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Quantum-Based Optimization And Inference: A Risk And Reliability Perspective

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Abstract

Quantum computing is a novel computational paradigm that holds the potential to revolutionize the approach we currently use to tackle complex computational challenges in science and engineering. Over the last few years, quantum computing has gained immense popularity, mainly due to the exciting advances in hardware development achieved by companies such as IBM and Google. These advances motivate the exploration of a novel set of quantum-based algorithms to assess under which circumstances an advantage with respect to traditional computers is achievable. However, despite the recent advancements in the field, a large gap remains between quantum computing research and its practical applications in engineering. Even though quantum computing is still in its early phases of development, we believe that it is important for the risk and reliability research community to become familiarized with these novel algorithms in order to be prepared for when high-capacity quantum hardware becomes readily available. This paper presents three main contributions aimed to help close the aforementioned gap. First, a probabilistic-based introduction to quantum computing theory is presented to the reader, focusing on the math behind the operations performed by a quantum computer and ignoring quantum mechanics whenever possible. Second, the paper provides a curated set of existing literature combining quantum computing algorithms with risk and reliability applications. For this, we focus the discussion on the fields that are believed to hold the greater potential for advantage: combinatorial optimization and sampling enhancement routines. Finally, we list several research avenues that, from the author's perspective, hold promise for the field of risk and reliability.

Keywords: quantum computing, combinatorial optimization, inference, sampling.

1. Introduction

Quantum computing is a novel set of techniques that holds the potential to surpass the current computational capabilities of traditional computers for a selected group of tasks in science and engineering. To achieve this theoretical advantage, quantum computers leverage the properties of quantum mechanics to perform computation at a larger scale. Quantum computers are machines built to manipulate and measure a physical system, using natural laws to perform computation. In that sense, they are more akin to mid-century analog computers (Lundberg, 2005) than to modern, traditional computers. Over the last five years, quantum computing has started to gain traction in research circles outside of quantum mechanics and computer science due to the exciting developments in quantum-focused hardware and software, pushed forward by companies such as IBM, Google, Xanadu, and others. The expectation is for quantum computers to reach the capacity required for practical applications in the next decade.

These advances in quantum hardware have motivated a surge of exploration analysis regarding quantum algorithms with the objective of identifying advantages over classical counterparts. Notable examples of advantages achieved by quantum computing include the Shor's algorithm (Shor, 1997) and the Grover's algorithm (Grover, 1996) which have been proved to surpass traditional approaches in the factorization of prime numbers and search tasks in unstructured databases, respectively. However, despite the recent developments in the field, there exists a substantial gap between quantum computing research and its practical implementation for engineering tasks. This gap can be attributed, in principle, to the notable disconnection between the mathematical and physical interpretations used in quantum mechanics versus other fields of engineering. Even though quantum computing is still in its early phases of development, we believe that it is important for the risk and reliability community to develop, explore, and test these novel algorithms to participate in the global discussion and to be prepared for when high-capacity quantum hardware becomes easily available.

To bridge the aforementioned gap, this paper presents three main contributions. First, an introduction to quantum computing theory is provided to the reader, which is centered around a probabilistic interpretation of quantum computers in order to trace parallels with the field of risk and reliability. Additionally, we place special emphasis on the mathematical description of the operations that a quantum computer performs in an attempt to isolate the explanation from quantum physics as much as possible. Our second contribution is the development of a curated set of references combining quantum computing algorithms with risk and reliability applications. The objective is for this set to serve as an introductory reading list to the capabilities and early exploration of quantum computing in our field. For this curated set, we focus the discussion on the fields that hold the greatest promise for achieving advantages over classical algorithms: combinatorial optimization, and probabilistic inference and sampling tasks. Our final contribution is the description of several future research avenues that, from the authors' perspective, hold promise for the field of risk and reliability.

The paper is structured as follows. Section 2 offers a quantum computing primer based on a probabilistic perspective. Section 3 continues with an overview of current applications of quantum-based optimization within the risk and reliability domain, centering the discussion on the Quantum Approximate Optimization Algorithm (QAOA). Section 4 reviews the existing applications of quantum computing for enhancing sampling and inference techniques, using the Quantum Amplitude Amplification Algorithm (QAAA) as the main tool. Finally, Section 5 presents our concluding remarks and outlines the main quantum computing research avenues that we believe hold great promise for the field of risk and reliability.

2. Quantum computing primer: a probabilistic perspective

A quantum computer is a physical machine capable of holding, measuring, and manipulating a quantum state. A quantum state is the mathematical representation that summarizes the knowledge about a quantum system. In quantum computing and quantum mechanics, states are represented using complex vectors. Through this section, we use the *ket* notation to denote complex vectors: $\vec{\psi} \in \mathbb{C}^N \rightarrow |\psi\rangle \in \mathbb{C}^N$.

