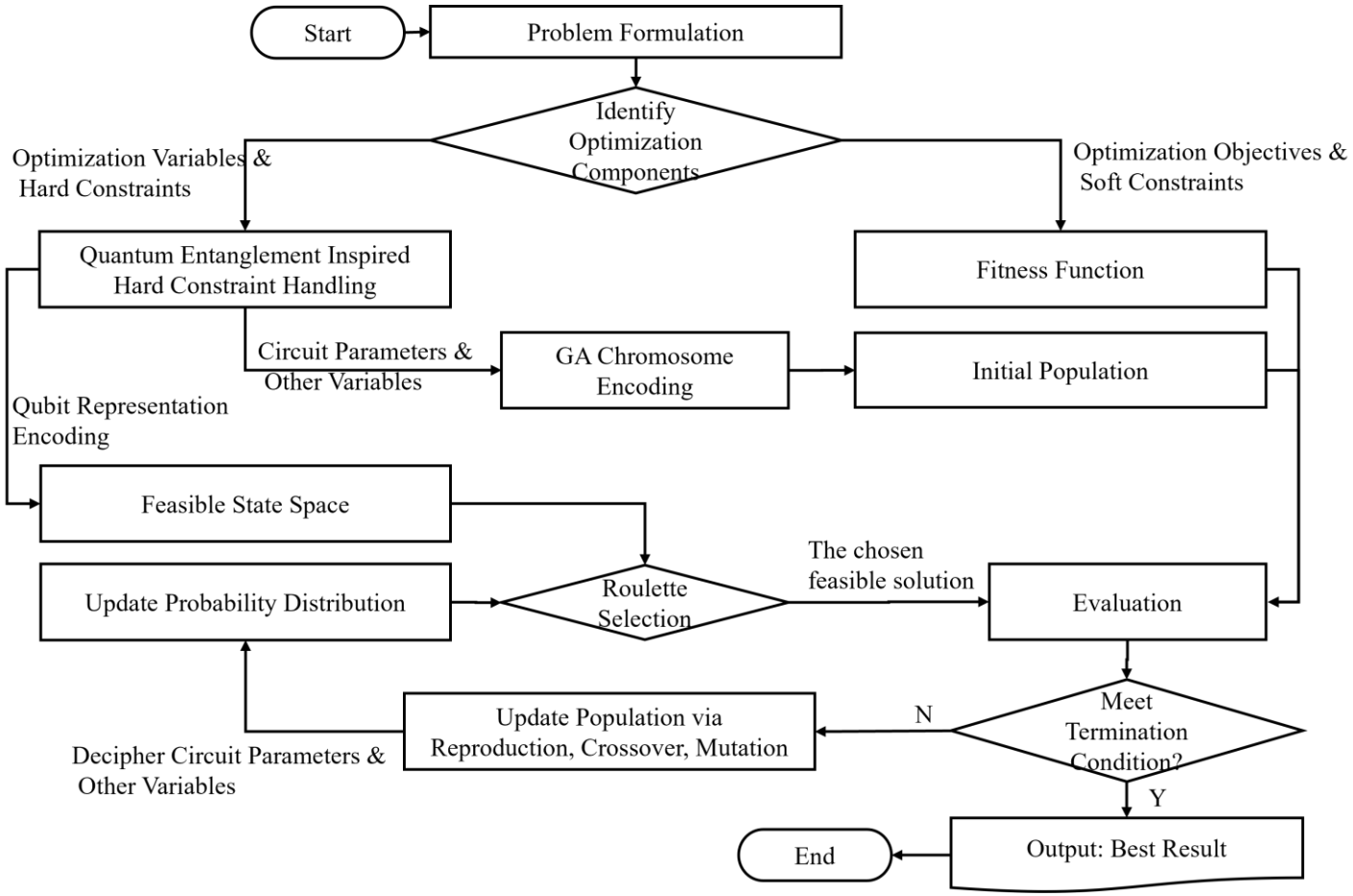


Figure 26. Flow Chart of QEI-GA

Noticeably, there are two encoding methods in this paradigm. One is the qubit representation encoding, which uses qubits and quantum circuits to generate quantum superposition. The feasible states in qubit representation can be precisely one-to-one mapped to the feasible solutions to the original COP, and the probability distribution among all feasible states are controlled by the parameters of quantum circuits. Using the same case example as above, this encoding method is shown in Figure 27. The other encoding method is the chromosome encoding using classical encoding strategy. The encoded chromosome includes the information of quantum circuits parameters, as well as some other information that cannot be handled by quantum entanglement inspired approach, as shown in Figure 28. The existence of both encoding methods enable the effectiveness of classical GA operation, since the quantum entanglement inspired section is not directly involved in the optimization process.

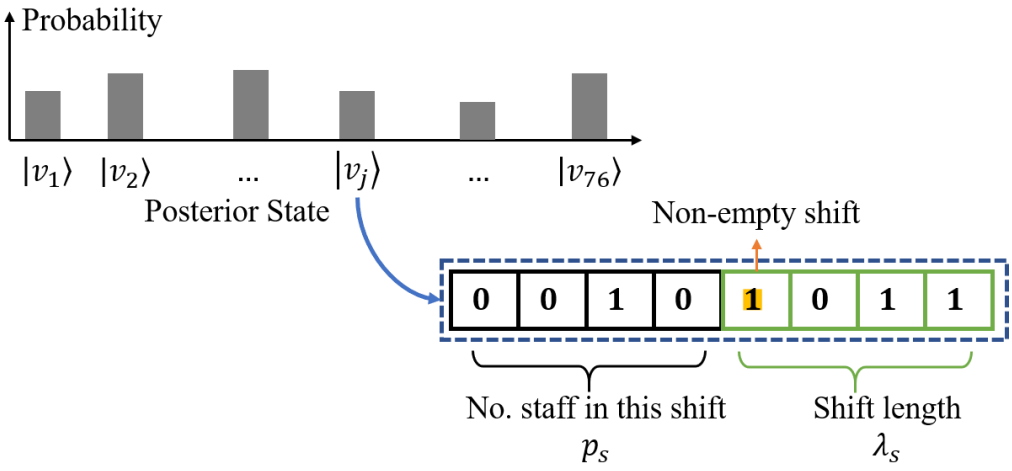


Figure 27. Interpretation of Feasible State

Next, the circuit parameters compose the chromosome of GA, as shown in Figure 28. All circuit parameters are rotation angles, which share the same range $[0,2\pi]$. The reproduce, selection, crossover, and mutation processes of GA do not change the feasibility

of chromosomes, while the fitness evaluation of each combination of circuit parameters is executed on the probabilistically selected posterior state of the corresponding circuit in the form of binary string.

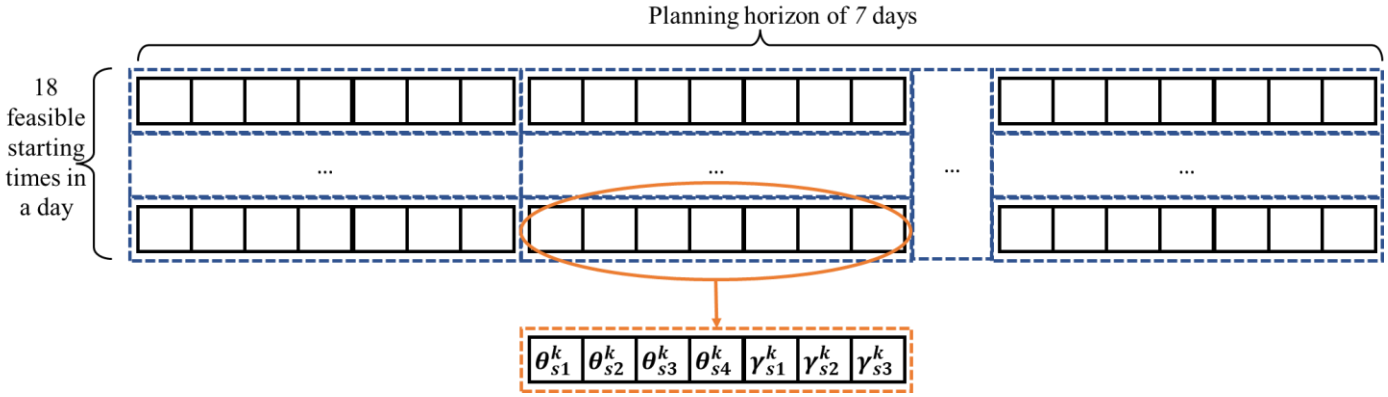


Figure 28. GA Chromosome

The computational complexity of the QEI-GA includes the complexity of classical GA with unconstrained optimization variables and the complexity of GEI hard constraint representation. The following parameters are used in the GA part: a population size P, a termination criterion: maximum number of iterations G, a chromosome with length L, a fitness evaluation function, a fixed crossover probability for one-point crossover, a fixed mutation probability for one-point mutation and a roulette-wheel selection process. The computation complexity of such a GA is given (Samanta et al., 2017) by:

$$\begin{aligned} &O(popluation\ size\ \times maximum\ iteration \times O(Fitness) \\ &\quad \times \big(Crossover\ probability \times O(Crossover) \\ &\quad + Mutation\ probability \times O(Mutation) \\ &\quad + O(Selection)\big) \\ &\quad = O(P \times G \times O(Fitness) \times (O(Crossover) \\ &\quad + O(Mutation) + O(Selection))) \end{aligned} \tag{35}$$

The following parameters are used in the GEI hard constraint representation part: a qubit chromosome with same length L, a quantum entanglement circuit with L quantum rotation gates, and a quantum observation process. The computation complexity of the GEI hard constraint representation part is given by:

$$
\begin{aligned}
&O(number\ of\ qubits \\
&\quad \times \big(O(quantum\ rotation) + O(qubit\ observation)\big)) \\
&\quad = O(L \times (O(Quantum\ rotation) \\
&\quad + O(Qubit\ observation)))
\end{aligned}
\tag{36}
$$

Therefore, the total computation complexity of the QEI-GA is given by:

$$
\begin{aligned}
&O(P \times G \times (L \times (O(Quantum\ rotation) + O(Qubit\ observation)) \\
&\quad + O(fitness)) \times (O(Crossover) + O(Mutation) \\
&\quad + O(Selection)))
\end{aligned}
\tag{37}
$$

6.4.2 Lightweight Version for Small Scale Personnel Scheduling

Personnel scheduling problems are often associated with various decisions that need to be made, one of the most commonly seen decisions is the assignment of work tasks. Especially when certain tasks have specific requirements, the assignment of work tasks is also coupled with the decisions of combining workers into subsets based on their distinct skill sets or locations.

In this section, a classical application domain of balanced nurse scheduling is used as an illustrate case about how a personnel scheduling problem can be formulated into a combinatorial constrained optimization mathematic model. Since nursing cost makes the largest portion of the personnel budget of a hospital (Mullinax and Lawley, 2002) and balanced workload distribution among nurses is known as an essential factor to ensure the

care quality (Svirsko, et al. 2019) and fairness of the work environment, the optimal nurse scheduling decisions are of critical importance.

6.4.2.1 Mathematical Modelling

Balanced nurse scheduling problem originated from the real-world scenarios of daily assignment of newborn infant patients to nurses in a hospital (Schaus, Hentenryck and Régin, 2009), where each patient may require a different level of care and the amount of care each patient type requires during one shift (also called the acuity) is nurse dependent. The workload of a nurse during one shift is the total amount of acuity required from the group of patients assigned, while another request to make the schedule reasonable is to limit the number of patients assigned per shift. This study aims to develop techniques for improving the balanced assignment of workload to staff nurses in an intensive care provider facility. There are a variety of different type of health care nurseries based on their size, shape, and care level. The size refers to the number of patients that need to be accommodated, where a small nursery may only have 10-12 infants while a large one can have up to 50 beds. The size characteristics is about the number of workstations, which also are referred as zones, separated by walls or floors. The care level refers to the types of patients admitted in the facility, from healthy newborns to critically ill infants that require surgery or extensive mechanical ventilation. The problem can be decomposed in two sub-tasks: nurse staffing and nurse-patient assignment. The former first assigns nurses to zones if there are more than one working zones, while the latter then assigns patients of each zone to nurses. The mathematical description of the above can be provided as: There are n patients $\{1, \dots, n\}$ in the given shift period with m nurses $\{1, \dots, m\}$, the acuity of patient i for nurse j is $a_{i,j}$. Noticeably, some patients can be out of a nurse's capability, where some

modelling methods set the corresponding acuity equals to infinity as penalty, while in this study, this constraint is represented as that each patient has a defined potentially available nurse set. The set of patients in zone k is denoted by $\mathcal{P}_k$, and the sets of patients from all p zones $\{\mathcal{P}_1, \dots, \mathcal{P}_p\}$ forms a partition of $\{1, \dots, n\}$. For each patient i, his/her assigned nurse is represented by the decision variable N_i, where the value of N_i must belong to the potentially available nurse set AN_i. The workload of nurse j is represented by $W_j = \sum_{i=1}^{n} c_{i,j} * a_{i,j}$, where $c_{i,j} = \begin{cases} 1, & N_i = j \\ 0, & N_i \neq j \end{cases}$. The workload balance level among nurses is indicated by the standard deviation σ among the workloads of nurses $\{W_1, \dots, W_m\}$.

The optimization objectives are:

- Optimize the overall workload by minimizing the total amount of acuity.
- Balance the workload among nurses by minimizing the standard deviation of the workloads. (Primary Target)

The embedded constraints in this problem include:

- There must be one and only one nurse assigned to each patient.
- A nurse can only work in one zone.
- A nurse can only be assigned to a patient within his/her capability.
- The number of patients a nurse is responsible should remain in a certain value range.

The problem can be formulated as follows:

$$Min\ \sigma, \sum_{j=1}^{m} \sum_{i=1}^{n} c_{i,j} * a_{i,j}$$

s.t.

- $c_{i,j} = \begin{cases} 1, & N_i = j \\ 0, & N_i \neq j \end{cases}, \forall i \in \{1, \dots, n\}, N_i \in AN_i \subseteq \{1, \dots, m\}$
- $\sum_{j=1}^{m} c_{i,j} = 1, \forall i \in \{1, \dots, n\}$
- $k_1, k_2 \in \{1, \dots, p\}, k_1 \neq k_2, \ \left(\bigcup_{i \in \mathcal{P}_{k_1}} N_i\right) \cap \left(\bigcup_{i \in \mathcal{P}_{k_2}} N_i\right) = \emptyset$
- $\forall j \in \{1, \dots, m\}, \ C_{min} \leq \sum_{i=1}^{n} c_{i,j} \leq C_{max}.$

A general version of the qubit-encoded chromosome structure and its corresponding evaluation procedure is given in Figure 29.

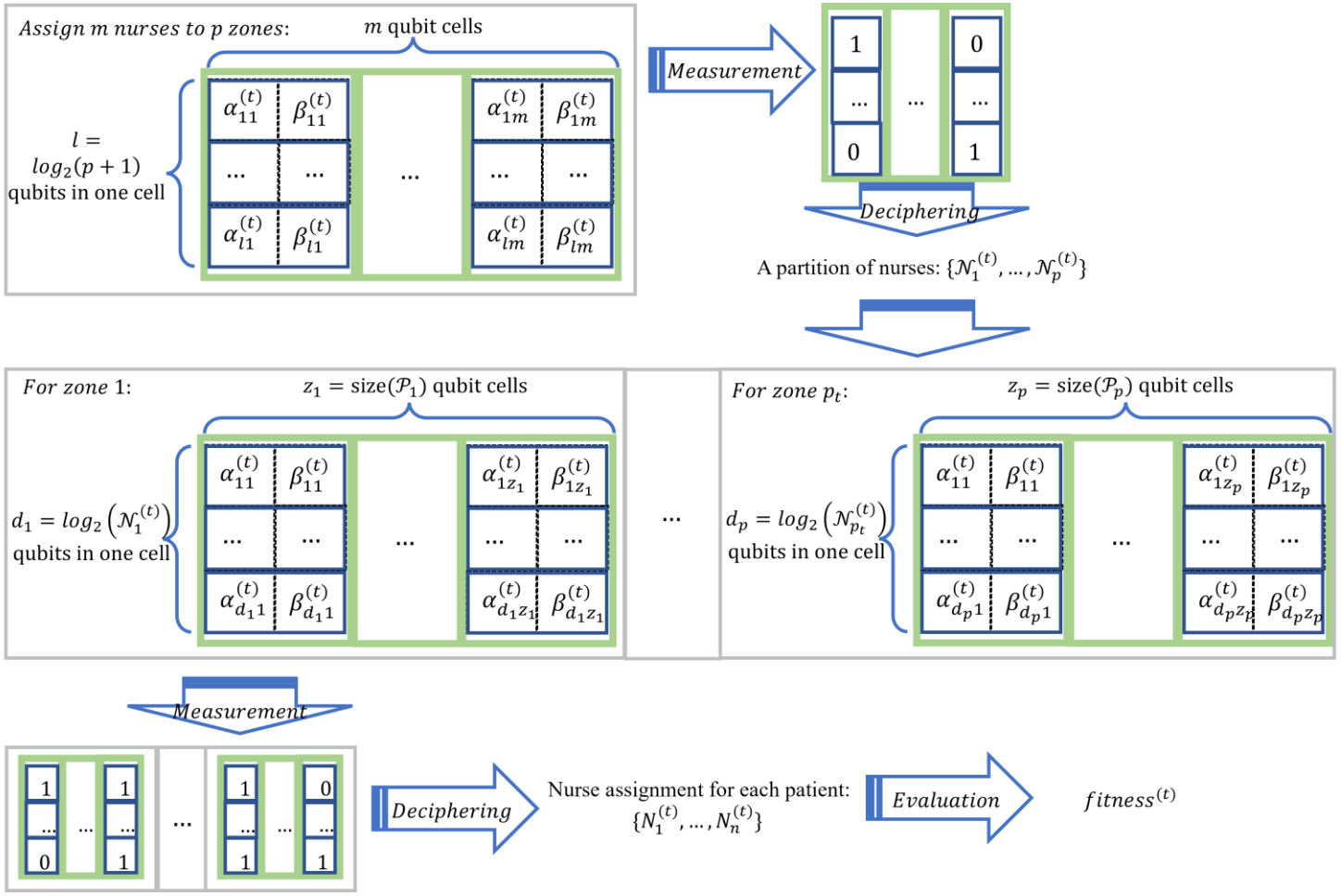


Figure 29. Qubit-encoded Chromosome for Multiple Zones Scenario and its Evaluation Procedure

Obviously, when there is only one working zone existed in the given scenario, the phase of assigning nurses to zones would be unnecessary, and the qubit chromosome would then be formulated into a matrix-like structure, as shown in Figure 30.

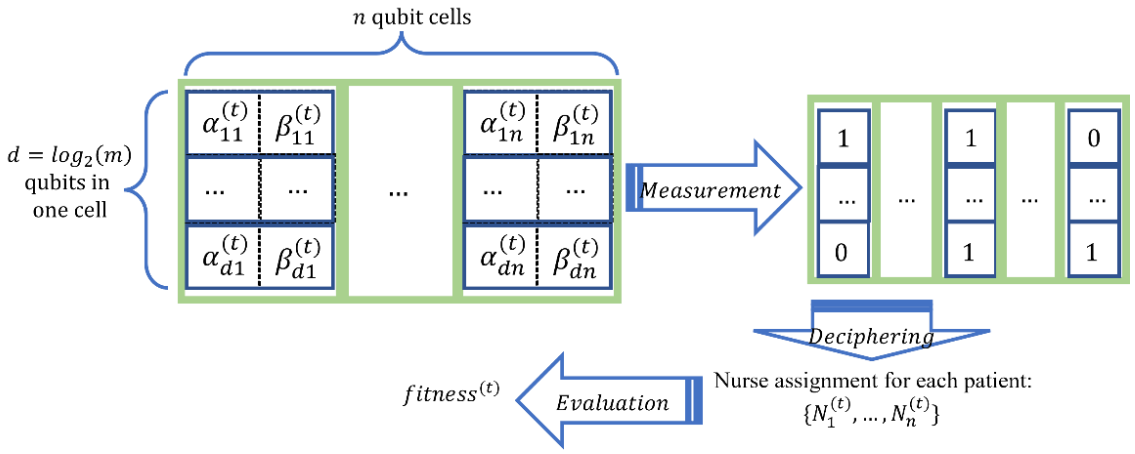


Figure 30. Qubit-encoded Chromosome for Single Zone Scenario and its Evaluation Procedure

Noticeably, qubit-encoded GA chromosome still uses data structure for constraint handling, which could result in very heavy chromosomes, this slows down the optimization process especially for the small-scale problems with less strict requirement of optimality but higher performance of agility and flexibility.

6.4.2.2 Lightweight Quantum Inspired Genetic Algorithm (LQIGA)

Similar to classical GA chromosome encoding method, current existing qubit encoding approaches could lead to a complicated chromosome data structure in order to represent constraint information, which can significantly increase the computation effort and re-programming work when applying to another scenario with different parameter settings. To overcome these difficulties, the proposed lightweight qubit encoding method

uses a simple single-dimension chromosome structure by leveraging the power of quantum circuits. Unlike the classical idea of using qubit to represent a binary decision variable, each single qubit in the lightweight qubit-encoded chromosome represents the parameterized probability distribution among all feasible nurse assignment decisions for each patient by embedding a case specific single parameter-controlled quantum circuit. Noticeably, the embedded quantum circuit can be represented as a unitary matrix for rapid computation due to the nature of quantum operation gates, which requires less computation efforts comparing to the deciphering process of a much more complicated chromosome.

An example of the lightweight qubit encoding method and its corresponding evaluation process in the single zone nurse scheduling scenario is given in Figure 31. The single parameter-controlled quantum circuits here are for the representation of nurse assignment information. When the number of available nurses happen to be the exact power of 2, the quantum circuit is consisted of only free qubits. One easy way to generate qubits in such a manner is to let one qubit goes through a parameterized rotation gate while the other goes through a Hadamard gate H. The posterior states of such a quantum circuit can be represented by the tensor product of all qubits, where the probability of each state is a function of the single rotation parameter. In a more generalized situation, the number of nurses is not exact power of 2, then quantum entanglement circuits would be required following the general design guideline (Zou., et al. 2022), in which case the posterior states can no longer be represented by the tensor product of all qubits and the usage of multiple quantum rotation gates enables the maximal parameterized control flexibility. In either way, the qubits in the lightweight qubit-encoded chromosome stay independent and can be updated separately. Noticeably, as a necessary result of the lightweight feature, the

quantum circuit controlled by single parameter would likely to have less flexibility in the control of each state. Considering the maximal control is not necessary in many small-scale cases, the proposed lightweight alternative is of more practical meaning for small scale problems rather than large scale ones. For instance, in the balanced nurse scheduling case, since each qubit in the chromosome bonds with one independent single parameter-controlled circuit, even the lightweight encoding method allows the available nurses for each patient be adjusted with independently, which can be used to represent the nurse capability constraints without using the indication of acuity being infinity.

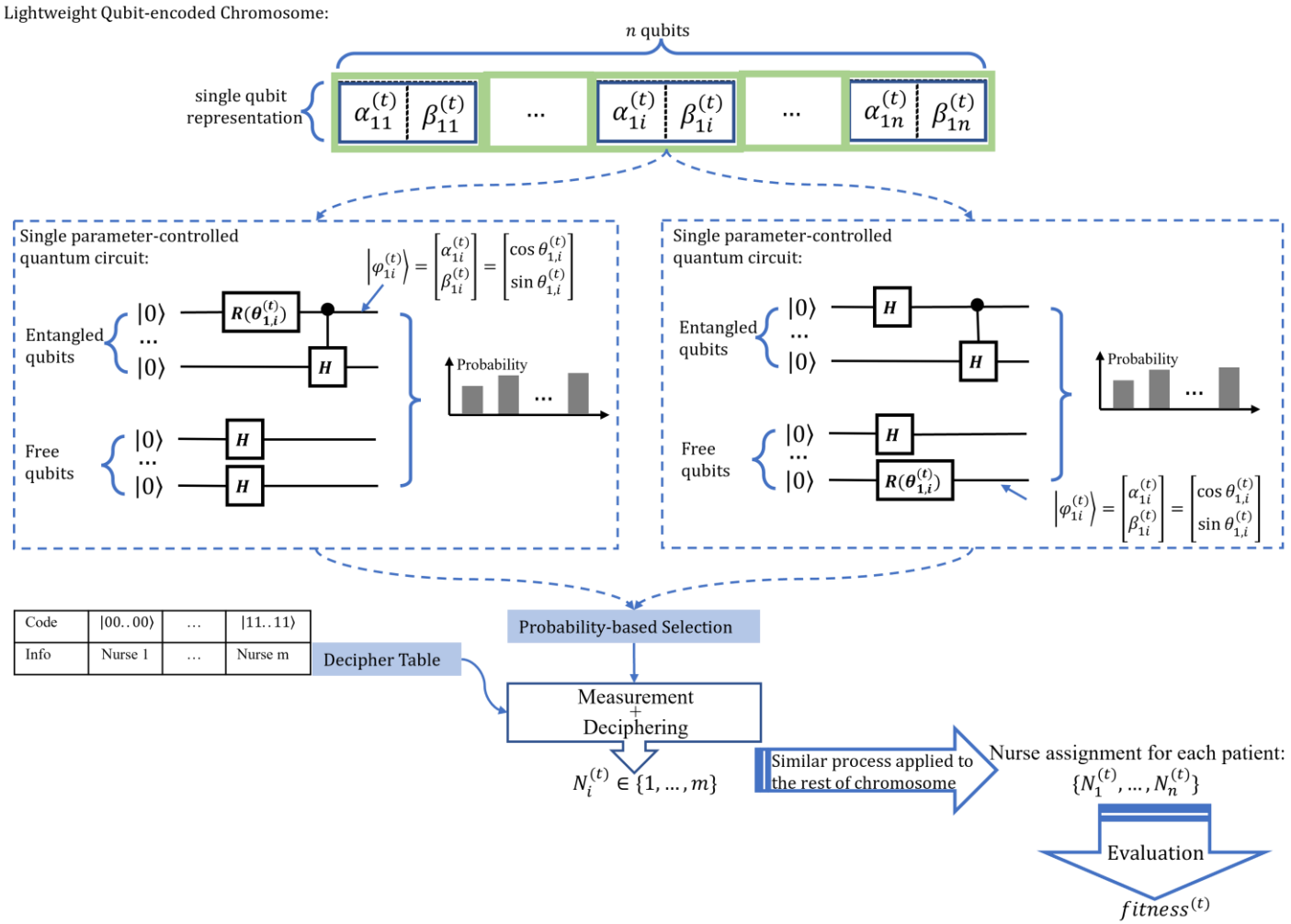


Figure 31. Lightweight Qubit-encoded Chromosome for Single Zone Scenario and its Evaluation

Using the proposed lightweight qubit encoding approach, a novel quantum inspired genetic algorithm with lightweight chromosome is developed, in order to provide a more agile solution especially for the small-scale personnel scheduling problems. A typical lightweight qubit-encode chromosome for the balanced nurse scheduling problem is a group of qubits. The statuses of qubits in the lightweight qubit-encoded chromosome are independent, which means each single qubit can still be applied with “update” process as well as the quantum inspired genetic operators. Also, the terminating condition can be set in any classical manner, which in this specific case, the number of iterations is used as a unified setting. A general workflow of this lightweight quantum inspired genetic algorithm (LQIGA) is shown in Figure 32.

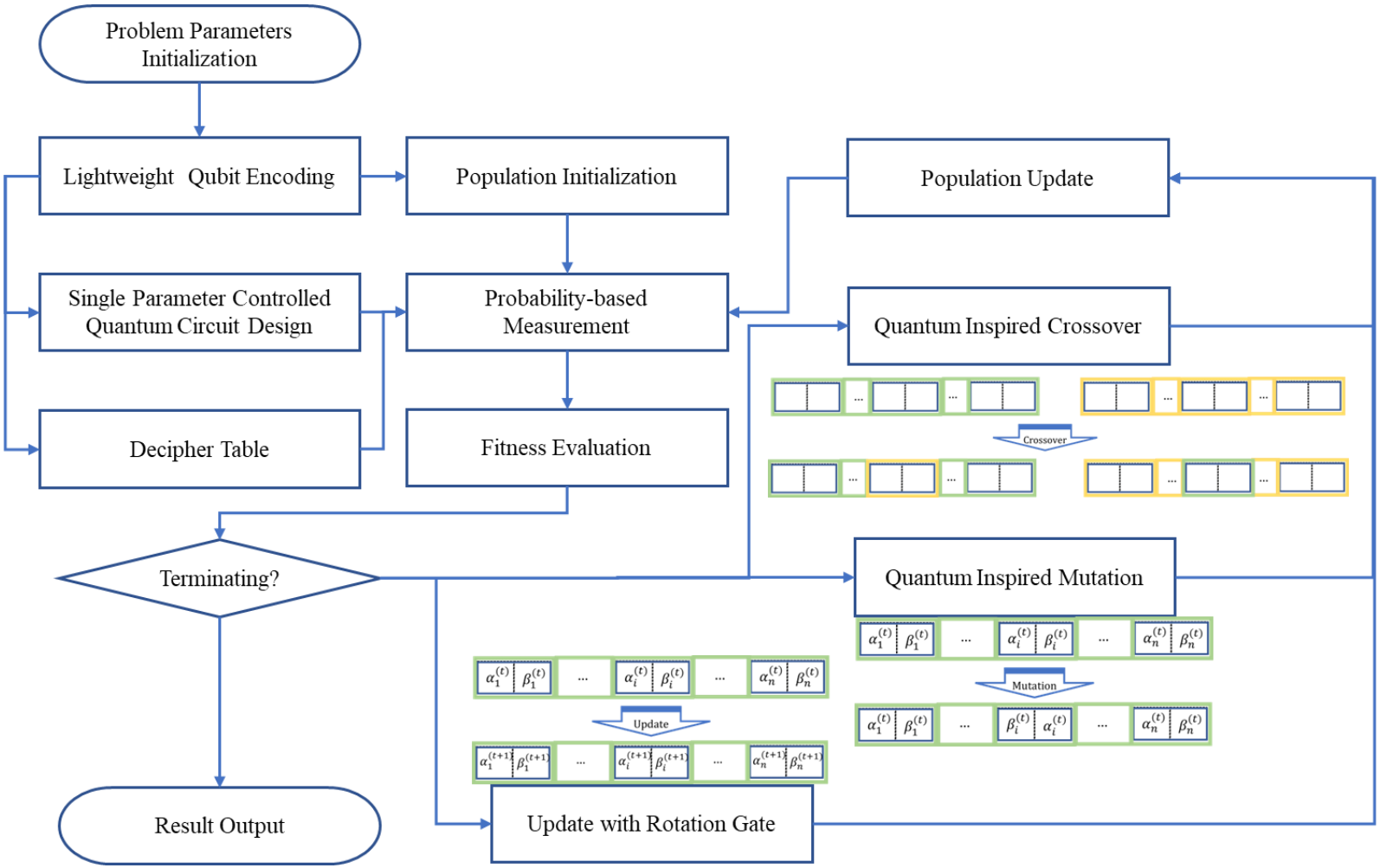


Figure 32. Complete Workflow of LQIGA

6.5 Application to Airport Shift Planning

6.5.1 Problem Context

Today's airline industry is confronting an enormous cost pressure, due to several crises that have considerable adverse influence on the business, including global health events and world economic situations. Consequently, airlines and airports are trying to cut their costs and increase competitiveness. Clearly, efficient planning of staff is crucial in controlling costs, as the size of airport operations can amplify the small improvements into large savings. Airport shift planning (ASP) is a very complex task, since it frequently involves high variations in demand, long planning horizon, small time granularity in work tasks and multitudes of constraints. As a real-world case study, the airport shift planning problem mentioned in this study aims to cover or minimize the deviation from the workloads/demand over a seven-day planning horizon by designing legally appropriate and overall cost-efficient shift duties.

In this problem, the discrepancy between the workforce demand D and the designed working shifts S are measured by the situation of understaff and overstaff, which are handled as the understaff cost f_u and overstaff cost f_o in the global objective function. Given by the airport, the corresponding weight values are $w_c = 1, w_u = 50, w_o = 1, w_p = 0$, indicating that the highest priority is to avoid understaff situation and no soft constraint preference is applied in this case study.