The simplest quantum state possible is represented by a 2D complex vector, $|\psi\rangle = [c_0 \quad c_1]^T$, commonly refer to as a quantum bit or *qubit*. Larger quantum states are formed by combining multiple qubits together using the Kronecker product operation. Consequently, a quantum state that results from the Kronecker product between K qubits will be a 2^K dimensional vector, as shown in Eq. (1).

$$|\Psi\rangle = \bigotimes_{i=1}^{K} |\psi_i\rangle = [c_0 \quad \ldots \quad c_{2^K}] \in \mathbb{C}^{2^K} \tag{1}$$

As with any other component of a vector space, a quantum state can be decomposed into a linear combination of basis vectors. The preferred base to perform this operation in quantum computing is the canonical base composed by the set $\{|e_i\rangle\}_{i=1}^{2^K}$, where $|e_j\rangle$ is a vector full of zeros, with a 1 in the *j*-th position. Using this basis, the quantum state $|\Psi\rangle$ can be decomposed as:

$$|\Psi\rangle = \sum_{i=1}^{2^K} c_i |e_i\rangle \tag{2}$$

An important limitation of quantum computers is that they cannot read a quantum state directly. This limitation is derived from the principles of quantum mechanics. To overcome this issue, quantum computers perform an operation known as *measurement*. When a measurement is performed over a quantum state $|\Psi\rangle$, the result is always one of its basis vectors $\{|e_i\rangle\}_{i=1}^{2^K}$. Which one is obtained in each measurement is determined by a probability distribution that directly depends on the set of complex numbers $\{c_i\}_{i=1}^{2^K}$, as shown in (3).

$$p(|e_i\rangle) = \|c_i\|^2 \tag{3}$$

Equation (3) reveals a fundamental interpretation of quantum computing: each quantum state $|\Psi\rangle \in 2^K$ can be interpreted as an object encoding a discrete probability distribution over the set of basis vectors $\{|e_i\rangle\}_{i=1}^{2^K}$. This probability distribution can be estimated by performing multiple measurement operations and recording their outputs.

Quantum computers are also capable of modifying quantum states. This modification is mathematically described in (4), where a set of unitary[1] matrices $\{U_j\}_{j=1}^{M}$, $U_j \in \mathbb{C}^{2^K} \times \mathbb{C}^{2^K}$ is applied to an initial quantum state $|\Psi_1\rangle$ to transform it into the new quantum state $|\Psi_M\rangle$. This application is given by traditional matrix multiplication.

$$|\Psi_M\rangle = \left(\prod_{j=1}^{M} U_j\right)|\Psi_1\rangle \tag{4}$$

These unitary gates can also be parametric, i.e., they can incorporate external information defined by a user, $U_j = U_j(\vec{x})$. The process of defining these unitary operations and their inputs is akin to the process of writing code for a digital computer. Equation. (4) can also be interpreted through a probabilistic perspective: by modifying the initial quantum state, the quantum computer is changing the probability weights assigned to each one of the basis vectors, thus transforming the original probability distribution.

So far, we have described from a mathematical point of view the operations performed by a quantum computer. Now, we contextualize these operations in a framework to solve practical problems. The underlying idea behind quantum computing is to identify the set of candidate solutions for a particular problem with the set of basis vectors $\{|e_i\rangle\}_{i=1}^{2^K}$, forming a one-to-one relationship. Then, starting from an initial quantum state encoding an uninformative probability distribution (for example, a uniform distribution), information about the problem is incorporated through the application of parameterized unitary matrices to the initial quantum state. Finally, the transformed quantum state is measured to estimate the resulting probability distribution. The expectation is for this final probability distribution to assign a high likelihood to the correct solution of the original problem. This framework is graphically depicted in Fig. 1.

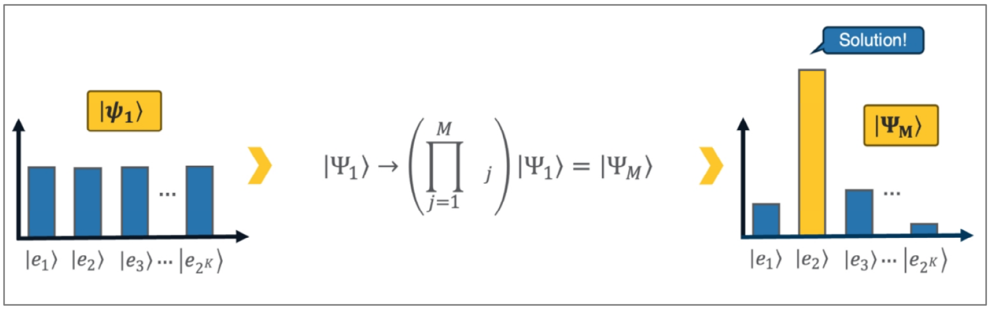

Fig. 1. Probabilistic framework used by quantum computing to solve practical problems.