6.5.2 Optimization Modelling

This case study is utilized in this study, not only because it is an example of the typical operations engineering optimization problem, but also because it is a benchmark case that has also been solved by other existing optimization algorithms (Gong et al., 2019).

The optimization model for this ASP case can be described as following:

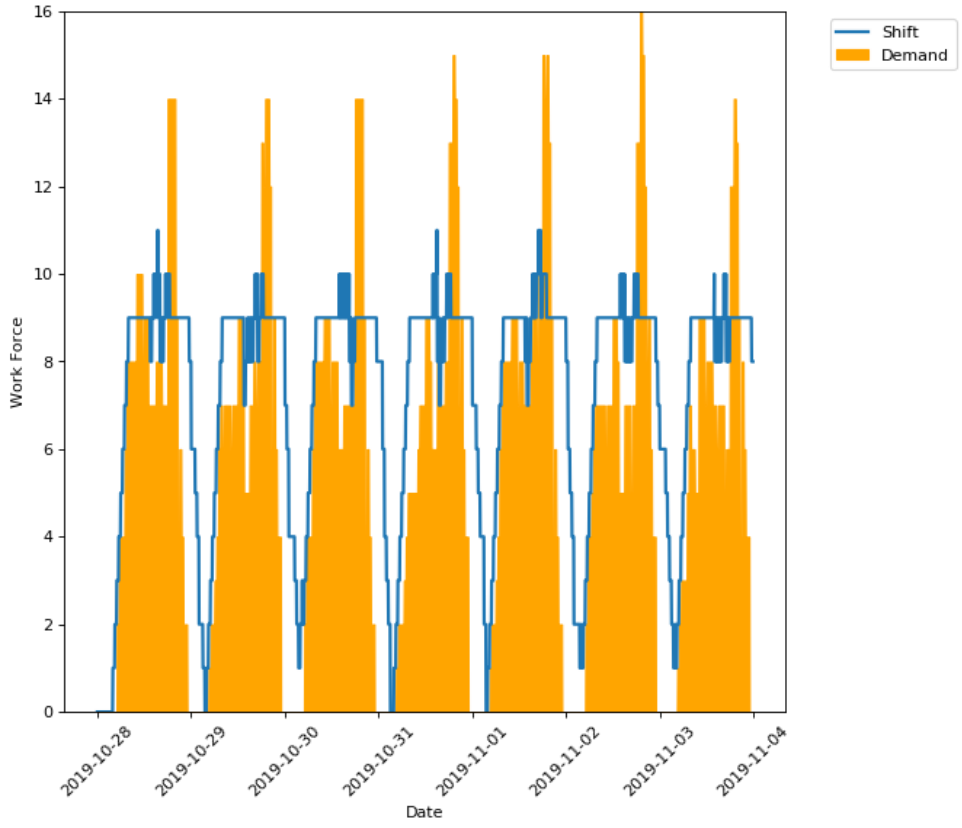
- $Objective$: $\min\{[w_u \cdot f_u(S) + w_o \cdot f_u(S)] \cdot f_c(S)\}$
  - $f_u(S) = [\sum_{s \in S, D^s > p_s}(D^s - p_s)]^3, f_o(S) = [\sum_{s \in S, D^s < p_s}(p_s - D^s)]^3, f_c(S) = \sum_{s \in S}|\lambda_s - 10| + 1$
- $subject\ to$:
  - $\forall s = (t_s, p_s, \lambda_s) \in S,$
  - $t_s \in D_1 =$ $\{04{:}00, 04{:}30, 05{:}00, 05{:}30, 06{:}00, 06{:}30, 07{:}00, 07{:}30, 08{:}00,$ $14{:}00, 14{:}30, 15{:}00, 15{:}30, 16{:}00, 16{:}30, 17{:}00, 17{:}30, 18{:}00\}$,
  - $p_s \in D_2 = \left\{0, 1, \ldots, \max_{k=1,\ldots,T}\{D_p^k\}\right\}$
  - $\lambda_s \in D_3 = \{0, 9, 9.5, 10, 10.5, 11\}$
  - if $p_s = 0$, then $\lambda_s = 0$; if $p_s \neq 0$, then $\lambda_s \neq 0$.
- $Output: S$

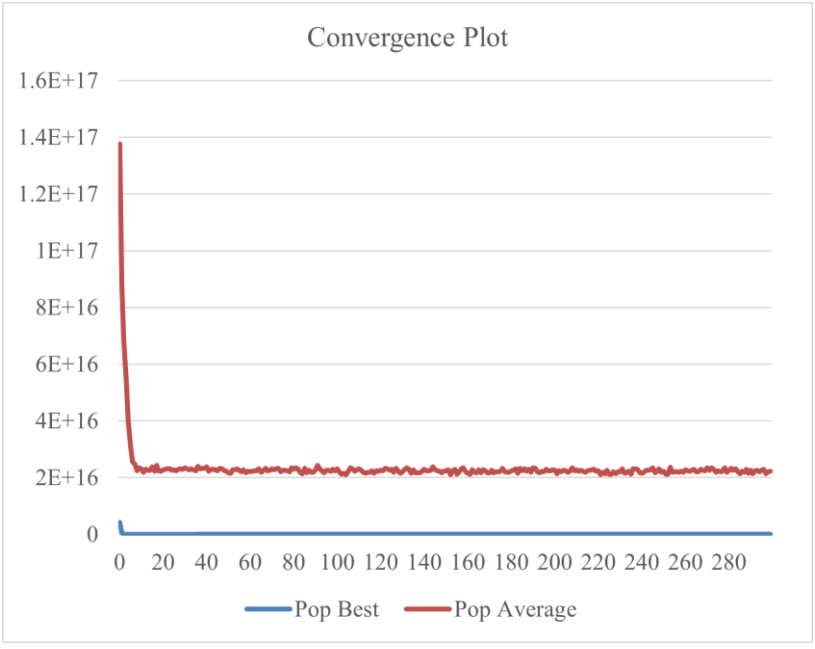
6.5.3 Result and Analysis

6.5.3.1 Validation of Effectiveness

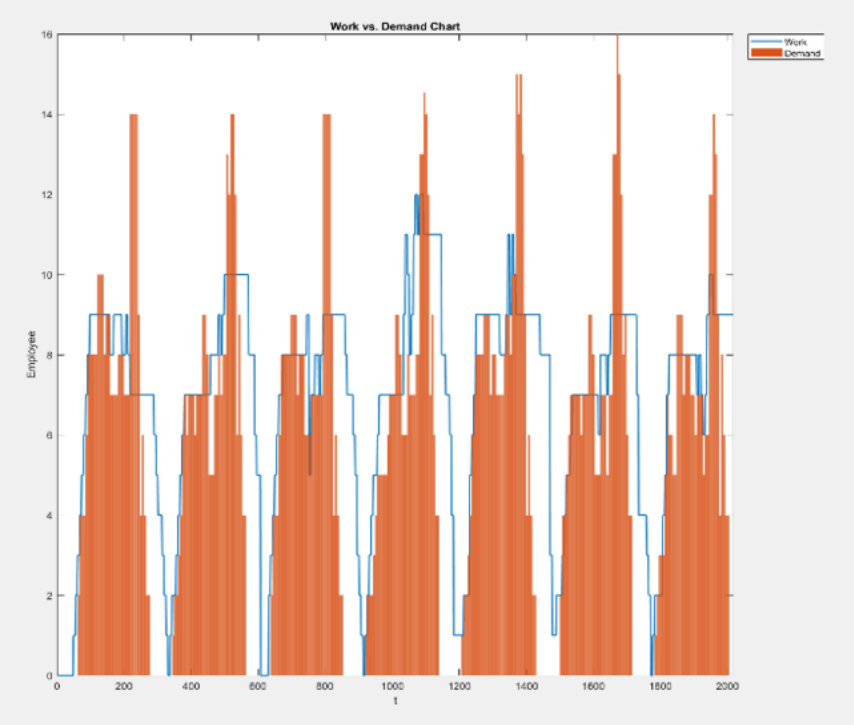
To validate the effectiveness of the proposed approach, QEI-GA is tested on a real-world case of 7-day horizon. The baseline results are obtained using the 2D-GA method (Gong et al., 2019), since the method is a chromosome structure modified version of classical GA to suit for the airport shift planning problem, where the GA chromosome is formed in a 2D structure with one dimension indicates the date information and the other daily-wise shift information. Correspondingly, the 2D-GA method applies crossover operators from both dimensions to guarantee the shift feasibility, due to the high interchangeability of each shift format. To handle the hard constraint that only one shift can be added at a feasible starting time, the 2D-GA method uses penalty function added to the fitness value. When no hard constraint is violated, their adjusted fitness function is equivalent to the original one. Additionally, another comparing object for GEI-GA is a multi-objective genetic algorithm NSGA-II (Deb et al., 2002), where an additional objective that consists of the constraint violation measure is used for constraint handling in the single-objective constrained optimization, and a concept of biased-dominance (Li and Zhang, 2014) is applied to compare or select individuals during the optimization process. The same 2D structure GA chromosome is used to fit NSGA-II into the particular case study.

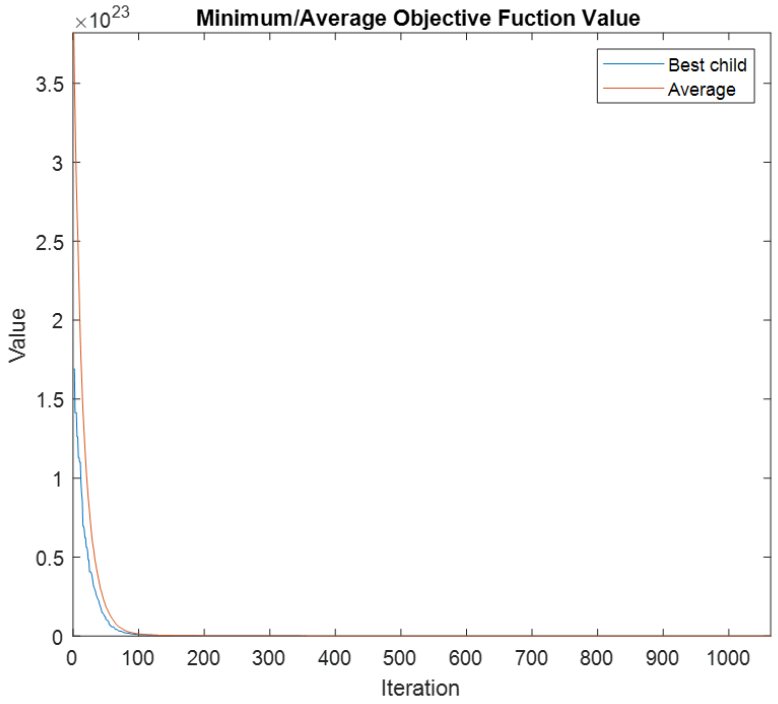
Due to the different design of GA chromosome structure, the crossover and mutation probability used in the quantum-entanglement inspired method and the two classical methods cannot be unified for comparison purpose, thus their corresponding best parameter are used. Using the same population size of 1875 and maximum iterations of 300 selected by the 2D-GA method, the results of shift coverage and convergence plots via the three methods are obtained and shown in Figure 33, with detailed results in Table 7.



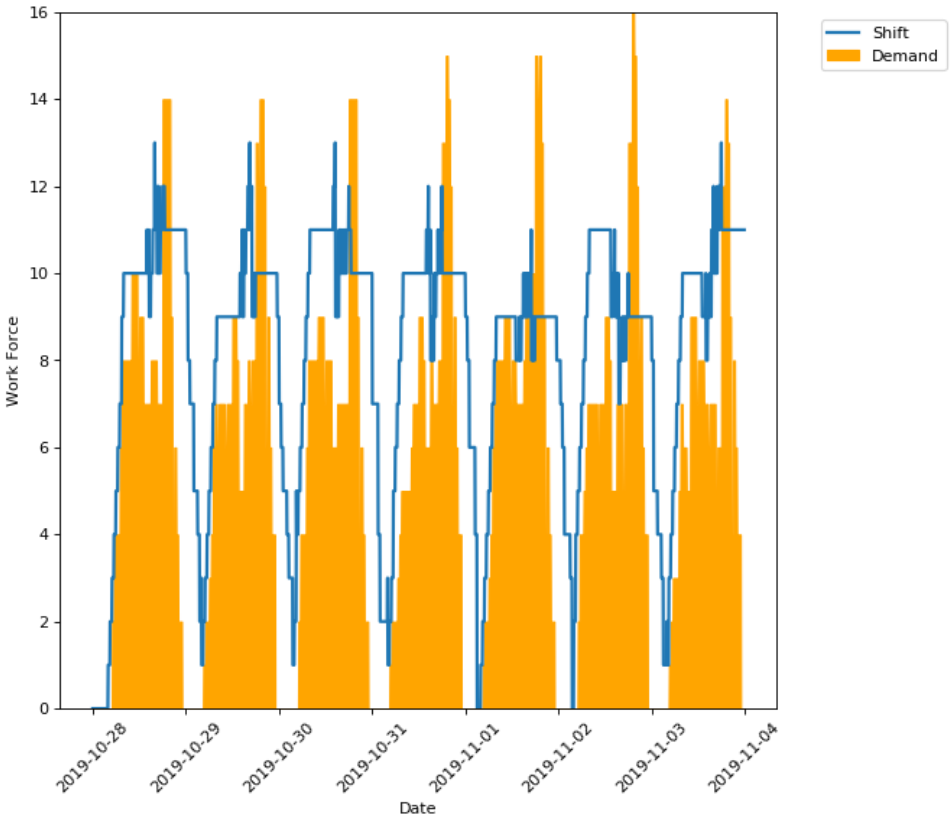


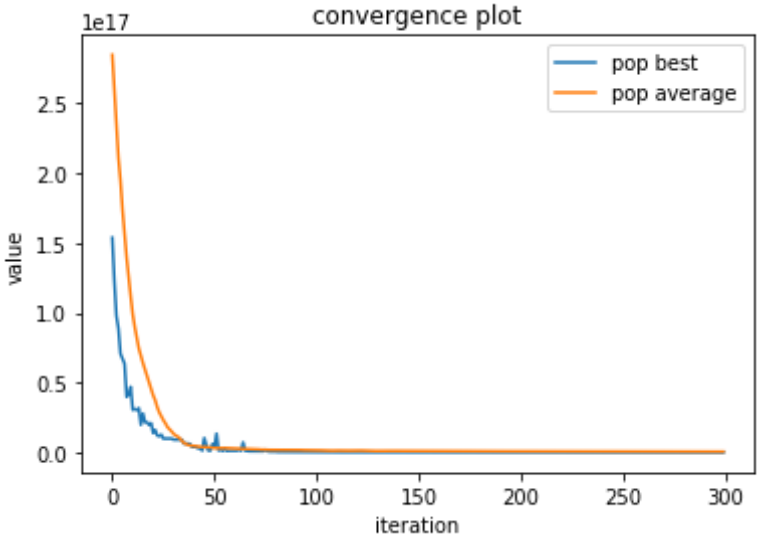
(a) Shift Convergence Result and Convergence Plot using QEI-GA





(b) Shift Convergence Result and Convergence Plot using 2DGA





(c) Shift Convergence Result and Convergence Plot using NSGA-II

Figure 33. Results of a 7-day Planning Task

Table 7. Detailed Results Comparison

	Best Fitness Value	No. Iteration at Convergence
QEI-GA	6.8438×10^{12}	~20
2D-GA	1.6205×10^{13}	~100
NSGA-II	1.7656×10^{13}	~50

Noticeably, QEI-GA converges significantly faster than 2D-GA and NSGA-II, while the best fitness value obtained is also better. It also can be seen that, unlike the two classical GA-based algorithms, QEI-GA consistently maintain higher diversity in the population. The underlying quantum mechanism of QEI-GA enables the efficient search with higher population diversity, and thus it might be able to reduce the requirement of population size to a great extent. The fact is, even with a commonly considered "small" population size 50, QEI-GA can still converge rapidly (shown in Figure 34) and obtained the best fitness value 7.5532×10^{12}, which is only about 10.36% worse than the best result obtained using a more than 300 times larger population size 1875. Therefore, the hypothesis is that QEI-GA only requires very small population size to obtain optimal or near-optimal solution within small number of iterations.

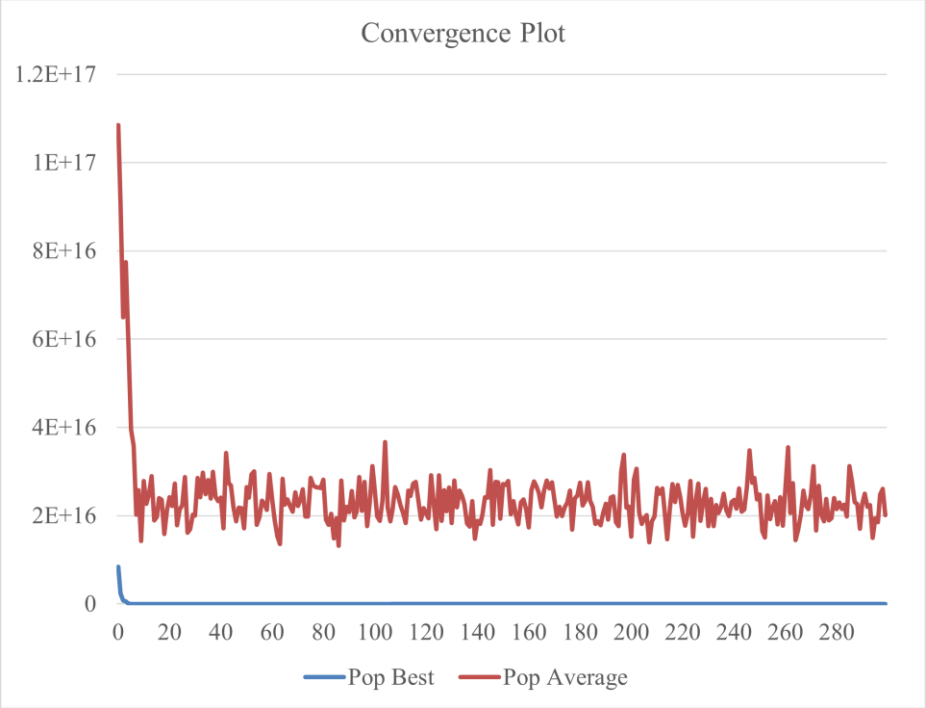


Figure 34. Convergence Plot of QEI-GA using Population size of 50

6.5.3.2 Exploration-Exploitation Behavior Analysis

Next, the analysis of the exploration-exploitation behavior is done and measured by the dimension-wise diversity measurement (Hussain et al., 2019), which treats the entire population as a whole and thus a good performance index for the population-based algorithms. The calculation of the dimension-wise diversity Div in the population of size n is given as:

$$Div_j = \frac{1}{n}\sum_{i=1}^{n}\left|median(x^j) - x_i^j\right| \tag{38}$$

$$Div = \frac{1}{D}\sum_{j=1}^{D} Div_j \tag{39}$$

where $median(x^j)$ is the median of dimension j in the population and it indicates the center of the population, x_i^j is the dimension j of the individual i , D is the dimension size of the solutions.

Once the population diversity of each iteration is captured, the percentage of exploration Xpl and the percentage of exploitation Xpt can be determined:

$$Xpl = \frac{Div}{\max\limits_{1 \le j \le D}(Div_j)} \times 100\% \tag{40}$$

$$Xpt = \frac{\left| Div - \max\limits_{1 \le j \le D}(Div_j) \right|}{\max\limits_{1 \le j \le D}(Div_j)} \times 100\% \tag{41}$$

Figure 35 demonstrates the visual tendency of exploration and exploitation in QEI-GA. It can be seen that, QEI-GA applies around 40%:60% exploration-exploitation ratio, which is a relatively balanced proportion assignment.

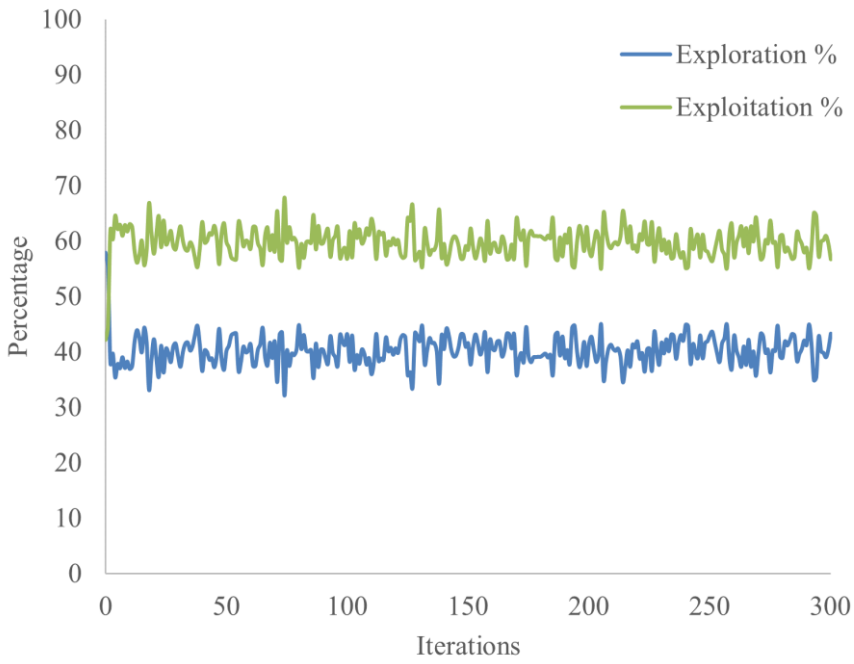


Figure 35. Exploration-Exploitation Behavior of QEI-GA

6.5.3.3 Robustness Test

Additionally, the robustness of the algorithm to the hyperparameters change is tested. Since the circuit parameters are treated as optimization variables in the unconstrained classical GA section, the hyperparameters of the quantum entanglement inspired algorithm are just limited to that of classical GA, namely, the population size, the crossover and mutation probabilities, and the maximum number of iterations (if it is used as the termination condition). Generally speaking, in the classical GA, the selection of crossover and mutation probabilities can be done based upon some simple guidelines or can be obtained from error-and-trial method, while increasing the population size and maximum iteration number can enlarge the search space, thus it is known as an effective way to enhance the probability of reaching better solutions. Since the quantum representation naturally carries more information than the conventional method, the test is

designed to see if this advantage is sufficient to obtain a better solution even with a much smaller population size. Four different scale of population size settings are shown in Table 8 and with each setting QEI-GA is ran for consecutive 10 repetitions to get an understanding of its robustness. Two types of performance measure are considered in the result analysis: best fitness value obtained, and the number of iterations at which the best result is obtained. The results obtained are shown in Figure 36 in the form of box-and-whisker plot.

Table 8. Different Scale of QEI-GA Population Size Settings

Setting	L-01	L-02	M	H
Population Size	50	100	300	500

From Figure 36, it is observable that increasing the population size actually has no significant improvement to the result performance over the 10 repetitions. This is possibly caused by the reason that quantum representation is able to introduce exponentially higher diversity and stochasticity to the population, and thus broadening the search horizon coherently compared to the conventional method of increasing population size and number of iterations. Therefore, choosing a practical small population size and maximum iteration numbers is still an effective way to get optimal solutions, given the limitation of time or computation resource.

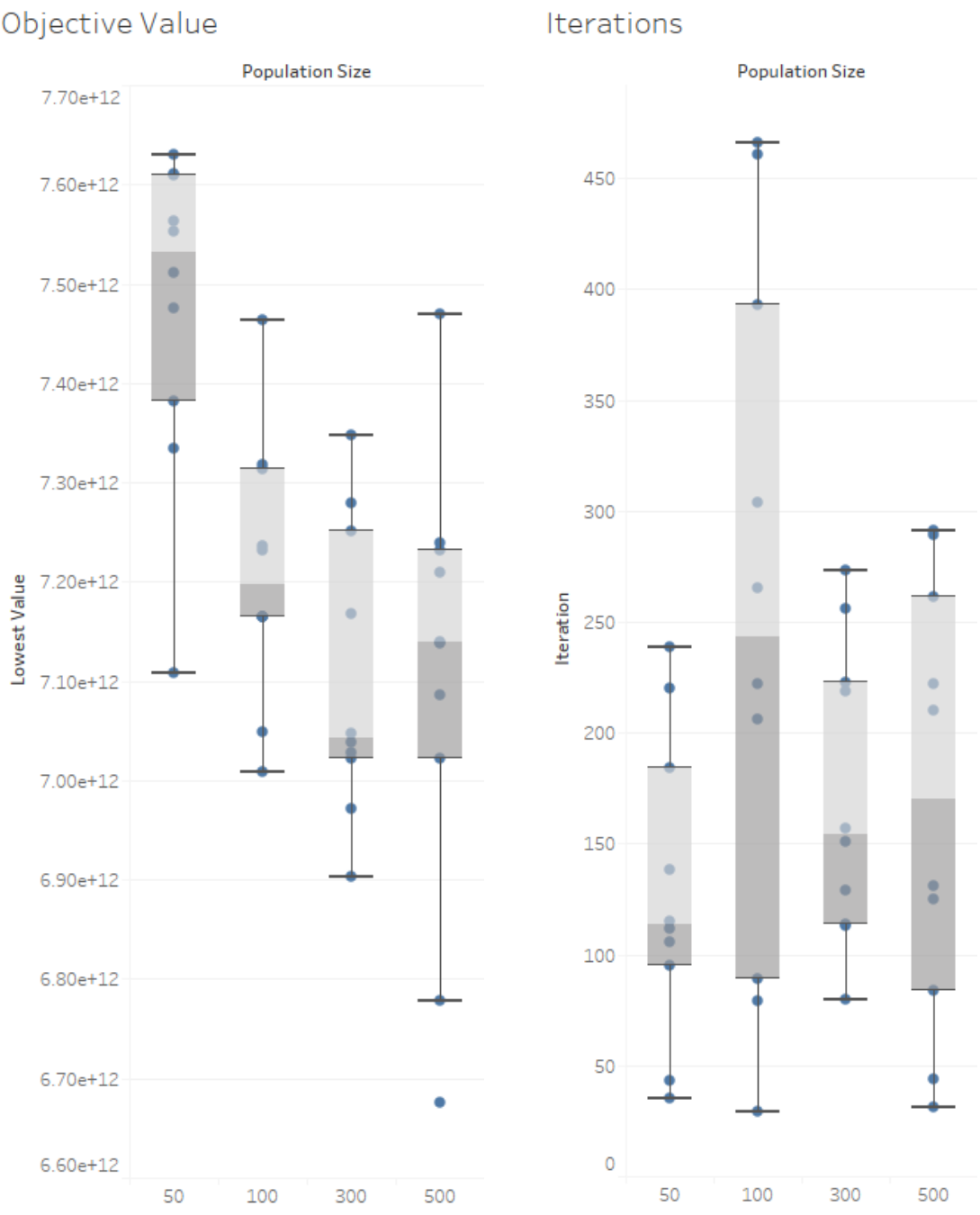


Figure 36. Box-and-whisker Plots of QEI-GA Results using Different Scale of Population Size Settings

6.6 Lightweight Application to Balanced Nurse Scheduling

6.6.1 Problem Context

Personnel scheduling copes with the allocation of work tasks, possibly physical locations and other resources to people. The studies regarding personnel scheduling problems have been conducted widely in the past several decades. Recently, due to the world-wide labor shortage and the corresponding economic considerations associated with the long-lasting influence of the pandemic, personnel scheduling has attracted significantly increasing attention in both research and practice. As for many workplaces, implementing an optimal personnel schedule is not only beneficial for economic considerations but also for providing solid service quality and remaining competitive in labor market (Porto, et al., 2019). Particularly, the healthcare industry has witnessed enormous pressures to meet the unusual high patient demand with the balancing constraints associated with increasing request of fairness in the work environments.

The benchmark instances used here are from the public benchmark problem library CSPLib, under the category of "Prob069: Balanced Nursing Workload Problem". The benchmark instances provided by CSPLib are of relatively small scale, with the number of nurses being 3 or 5, 17-33 patients all in one zone are grouped into 5 types and has the acuity associated with each patient type being nurse dependent. None of the patient is out of the capability of any nurse.

As it mentioned earlier, the optimization task of such problems is usually to minimize the total workload and workload standard deviation. The constraint that the number of patients a nurse is responsible should remain in a certain value range ($\forall j \in \{1, \dots, m\},\ C_{min} \leq \sum_{i=1}^{n} c_{i,j} \leq C_{max}$), is more of a preference and can be optimized simultaneously with the objectives, thus this constraint is treated as a penalty function

added to the objective function. Therefore, the mathematic modelling is then updated to the following:

$$Min\ [\alpha * \sigma\{\sum_{i=1}^{n} c_{i,1} * a_{i,1}, \dots, \sum_{i=1}^{n} c_{i,m} * a_{i,m}\} + \beta * \sum_{j=1}^{m}\sum_{i=1}^{n} c_{i,j} * a_{i,j} + \gamma$$

$$* \sum_{j=1}^{m} \max(0, (\sum_{i=1}^{n} c_{i,j} - C_{max}), (C_{min} - \sum_{i=1}^{n} c_{i,j}))^2]$$

s.t.

- $c_{i,j} = \begin{cases} 1, & N_i = j \\ 0, & N_i \neq j \end{cases}, \forall i \in \{1, \dots, n\}, N_i \in \{1, \dots, m\}$
- $\sum_{j=1}^{m} c_{i,j} = 1, \forall i \in \{1, \dots, n\}$

The goal is to obtain the patient-nurse assignment set $\{N_1, \dots, N_i, \dots, N_n\}$ that can minimize the workload standard deviation among nurses (primary target), the total workload, and deviation of number of patients each nurse being assigned away from the preference range, as well as following all the hard constraints. Therefore, the weights of the multiple objectives are set as $\alpha = 1, \beta = 0, \gamma = 99$. When the output result has no violation of the constraint in number of patients per nurse, the fitness value equals to the standard deviation σ among nurses.

6.6.2 Modelling and Implementation of LQIGA

In the application of this group of benchmark instances, the lightweight solution is to employ single parameter-controlled quantum circuit to represent nurse assignment. Obviously, neither 3 nor 5 can be represented by 2 to the power of an integer, thus the quantum circuits require the usage of controlled Hadamard gate with the control qubit

corresponding to the qubit in the chromosome. The detailed implementation of lightweight qubit-encoded chromosome and quantum circuits is shown in Figure 37.