It is important to note that quantum computing does not represent a universal approach to perform computation, but just an alternative way of solving a certain type of challenges that can be interpreted as finding a suitable probability distribution over a set of candidate solutions. While in principle limited, many relevant tasks within the risk and reliability field fall into this category. For example, classification problems, widely used for the diagnosis and prognosis of health states, can be looked through this lens. For this paper, we focus on how combinatorial optimization inference and sampling problems can be solved using the framework described in Fig. 1.

But before delving into those two applications, we first provide motivation for why scientists and practitioners believe quantum computing can offer advantages over traditional computation. First, note that a quantum computer is a physical system. As such, all the transformation and measurements that occur inside of it are not a digital simulation, but an actual physical system that responds *instantly* to the changes it is subjected to. In this sense, a quantum computer is much more akin to an analog computer (Lundberg, 2005) than to a traditional, digital computer. Second, as shown in (1) and (4), quantum computing allows the multiplication of exponentially large matrices given a relatively reduced set of K qubits. As an example, for a system with $K = 50$ qubits, the transformation of quantum states involves the multiplication of a vector of dimension

[1] A unitary matrix fulfils that its inverse is also its conjugate transpose, i.e., $UU^\dagger = U^\dagger U = I$.

$2^{50} = 1.125 \times 10^{15}$ with a matrix of dimension $2^{50} \times 2^{50} = 1.267 \times 10^{30}$. Even though that operation is impossible to perform in a traditional computer, it is instantly computed in a quantum computer by just letting "nature" follows its course. We just need to estimate the result by measuring the final quantum state. The challenge that quantum computing faces now, other than the actual development of capable, error-corrected hardware, is of algorithmic nature: how should we design these unitary matrices to solve practical problems? In this paper, we will provide the status of this question for two fields: combinatorial optimization, and probabilistic inference and sampling.

The current landscape in quantum hardware is usually referred to as NISQ: Noisy Intermediate-Scale quantum era (Lau et al., 2022). These machines are characterized by a low count of qubits and a high rate of measurement errors. The development focus is currently placed on solving these two issues. However, while increasing the number of connected qubits has shown steady progress over the last few years, decreasing the error rate has proved more challenging. Due to quantum computers being physical systems, they naturally interact with the environment around them. Quantum systems, in particular, are extremely sensitive to environmental changes, including changes in electromagnetic fields, temperature, and vibrations. All these perturbations can induce unsolicited alterations in the internal complex coefficients of the quantum state and produce errors in the final computation. How to minimize this perturbations and control for the inevitable ones is an active area of research in quantum hardware.

For the challenges mentioned above, most researchers and practitioners use simulation environments to explore the capabilities of quantum algorithms. These simulation environments are software programs that are executed on traditional computers with the objective of perfectly simulate the behavior of an error-corrected quantum computer. While the evident advantage of this approach is the lack of measurement errors, the disadvantage is that the capacity of such simulators is limited to the capacity of traditional computers. Consequently, only quantum systems up to 20 or 25 qubits can be efficiently simulated in this manner.

In what follows, we show how quantum computing is currently being used to solve combinatorial optimization and probabilistic inference problems within the Risk and Reliability context, and what developments in the area are good alternatives to explore in a near future.

3. Quantum-based combinatorial optimization

Why quantum computers are thought to present an ideal environment to solve optimization problems? As mentioned before, a quantum computer is a physical system. Consequently, it will inherently have all the properties we usually recognize in them, such as an energy level. The energy level of a quantum computer directly depends on its quantum state. As with any other physical system, if the quantum computer is left to naturally evolve its internal system, it should reach a state of local minimal energy. This evolution process is the basis for quantum-based combinatorial optimization. The general idea is to first identify each of the basis vectors of the quantum state with one of the candidate solutions for the optimization problem. Then, the objective function is encoded into a set of unitary operations. These operations are expected to assign a higher likelihood to the set of states that are optimal or near optimal.

From a practical point of view, the process of slow evolution is implemented in a quantum computer using an approach called Quantum Approximate Optimization Algorithm (QAOA), proposed by Farhi et al. in 2014 (Farhi et al., 2014). The QAOA is graphically depicted in Fig. 2.