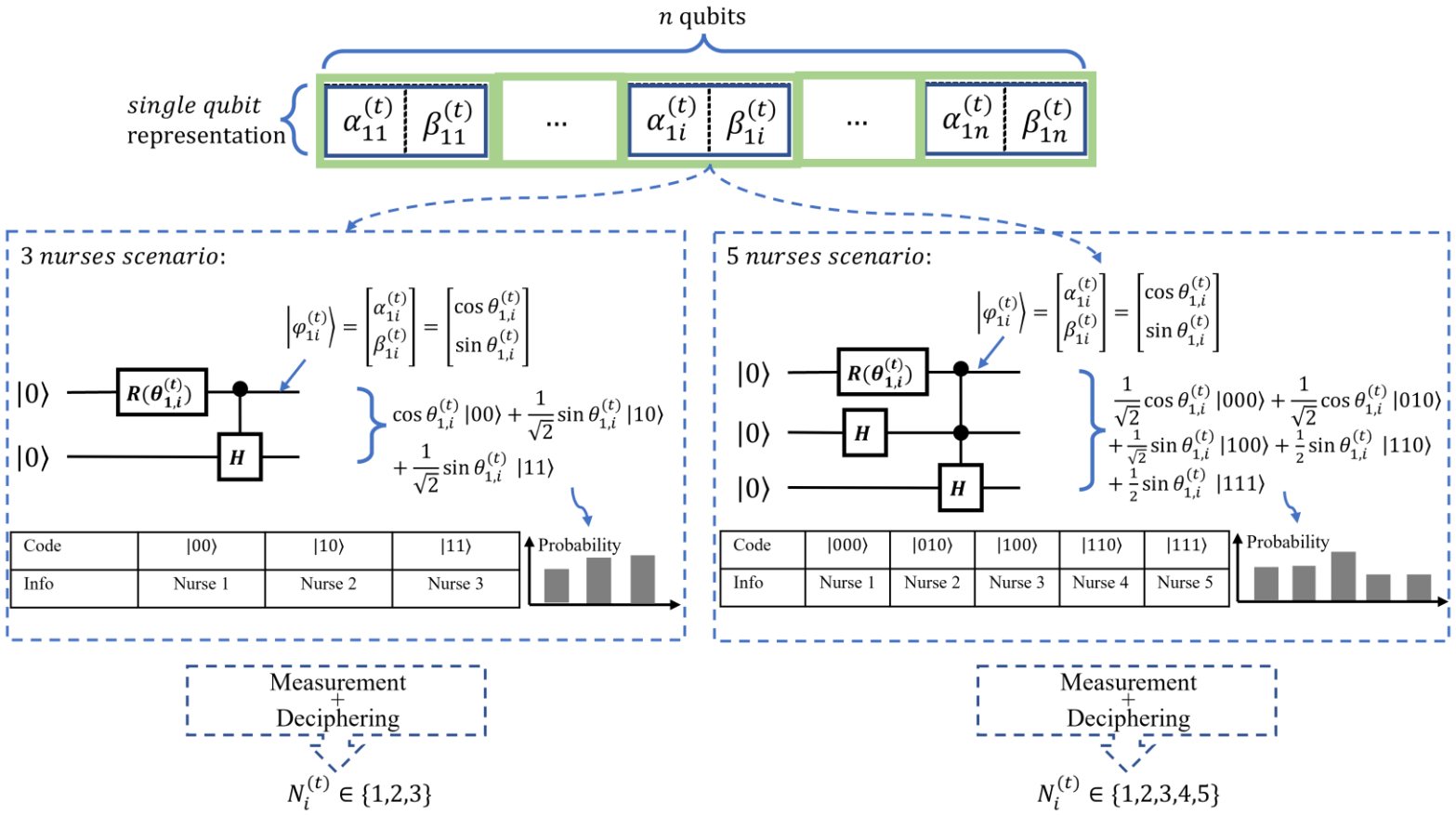


Figure 37. Lightweight Qubit-encoded chromosome with Case Specific Quantum Circuits

The above lightweight qubit encoding method can guarantee the constraints that every patient has one and only one assigned nurse, additionally, the usage of quantum entanglement circuit ensures the exact number of posterior states, thus no repair operation is even required in the following optimization process.

6.6.3 Results and Analysis

The parameter setting used in the benchmark instances experiment are shown in Table 9, the population size and number of iterations are chosen to achieve optimal or near-optimal solution within reasonable time, and the rest of parameter values are results based on trial-and-error. Each instance is tested for 15 repetitions in order to verify the effectiveness and robustness. The basic information of each instance, the best results obtained for each instance, and the 95% confidence interval (CI) over 15 repetitions for each instance, which consists of the sample mean value and the CI halfwidth value, are given in Table 10. According to the results shown in Table 10, the proposed LQIGA can effectively solve the 6 benchmark instances by achieving the optimal or near optimal results consistently.

Table 9. Parameter Setting used in the Benchmark Testing

Parameter	Population size	No. Iterations	Elite Rate	Crossover Rate	Mutation Rate	Rotation Angle Threshold
Value	500	500	0.1	0.85	0.4	0.01π

Table 10. Results from the Benchmark Instances

Instance	3nurse5patientType0	3nurse5patientType3	3nurse5patientType5	5nurse5patientType0	5nurse5patientType3	5nurse5patientType5
No. Nurse	3	3	3	5	5	5
No. Patient	17	22	23	26	32	33
No. Patient Type	5	5	5	5	5	5
$[C_{min}, C_{max}]$	[4, 8]	[4, 8]	[4, 8]	[4, 8]	[4, 8]	[4, 8]
Best Result	0	0	0	0.40	0.40	0.89
95% CI	0 ± 0	0 ± 0	0.031 ±0.067	0.921 ±0.281	0.903 ±0.327	1.448 ±0.193

6.7 Chapter Summary

The emerging quantum computing paradigm provides some unconventional but promising directions for computational problem solving, however, the practical and in-depth applications of quantum physics concepts and mechanism into engineering problem solving are still in an early stage. This chapter provides a promising attempt to solve operations engineering optimization problem in order to inspire further research interests into this field.

The proposed quantum entanglement inspired hard constraint handling approach provides a novel insight of discrete constrained optimization problem solving. First of all, different from the conventional representations, the quantum entanglement inspired representation of constraint relationship aims to map the original optimization variables with the hard constraints into unconstrained new variables through the quantum circuit, which reduces the difficulty of optimization modelling. Secondly, the qubit encoding method allows exponentially higher information density in the representation, thus helping broaden the search horizon significantly and maintain population diversity even with a much smaller population size. The efficient exploration of solution space enables a better exploration-exploitation balance, since the extra computation resources can be assigned to local search refinement if available. Lastly, the mechanism of quantum entanglement assures the feasibility of candidate solutions during the entire optimization process, which aligns with the requirement of practical applications. An example of assembling this proposed approach with the existing optimization strategy GA into QEI-GA was given to demonstrate its practical usability.

By embedding the quantum entanglement inspired hard constraint handling approach in GA, the proposed algorithm QEI-GA is designed to solve operations engineering optimization problems. The application of QEI-GA to a real-world airport shift planning case study shows that QEI-GA can obtain a better solution with a much smaller population size and with fewer iterations when compared to a case-tailored algorithm 2D-GA using penalty function and a multi-objective algorithm NSGA-II using constraint violation as additional objective.

Similarly, a lightweight quantum inspired genetic algorithm (LQIGA) for the constrained combinatorial optimization problem solving in the domain of personnel scheduling is proposed. Specifically, this method aims to provide a lightweight decision support for small scale personnel scheduling problems, where the term "lightweight" means LQIGA uses a much simpler chromosome structure (one dimension, unconstrained) comparing to the classical encoding method of complex chromosome data structure for constraint representation, yet still be able to effectively represent problem-specific constraints in the chromosome with flexibility and leverage the power of qubit representation to maintain high population diversity and thus potentially better optimization performance. The lightweight qubit-encoded chromosome structure also reduces the efforts required for the corresponding operations of the algorithm, and thus provides agile decision support for small scale personnel scheduling scenarios, such as the balanced nurse scheduling issue in a small nursery. Based on the experimental result of applying the proposed algorithm on benchmark instances of balanced nurse scheduling problem from CSPLib, the effectiveness of the algorithm can be validated, since it can

always achieve optimal or near-optimal solutions with the 95% confidence interval of the results over 15 repetitions staying within reasonable range.

CHAPTER 7. HYBRID QUANTUM INSPIRED SEMANTIC NEURAL NETWORK FOR DOMAIN CONTEXT-AWARE INTELLIGENT LEARNING

This chapter presents a novel quantum inspired neural network model consisting of quantum inspired semantic and classical neurons. The quantum inspired semantic neurons are used to represent domain knowledge in the form of semantic network and embed the domain knowledge in the neuron structure for data processing. The proposed structure can leverage the power of quantum superposition and maturity of classical artificial neural network techniques. The effectiveness, robustness, and computational performances of the proposed hybrid quantum inspired semantic neural network (HQISNN) are tested through applications of two engineering case studies: (1) a machine predictive maintenance case and (2) a customer segmentation case. The proposed model is also compared to a classical backpropagation neural network model with the same number of hidden layers and neurons to demonstrate the potential benefits of domain context-aware learning in engineering decision-making applications, which require very specific case-dependent domain knowledge.

7.1 Quantum Inspired Semantic Neuron Modelling

The quantum inspired sematic neuron is the key component of the HQISNN model as it has some domain knowledge embedded. In the example shown in Figure 38, the n input attributes can be grouped into d categories in the form of sematic network to represent

the underlying domain knowledge associated with the input attributes. These attributes that belong to the same category should be given some group attributes before the almost "black-box" manner of information processing in the classical neural network framework.

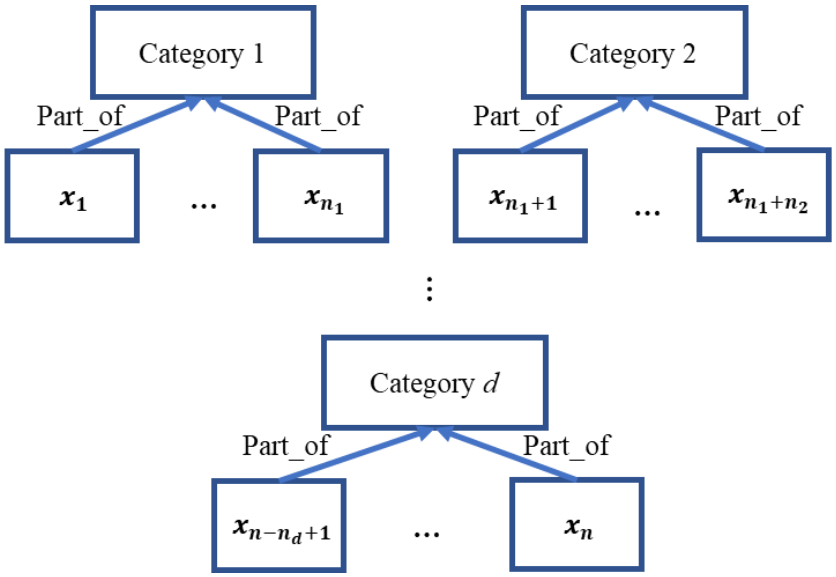


Figure 38. A Sematic Network Example

The original value of the attributes, of course, could not be processed by the quantum inspired neuron directly, they need to be first transformed into qubit representation using similar idea from a classical normalization method. The original value is normalized to the range of [0, 1] based on the minimal and maximal value existed in the dataset, the normalized value is then multiplied by a constant $\frac{\pi}{2}$ to adjust the range to [0, $\frac{\pi}{2}$], which can then be used as the angle parameter in qubit representation. Suppose that the *k*th sample in *n*-dimension input space $\{X^k\} = [\{x_1^k\}, \dots, \{x_i^k\}, \dots, \{x_n^k\}]^T$, where $k = 1, \dots, M$, M is the total number of samples in the given dataset. The corresponding pre-process of the original input attribute is given as follow:

$$\{|X^k\rangle\} = [\{|x_1^k\rangle\}, \dots, \{|x_i^k\rangle\}, \dots, \{|x_n^k\rangle\}]^T \tag{42}$$

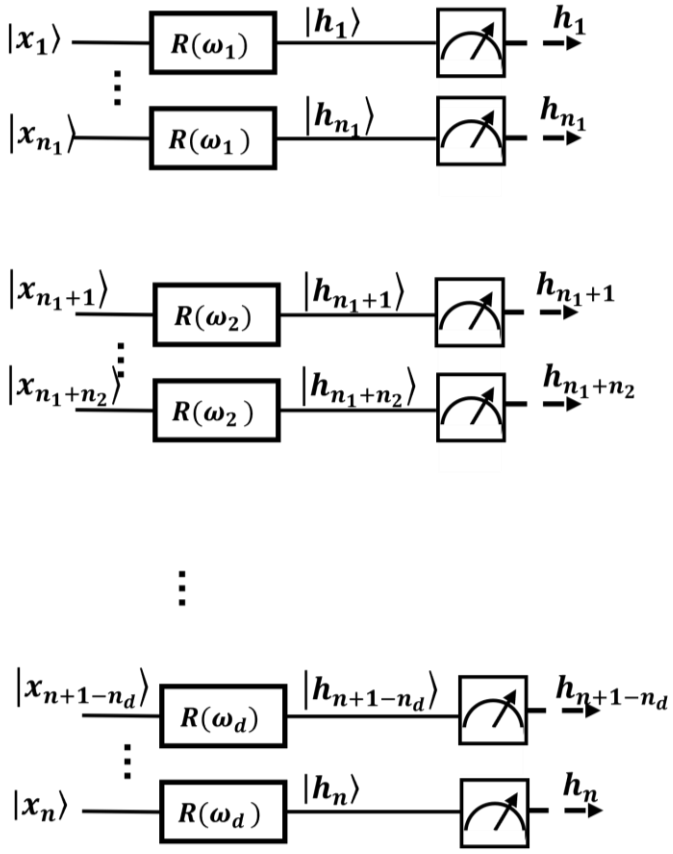
$$|x_i^k\rangle = \cos\theta_i^k\,|0\rangle + \sin\theta_i^k\,|1\rangle, i = 1, \dots, n, k = 1, \dots, M \tag{43}$$

$$\theta_i^k = \frac{\pi}{2} \times \frac{x_i^k - \min\{x_i^1, \dots, x_i^M\}}{\max\{x_i^1, \dots, x_i^M\} - \min\{x_i^1, \dots, x_i^M\}} \tag{44}$$

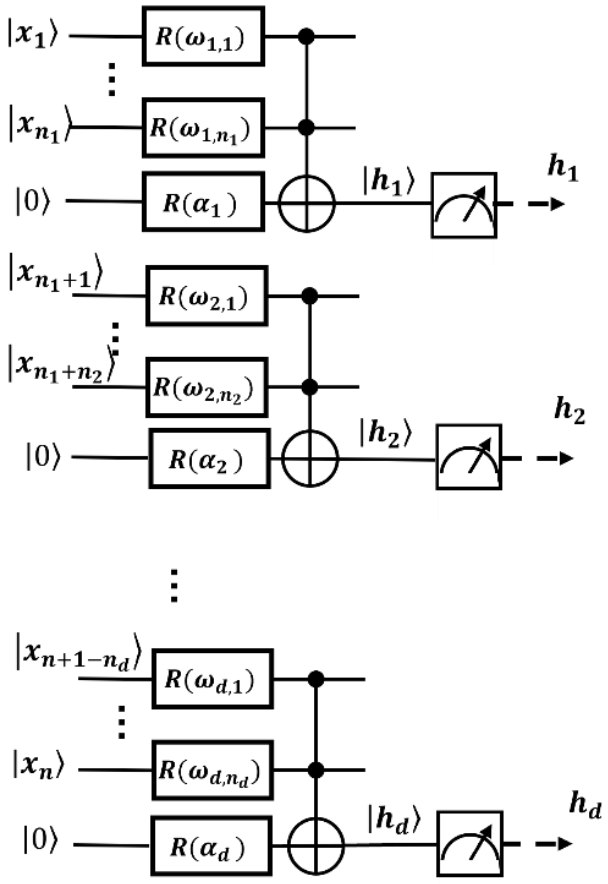
To match with the defined output value of the quantum inspired sematic layer and the follow-up classical neural layers, the output values also need to be normalized correspondingly. Suppose that the *k*th sample in *m*-dimension out space $\{Y^k\} = [\{y_1^k\}, \dots, \{y_j^k\}, \dots, \{y_m^k\}]^T$, where $k = 1, \dots, M$. The normalization of the original output values is given by:

$$\hat{y}_j^k = \frac{y_j^k - \min\{y_j^1, \dots, y_j^M\}}{\max\{y_j^1, \dots, y_j^M\} - \min\{y_j^1, \dots, y_j^M\}}, j = 1, \dots, m. \tag{45}$$

After the preprocessing stage, these input variables would go through the quantum inspired sematic neuron. There are two forms of quantum inspired sematic neurons can be applied here, as shown in Figure 39.



(a) Type I: Neurons with Shared Parameter



(b) Type II: Neurons with Shared $C^n(X)$

Figure 39. Quantum Inspired Sematic Neurons

The type I quantum inspired semantic neuron (Figure 39 (a)) is a single input and single output unit without quantum entanglement, each input passes through a single qubit rotation gate where these input attributes that belong to the same sematic category share the same rotation parameters. The corresponding output of those neurons are given by:

$$|h_i\rangle = \cos(\theta_i + \omega_s)\,|0\rangle + \sin(\theta_i + \omega_s)\,|1\rangle, where\ x_i \in category\ s,$$
$$i = 1, \dots, n, s = 1, \dots, d. \tag{46}$$

$$h_i = \sin(\theta_i + \omega_s) \tag{47}$$

The type II quantum inspired semantic neuron (Figure 39(b)) consists of multi-qubit controlled-NOT gates, where the control qubits of each gate are associated with the same sematic category. Each control qubit $|x_i\rangle$ passes through an independent single qubit rotation gate $R(\omega_{s,j})$ first, and the joint result of the control qubits operates on the target qubit and then generates output. The corresponding output of those neurons are given by:

$$|x_i'\rangle = \cos\left(\theta_i + \omega_{s,j}\right)|0\rangle + \sin\theta_i\,|1\rangle, where\ x_i \in category\ s.$$
$$i = 1, \dots, n, j = 1, \dots, n_s, s = 1, \dots, d. \tag{48}$$

$$|h_s\rangle = \sqrt{1 - P_s}|0\rangle + \sqrt{P_s}|1\rangle \tag{49}$$

$$h_s = P_s = (\sin\alpha_s)^2 - \left[\left(\prod_{j=1}^{n_s} \sin(\theta_i + \omega_{s,j})\right)\sin\alpha_s\right]^2 + \left[\left(\prod_{j=1}^{n_s} \sin(\theta_i + \omega_{s,j})\right)\cos\alpha_s\right]^2 \tag{50}$$

The two types of quantum inspired sematic neurons can be used solely or mixed to generate the quantum inspired sematic layer according to the specific application scenarios. The advantage of type I neuron is that the output is a simple function of the training parameter and thus can be trained using classical learning methods like gradient-based algorithms. As a comparison, type II neuron tries to leverage the power of quantum entanglement and its output is a more complicated function of the training parameters.

Thus, the learning associated with the type II neurons can view the entire quantum inspired neuron as a black box and calculate the gradient using the parameter shift rule (Crooks, 2019). Another approach for training the type II neurons is to use other algorithms that are not based on gradient, such as heuristic based optimization algorithms.

7.2 Hybrid Quantum Inspired Semantic Neural Network (HQISNN)

The HQISNN model is a hybrid model of quantum inspired semantic layer and classical fully connected layers, where the quantum inspired semantic layer is based on the domain knowledge associated with the input attributes and can be constructed using type I or type II quantum inspired semantic neurons. A HQISNN model with pure type I and type II neurons are shown in Figure 40 and Figure 41 separately. In a practical scenario, the two types of quantum inspired semantic neurons can be mixed and used, and the best practice can be case dependent.

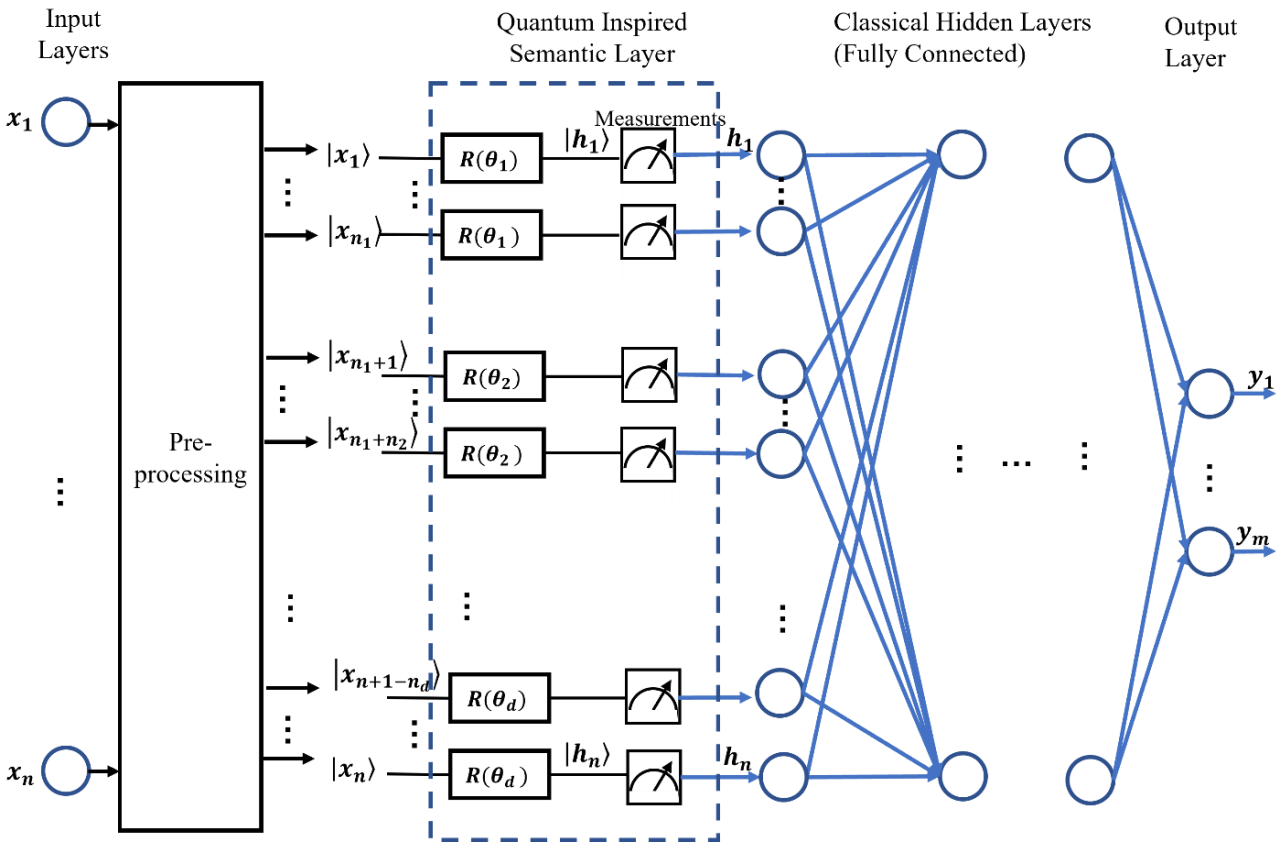


Figure 40. Structure of the HQISNN Model using Type I Neurons

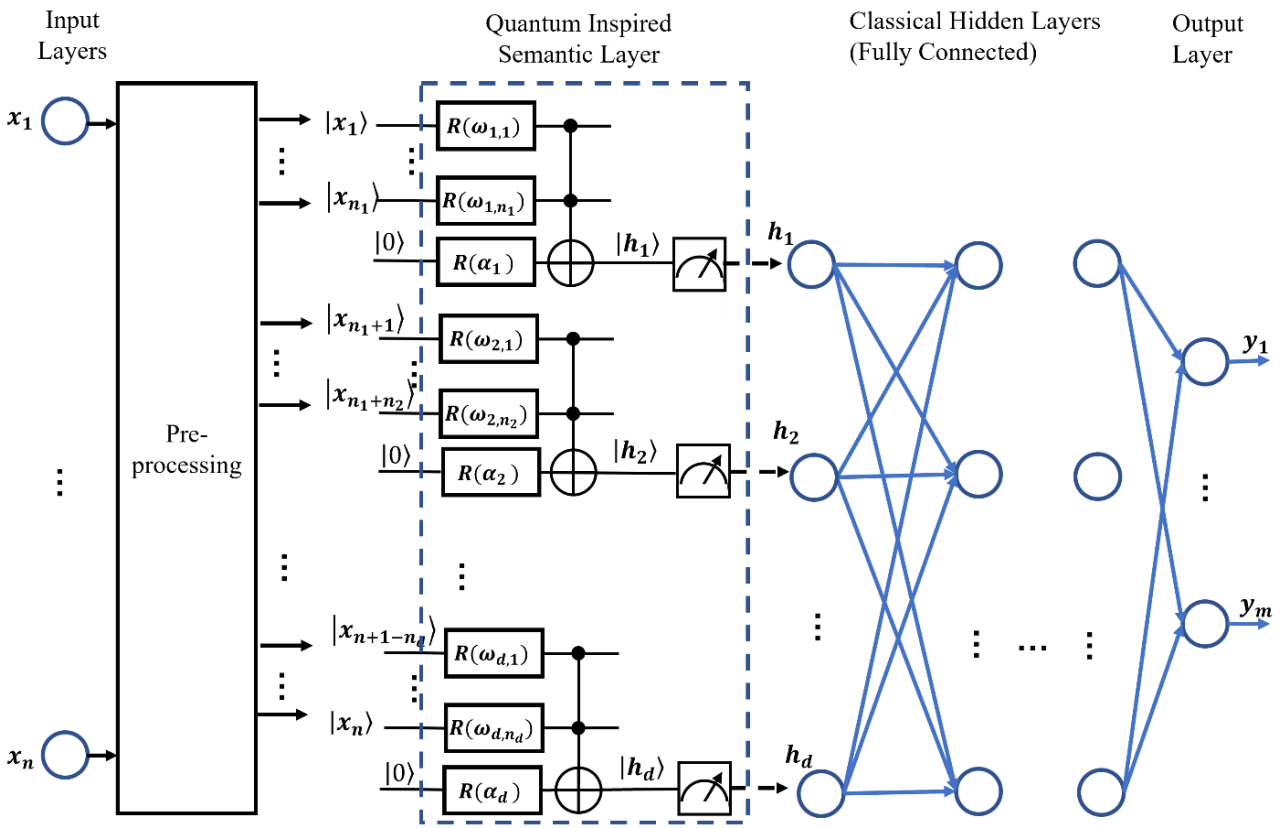


Figure 41. Structure of the HQISNN Model using Type II Neurons

Based on the description above, when the machine learning task in a specific domain application is given as well as the corresponding dataset, the workflow of conducting domain context-aware learning and obtaining the prediction model using the proposed HQISNN model is shown in Figure 42.

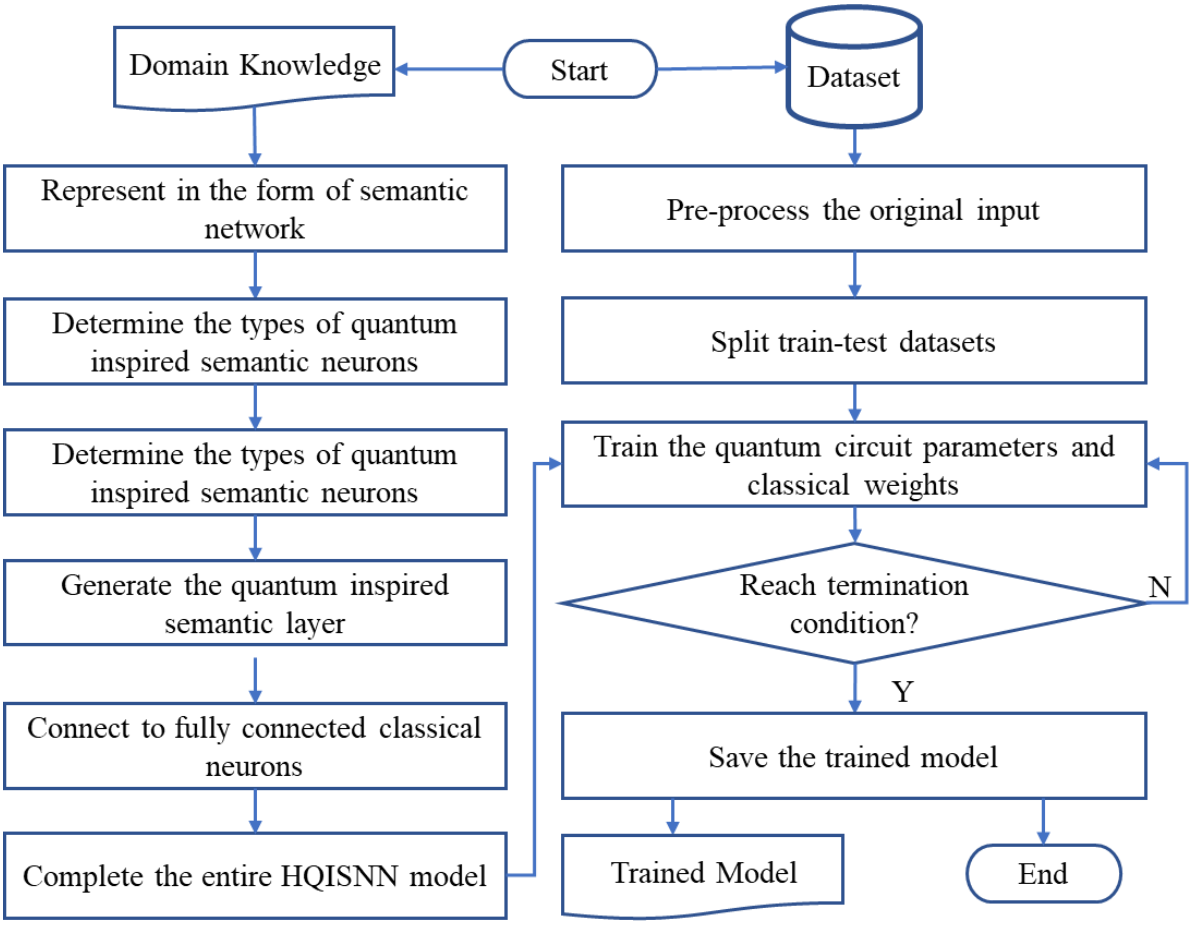


Figure 42. Workflow of Domain Context-aware Learning using the HQISNN Model

7.3 Applications to Predictive Machine Maintenance

7.3.1 Problem Context

Predictive maintenance refers to the intelligent monitoring of equipment to avoid future failures using advanced signal processing and pattern recognition techniques

(Paolanti et al., 2018), for instance artificial neural networks. Predictive maintenance largely relies on the collected data from sensors and analysis algorithms. In this case study, a public dataset (Dua and Graff, 2019) from UCI machine learning repository is used. The dataset consists of 10,000 data points with 7 input attributes ($\{x_1, x_2, \dots, x_7\}$), which include attributes describe different aspects of the conditions, and 1 output target, which indicates whether a failure was detected later. The domain knowledge indicating the categorization of the input attributes in the form of semantic network is given in Figure 43.

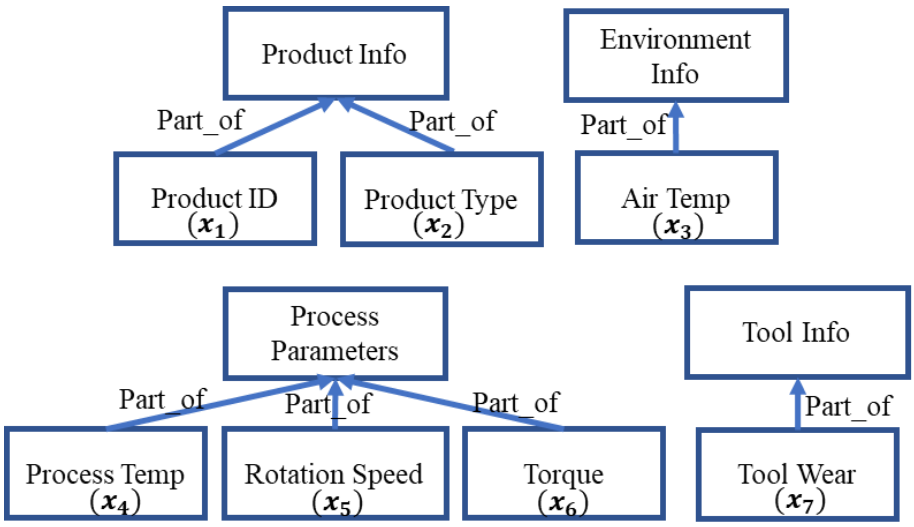


Figure 43. Sematic Network in the Machine Predictive Maintenance Case

7.3.2 Modelling

Based on the domain associated semantic network, the structure of the quantum inspired sematic layer can be constructed by using a mix of type I and type II quantum inspired sematic neurons, as shown in Figure 44. The quantum inspired semantic layer here would map the initial 7 input attributes $\{x_1, x_2, \dots, x_7\}$, to 4 intermediate outputs $\{h_1, h_2, h_3, h_4\}$, based on the prior knowledge represented by the corresponding semantic

network. The intermediate outputs are then delivered to next neural network layer, which consists of classic neurons, until the final output is reached.

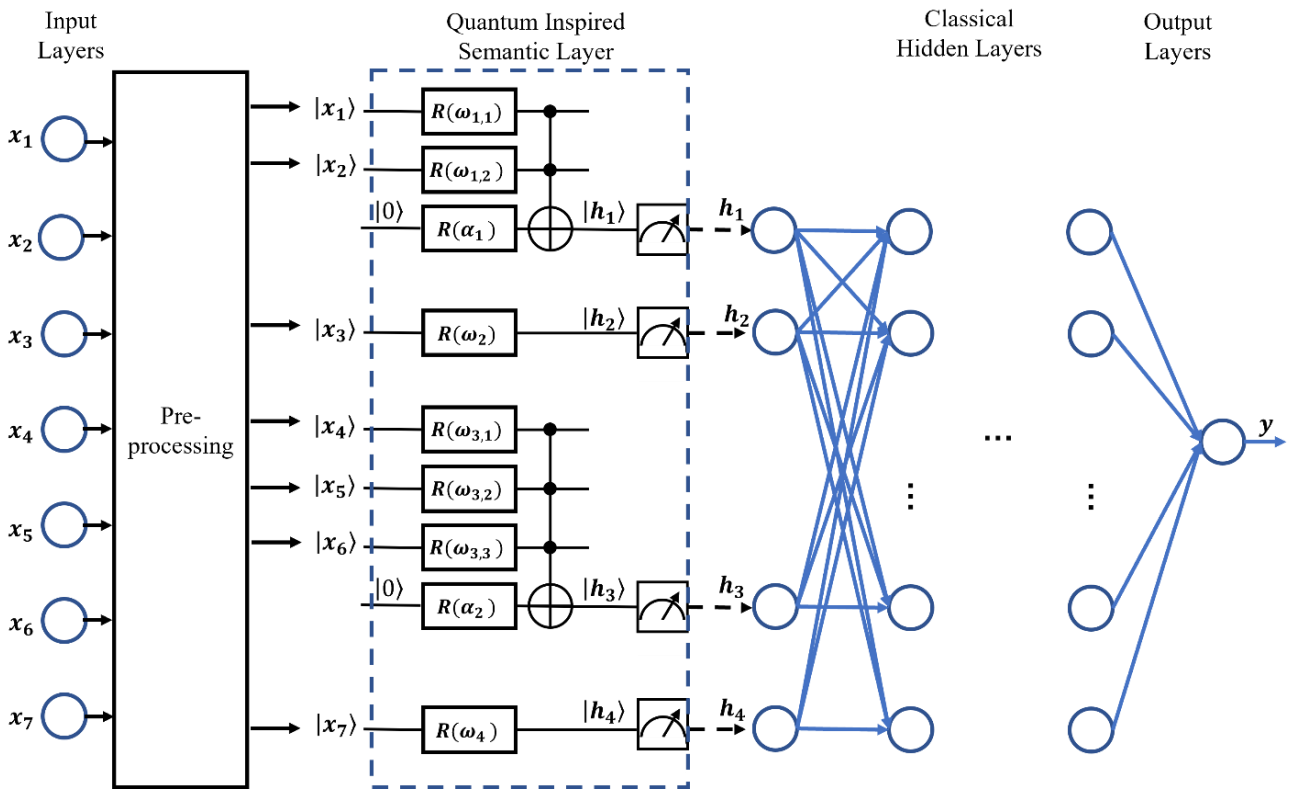


Figure 44. HQISNN Model for the Machine Predictive Maintenance Case

7.3.3 Results and Analysis

For the purpose of model testing, it is necessary to split the original data set into training data set and testing data set. However, due to the nature of machine breakdown happening in a real-world scenario, this dataset is heavily imbalanced, with 97% of data points have the output of "No Failure". The condition of data imbalance is handled using oversampling technique (Mohammed et al., 2020). Additionally, the creation of training-testing data sets was carefully conducted to ensure the similar distribution with a training-testing split ratio of 80%-20%. The cost function used here is cross-entropy function, as given below:

$$cost(y, \hat{y}) = -\sum_{i} y_i \log \hat{y_i} \tag{51}$$

The desired model here for machine predictive maintenance obviously has a preference on higher fraction of relevant instances being retrieved, since a failure case failed to be predicted can cause practically more expensive consequence. Thus, the performance measurement metric used here is sensitivity (also known as recall), which is used to measure the fraction of positive patterns that are correctly classified (Hossin and Sulaiman, 2015), as given below:

$$sensitivity = \frac{true\ positive}{true\ positive + true\ negative} \times 100\% \tag{52}$$

The number of follow-up classical hidden layers of HQISNN is set to 2. The performance results of HQISNN on the testing set over 16 repetitions was compared to that

of a fully connected classical backpropagation neural network (BPNN) model with same number of hidden layers and neurons, as shown in Table 11. The convergence behaviors comparison is given in Figure 45.

Table 11. Performance Comparison of the proposed HQISNN Model from a Similar Classical BPNN Model in Predictive Maintenance Case Study

Model	Learning Method	Num. Iterations	Avg. Performance Measure on Training (*sensitivity*)	Avg. Performance Measure on Testing (*sensitivity*)	Best Performance Measure on Testing (*sensitivity*)
HQISNN	Gradient Descent	2500	84.7%	96.6%	97.1%
BPNN	Gradient Descent	2500	88.1%	90.4%	96.6%

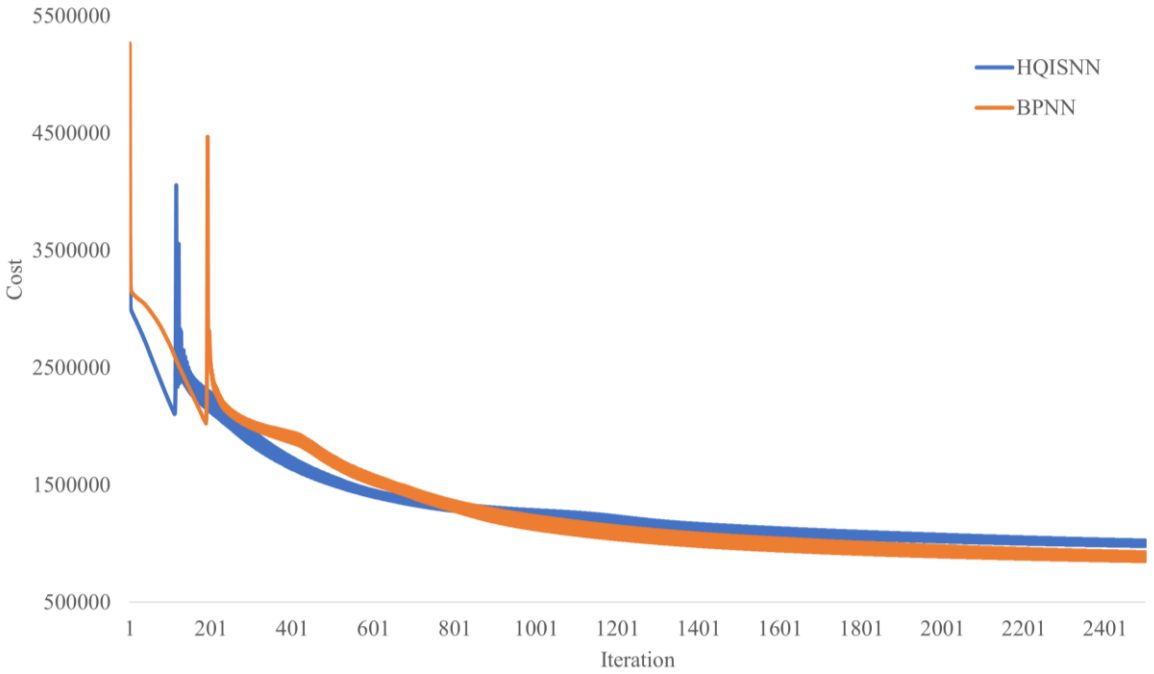


Figure 45. Comparative Convergence Behavior of the two Models during Training

The best performance measure results on the testing set of the two models are close, with the proposed model slightly better. However, the average performance over 16 repetitions for the HQISNN model is as good as the best performance the BPNN model can reach over the same 16 repetitions, and only 0.5% lower than the best performance HQISNN model can reach, which demonstrates the consistency and robustness of the proposed HQISNN model. Also, the proposed HQISNN model has an about 6.9% increase on the average performance on the testing set, while its average performance on the training set has a slight decrease, which indicates a higher generalization ability of the HQISNN model.

The convergence behaviors of the two models are very similar, which is probably due to the fact that both models applied gradient descent algorithm for training, and the majority of HQISNN model is still a classical neural network structure. However, it is noticeable that the convergence plot of HQISNN has a horizontal shift left comparing to that of BPNN, which indicates a faster convergence speed for HQISNN.

7.4 Applications to Customer Segmentation

7.4.1 Problem Context

The decision-making support to the manufacturing industry requires machine learning procedure for appropriate customer segmentation, due to the complexity and uncertainty in the market, in order to build characterized manufacturing solutions tailored to the specific customer profile (Simeone et al., 2021). In this case study, a public dataset (Kuila, 2021) from Kaggle is used. The dataset consists of 10,695 data points with 8 input attributes ($\{x_1, x_2, \dots, x_8\}$), which include attributes describe different aspects of the

customer profiles, and the output target is to find out which customer segment of the given customer should be assigned to (4 possible segments in total). The domain knowledge indicating the categorization of the input attributes in the form of semantic network is given in Figure 46.

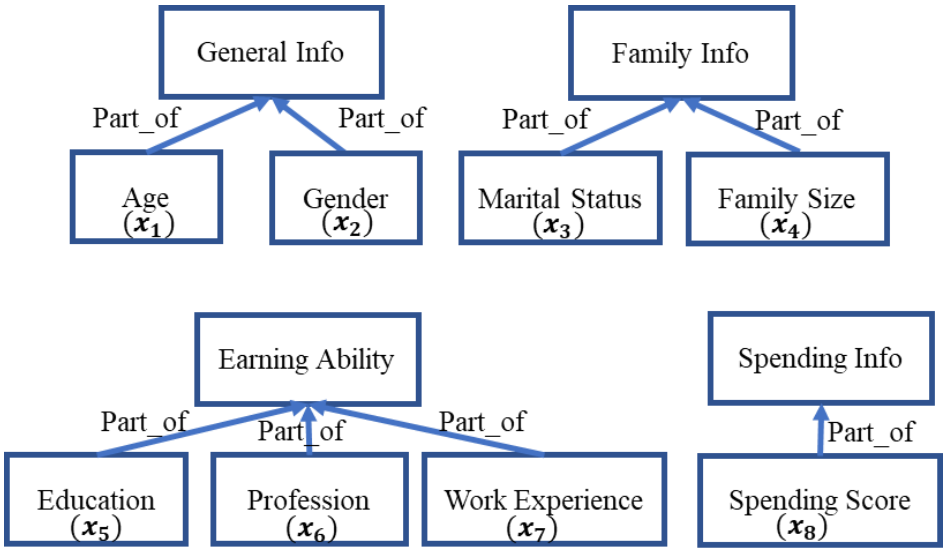


Figure 46. Sematic Network in the Customer Segmentation Case

7.4.2 Modelling

Similarly, the structure of the quantum inspired sematic layer can be constructed by using a mix of type I and type II quantum inspired sematic neurons based on the domain associated semantic network, as shown in Figure 47. The quantum inspired semantic layer here would map the initial 8 input attributes $\{x_1, x_2, \dots, x_8\}$, to 4 intermediate outputs $\{h_1, h_2, h_3, h_4\}$, based on the prior knowledge represented by the corresponding semantic network. The intermediate outputs are then delivered to next neural network layer, which consists of classic neurons, until the final outputs are reached.

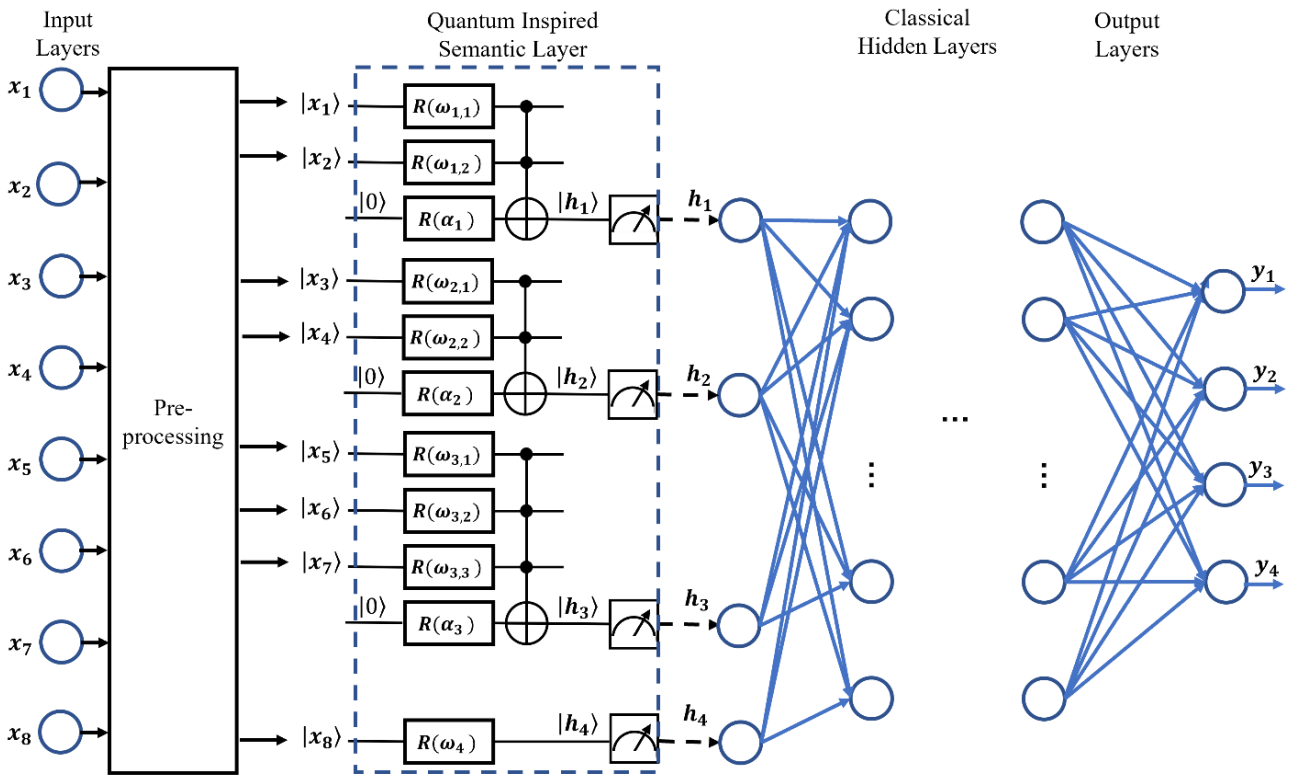


Figure 47. HQISNN Model for the Customer Segmentation Case

7.4.3 Results and Analysis

To generate meaning testing result, the original data set was split into training data set and testing data set with an 80%-20% split ratio. The desired prediction model in the customer segmentation case is a multi-class classification model, where the cost function used here is also cross-entropy function. Considering there is no prior knowledge of the preference in the prediction bias, the performance measurement metric used here is balanced F-measure F_1 (Hossin and Sulaiman, 2015), which represents the harmonic mean between precision and sensitivity values, where are the averaged value of per-class measurements in the multi-class case, as given below:

$$F_1 = \frac{2 \times precision \times sensitivity}{precision + sensitivity} \times 100\% \tag{53}$$

$$precision = \frac{1}{4}\sum_{i=1}^{4} \frac{true\ postive\ for\ class\ i}{true\ postive\ for\ class\ i + false\ postive\ for\ class\ i} \tag{54}$$

$$sensitivity = \frac{1}{4}\sum_{i=1}^{4} \frac{true\ postive\ for\ class\ i}{true\ postive\ for\ class\ i + false\ negative\ for\ class\ i} \tag{55}$$

Again, the number of follow-up classical hidden layers of HQISNN is set to 2. The performance results of HQISNN on the testing set over 16 repetitions was compared to that of the classical alternative, which is a BPNN model with same number of hidden layers and neurons, as shown in Table 12. The convergence behaviors comparison is given in Figure 48.

Table 12. Performance Comparison of the proposed HQISNN Model from a Similar Classical BPNN Model in Customer Segmentation Case Study

Model	Learning Method	Num. Iterations	Avg. Performance Measure on Training (F_1)	Avg. Performance Measure on Testing (F_1)	Best Performance Measure on Testing (F_1)
HQISNN	Gradient Descent	5000	68.4%	67.2%	71.6%
BPNN	Gradient Descent	5000	68.5%	66.9%	69.8%

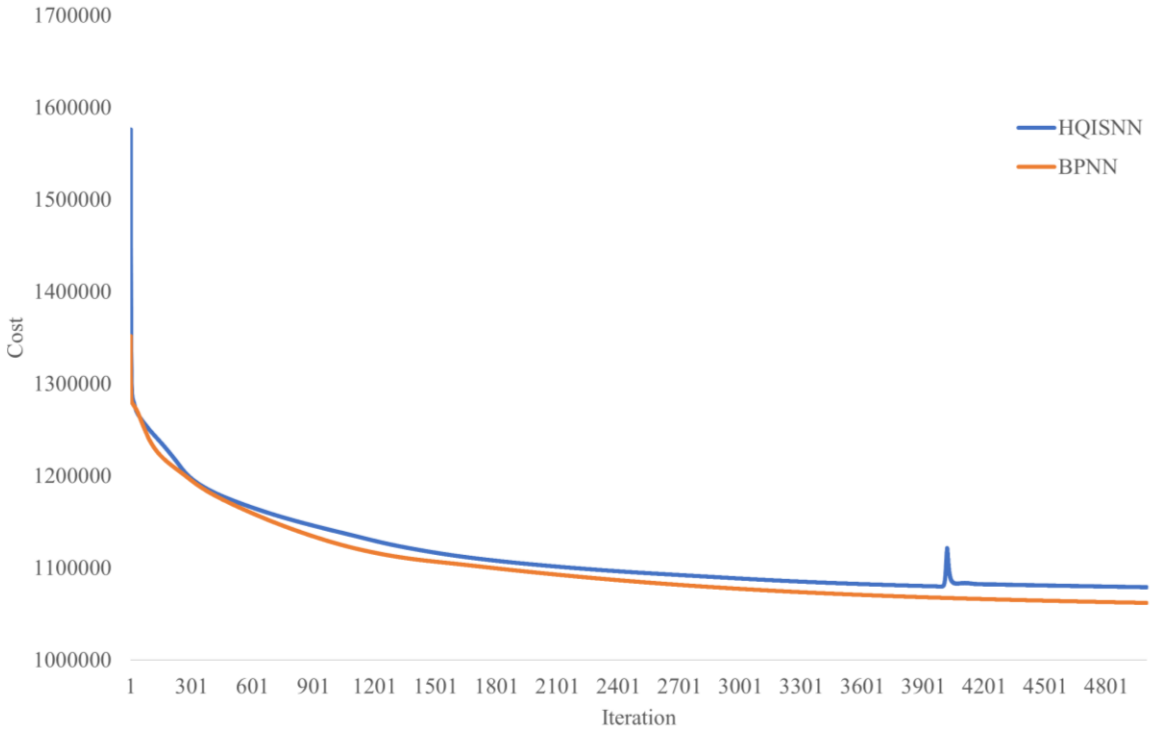


Figure 48. Comparative Convergence Behavior of the two Models during Training

What different from the results in case study 1 is that the average performance measure results over the 16 repetitions on the testing set of both models are lower than that

on the training set. This could be caused by the essential nature of the problem being a multi-class classification. The performance measure results of both models are generally matchable; however, some subtle performance improvements can still be seen in the results of the proposed HQISNN model comparing to the classical BPNN model, with a 2.6% increase in the best obtained performance. The convergence behaviors of the two models in this case study are also very close, while that of the HQISNN model has a small turbulence towards the end, which can be caused by the randomness introduced by its quantum inspired mechanism.

7.5 Chapter Summary

Inspired by the similarity between semantic network and classical neuron structure, and the emergence of quantum inspired neural networks, this chapter proposes two types of quantum inspired semantic neurons, which utilize the qubit representation and quantum gates to form the information processing units, and further proposed hybrid quantum inspired semantic neural network (HQISNN) model using the proposed quantum inspired semantic neurons and classical neurons. The proposed HQISNN model aims to provide a novel insight of representing domain knowledge in the neural network structure to enable domain context-aware ability of the neural network learning, which could consequentially lead to better data-driven decision-making problem-solving result.

Two engineering application case studies with different underlying essentials are conducted for verification and validation purpose here. Based on the results obtained from the case studies, the feasibility and effectiveness of the proposed HQISNN model can be clearly validated. Either in binary classification case study or multi-class classification case

study, the proposed HQISNN model can be trained on the given dataset and constantly converge to decent results. Noticeably, in the machine predictive maintenance case study, which requires a binary classification model, the obtained HQISNN prediction models can obtain not only higher prediction performance in the best result comparing to that of the corresponding classical alternatives, which are the BPNN models with the closest possible structure, but also better average performance measure results over 16 repetitions. While in the other case study of customer segmentation, although the proposed HQISNN model can still obtain matchable performance consistently, the possible advantage of the proposed model is not so obvious, which would require some future work for further exploration and refinement.

CHAPTER 8. CONCLUSIONS, LIMITATIONS & FUTURE WORK

In this chapter, the research contents presented in this dissertation are concluded regarding their consistency with the research objectives. The scientific merits and contributions associated with this research are identified and presented, as well as the limitations and possible future work for improvement.

8.1 Conclusions

With the aim of reaching the three identified research objectives, this research has planned, implemented, and presented the work associated with the following research tasks. Both qualitative and quantitative methods have been employed, the domain problem context and research hypothesis have been verified, the theoretical models and algorithms as well as technical concepts and solution performance have been assessed and validated, along with the benchmark case testing and real-world industrial case studies.

8.1.1 Quantum inspired genetic Algorithm for Computationally Efficient Combinatorial Optimization

Many efforts of QIGAs have been reported and demonstrated improvement in computational efficiency. However, existing QIGAs, including many variations and applications of quantum inspired evolutionary algorithms, only implement the mutation operator based on quantum phase shifting gates for iterative solution update. However, the use of crossover operator to update the population has not been addressed in line with the quantum inspired mechanism. Given the complexity of diverse categories of combinatorial

optimization problems in relation to different problem contexts of operation engineering, this simplification in the iterative solution process by a single updating procedure is not insufficient. In terms of domain problem solving, the core of a successful evolutionary computation is associated with a generic population-based metaheuristic and the corresponding strategies to handle the exploration-exploitation tradeoff, where the main iterative solution update is achieved by both the mutation and crossover operators. In this regard, a new twofold update quantum inspired genetic algorithm is developed to enable both a quantum inspired update procedure at the qubit level and a population-based metaheuristic update procedure at the solution structure level.

Results and analysis of an engineering system design case study show that the proposed TU-QIGA can obtain the best fitness value comparing to QIEA, CGA and PSO. Robustness analysis results also demonstrate that TU-QIGA is robust within a certain value range of parameter settings. Therefore, as an approach that coherently inherits the framework of the novel computation paradigm QIEA and the search strategy of most popular optimization method GA, TU-QIGA is a powerful next-generation alternative method in solving the combinatorial optimization problems in operations engineering.

8.1.2 Quantum Entanglement Inspired Hard Constraint Handling Approach for Solution Feasibility Assured Constrained Optimization

Quantum entanglement is a unique quantum-mechanical phenomenon where the individual qubits in the entangled quantum states are connected as an inseparable whole. Any action performed on one qubit affects the rest instantaneously in accordance with the entanglement logic, which is executed using quantum circuits. This behavior is

semantically similar to the influence of hard constraints on feasible solution, thus inspiring the novel hard constraint handling methodology in this study. The proposed quantum entanglement inspired hard constraints handling approach can express the domain constraints and conditional constraints into forms of quantum entangled states, and thus guarantee the feasibility of candidate solutions.

By embedding the quantum entanglement inspired hard constraint handling approach in GA, the proposed algorithm QEI-GA is designed to solve operations engineering optimization problems. The application of QEI-GA to a real-world airport shift planning case study shows that QEI-GA can obtain a better solution with a much smaller population size and with fewer iterations when compared to a case-tailored algorithm 2D-GA using penalty function and a multi-objective algorithm NSGA-II using constraint violation as additional objective.

8.1.3 Quantum Inspired Neural Network for Domain Context-aware Learning

As a subclass of quantum inspired algorithms, quantum inspired neural network inherits most of the artificial neural network concepts while using quantum circuits with parameterized gates to convert the classical binary concepts into quantum ones. The proposed quantum inspired neural network model HQISNN is built upon a mixed of parameterized quantum gates as neurons and classical artificial neurons to enable quantum concepts to efficiently represent information as well as coupling with partial semantic network to represent domain problem context awareness.

Based on the results obtained from the case studies, the feasibility and effectiveness of the proposed HQISNN model can be clearly validated. Either in binary classification

case study or multi-class classification case study, the proposed HQISNN model can be trained on the given dataset and constantly converge to decent results, by not only obtaining higher prediction performance in the best result comparing to that of the corresponding classical alternatives, which are the BPNN models with the closest possible structure, but also better average performance measure results over multiple repetitions.

8.2 Scientific Merits and Contributions

Future operations environment will see the advancement of quantum computers and super computational power, as well as more complex than ever decision-making processes. Industries, therefore, need to focus on developing frameworks and algorithms that can take advantage of these advancements in computational technologies to support decision-making as soon as they are available. The early application of quantum algorithms and quantum inspired algorithms have shown promising results in terms of computational effectiveness and efficiency. These strengths can be leveraged to solve large-scale combinatorial optimization problems which typically occur in the field of operations engineering. The proposed quantum computation inspired constraint handling and intelligent learning for data-driven decision-making approach goes beyond the conventional decision-making approaches in the following aspects:

8.2.1 Theoretical Foundation and Problem Formulation Framework for Quantum Inspired Optimal Combinatorial Decision Making

Though extensive research has been done in the field of quantum and quantum inspired computation, their application to real-world problems is extremely limited. A framework is proposed to transform real-world operational engineering problems into

quantum inspired combinatorial optimization problems. The proposed framework takes advantage of existing research in these fields and develops the required simplification and assumption to apply them to real-world problems.

By examining common operations engineering applications and identifies representative generic mathematical models, a quantum inspired formulation method and modeling technique is presented, which can shed light on the application of quantum inspired modeling in the broader decision science field.

8.2.2 Novel Quantum Inspired Hard Constraint Handling and Domain Context Representation

In many engineering scenarios, the domain context information, as well as other problem definition information, can only be specified in a set of constraints on the decision variables. A novel hard constraint handling approach inspired by quantum entanglement is proposed, to efficiently satisfied hard constraints in optimization problems. The proposed approach expresses domain context related hard constraints into forms of quantum entangled states using parameterized quantum gates, and thus guaranteeing the feasibility of candidate solutions. The potential of applying quantum entanglement feature in constraint representation and handling has not been explored before.

By embedding the quantum entanglement inspired hard constraint handling approach in classical optimization paradigm, many operations engineering constrained optimization problems can be solved in an unconventional and promising way. A substantial advantage of quantum inspired representation is that it allows for the encoding

of exponentially more information in each potential solution, which enables more efficient exploration of the search-space.

8.2.3 Advanced Quantum Inspired Methodologies and Algorithms for Operational Problem Solving

Based on the quantum inspired optimal combinatorial decision-making framework, hard constraint handling approach, and domain context representation, several advanced quantum inspired methodologies and algorithms are proposed:

(1) Twofold update quantum inspired genetic algorithm (TU-QIGA): The proposed twofold update mechanism enables QIGAs to be operated through iterative computation of both the deterministic and probabilistic schemes simultaneously, and thus to the largest extent to augment the exploration capability over the search space. Quantum inspired probabilistic search is conducive to cost-effectiveness of the solution process as each computational run can explore the search space more thoroughly than conventional deterministic search strategies.

(2) Quantum Entanglement Inspired Genetic Algorithm (QEI-GA) and its lightweight variant Lightweight Quantum Inspired Genetic Algorithm (LQIGA): The mechanism of quantum entanglement assures the feasibility of candidate solutions during the entire optimization process, which aligns with the requirement of practical applications. The power of qubit representation also enables the maintenance of high population diversity and thus better optimization performance.

(3) A Hybrid Quantum Inspired Semantic Neural Network (HQISNN) model: Given the data and information that narrates the uncertain operation process, with the support of semantic network knowledge representation and quantum inspired prediction modelling, the proposed model has its ability to firm the relatively static domain semantics in the model and learn the dynamic uncertainties in the scenario when needed.

8.3 Limitations and Future Work

Despite all the above inspiring powers and potentials, the limitations in this research are also obvious. The limitations are discussed in the following aspects, along with the possible future works to overcome them.

8.3.1 Generality of Problem Formulation and Modelling

The mathematical modelling of combinatorial optimization problems has a limited coverage of the combinatorial decision-making problems in operations engineering. Due to the nature of qubit superposition, the combinatorial optimization modelling in this study is derived from the classical modelling method using binary variables, in order to introduce qubit representation as the quantum inspired alternative of the original binary variables. However, not all the combinatorial optimization problems in operation engineering can be modelled in this way. The limitation of this modelling method would inevitably lead to the infeasibility of the proposed algorithms into solving the combinatorial decision-making problems that are outside of the current model.

Due to the crucial importance of problem formulation and modelling in the combinatorial optimization problem solving, one possible future direction of solving these limitations in the application scope of quantum inspired combinatorial optimization is to explore the possibility of new problem formulation models that can cover more types of combinatorial optimization problems and thus fully leverage or be inspired by the power of quantum computation.

In addition, the mathematical modelling in this study is designed to suit the usage of population-based stochastic searching algorithms, which could also limit the extension of the modelling framework to the domain of searching techniques.

8.3.2 Universality of Hard Constraint Representation and Handling

The proposed quantum entanglement inspired hard constraint handling approach has a very limited scope of application, it is only suitable for hard constraint handling in discrete COPs, but not any continuous ones. Due to its assumption of discrete variables on finite sets, it also lacks the general ability to handle inequality constraints, while inequality constraints are also widely seen in many operations engineering application scenarios. The extension of quantum entanglement inspired hard constraint representation would be the next step of work here.

Similarly, the exploration of domain knowledge representation in the combinatorial optimization problem solving procedure in this research has demonstrated good potential, yet it is still very limited. The extension of application scope to a higher variety of constraints, and in the form of more complex semantic network should also be considered, with the aim of more complex domain knowledge representation. Future research can also

be focused on the expansion of the proposed approaches to accommodate more variants of operations engineering problems, as well as embedding the quantum computation inspired combinatorial optimal decision-making supporting methodologies with more classical and exemplary optimization strategies.

Additionally, the usage guideline of hard constraint representation and handling approach presented in this study is rather complicated, which would require the user to master some quantum computation background knowledge and experience. To attract more application interests, a more automatic and user-friendly design pipeline should be considered and developed.

8.3.3 Enhancement in Learning Ability with Limited Computational Resources

Quantum inspired neural networks in this study are implemented in digital computer with simulated quantum behaviors, which would require large volume of computational resources when the learning model is getting complicated. Noticeably, in the machine predictive maintenance case study, which requires a binary classification model, the obtained HQISNN prediction models can obtain not only higher prediction performance in the best result comparing to that of the corresponding classical alternatives, which are the BPNN models with the closest possible structure, but also better average performance measure results over multiple repetitions. While in the other case study of customer segmentation, although the proposed HQISNN model can still obtain matchable performance consistently, the possible advantage of the proposed model is quite subtle, which would require some future work for further exploration and refinement.

Moreover, the semantic networks applied in this study are limited to single type of semantic networks, which is an obvious limitation of the proposed model. The future work would not only require enhancing the generalizability of the quantum inspired neural network, but also adapt the limited computational resources within a practical engineering scenario.

In summary, theoretically, the main limitations of the quantum inspired combinatorial optimal decision-making methods in this research are the inability to solve a wide range of problems, limited hard constraint handling, and the subtle enhancement of learning ability when computational resources are limited. Additional challenges also exist when applying the proposed methodologies to the practical scenarios as it requires not only a good understanding of the application domain, but also the basic understanding of quantum inspired computation. To overcome these roadblocks, some cooperative future work should be planned, which includes but not limited to the development of general guidelines, the construction of open-source quantum inspired combinatorial decision-making frameworks & platform, and the establishment of the quantum inspired industry solutions.

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