As Fig. 2 shows, the QAOA approach repeatedly applies a set of unitary operations $\{U_C^j, U_M^j\}_{j=1}^{M}$. The Cost unitary operation (U_C) is the one in charge of encoding the objective function into the quantum computer. The Mixing unitary operation (U_M), is tasked with the exploration of the set of candidate solutions, making sure that all possible combinations are considered. Fig. 2 shows this set of operations applied to the initial quantum state a total of P times. In accordance with quantum computing theory, the higher the number of operation applications, P, the better the process of slow evolution is approximated by the QAOA, and consequently higher-quality solutions should be achieved. For a complete review of the QAOA, the reader is refer to (Choi and Kim, 2019; San Martin and Lopez Droguett, 2023).

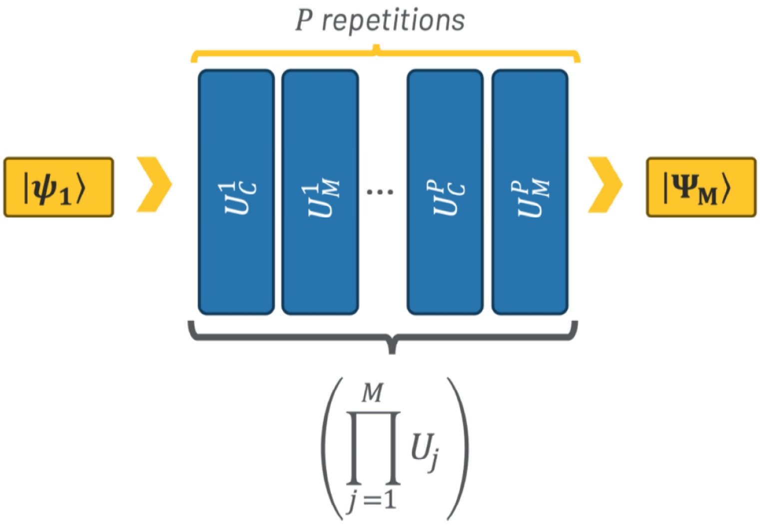

Fig. 2. Unitary operations that compose the Quantum Approximate Optimization Algorithm (QAOA).

An important limitation of the QAOA approach is that it is designed to exclusively Quadratic Unconstrained Binary Optimization (QUBO) problems. This is a relevant restriction, as a large percentage of relevant optimization problems in science and engineering fields are not QUBOs. A significant portion of the current research effort concerning the application of the QAOA is dedicated to exploring approaches to transform relevant optimization problems into QUBOs (Akrobotu et al., 2022; Glover et al., 2019; Papalitsas et al., 2019).

Early exploration of the QAOA algorithm has primarily been conducted in fields related to Operations Research and Finance. For example, Brandhofer et al. (Brandhofer et al., 2022) presents a complete assessment of the QAOA performance for the task of portfolio optimization. In their assessment, it is shown the effect of utilizing different mixing operations for the solution finding process. Additionally, design guidelines related to the cost unitary operation are also provided. The QAOA has also been applied in risk and reliability applications, using smaller case studies and quantum simulation environments to study under which conditions it can produce suitable results.

Indeed, San Martin and Lopez Droguett (San Martin and Lopez Droguett, 2023) proposed an approach to perform sensor placement optimization in civil infrastructure using the QAOA algorithm. In this approach, the Modal Strain Energy (Tan and Zhang, 2020) criteria is transformed into a QUBO objective function, and then the QAOA is used to find near-optimal sets of sensor configurations. The approach is validated using two numerical case studies concerning relevant civil structures: a shear building and a Warren truss bridge. Another example of the use of quantum-based optimization within the field of sensor placement optimization it presented by Speziali et al. (Speziali et al., 2021). In their paper, the authors proposed a methodology for identifying optimal configurations in Water Distribution Networks (WDN). For this, pipes and pumping stations within the WDN are first characterized as a mathematical graph. Then, a QUBO problem is formulated to find the minimum vertex cover in the resulting graph. The minimum vertex cover problem finds the smallest set of nodes (pumping stations) in the graph such that all edges (pipes) are at least incident to one of them. In practical terms, this solution strategy ensures that the resulting sensor configuration will facilitate the fast identification of anomalies within the network while installing minimum equipment.

Quantum computing theory has also been used to inspire the modification of traditional optimization techniques. This approach is usually referred to in the literature as "quantum inspired" algorithms (Gharehchopogh, 2023). We provide two relevant references regarding this type of approach. First, the paper presented by Araújo et al. (Araújo et al., 2022) provides a review of quantum-inspired algorithms to solve system reliability challenges. This review focuses on "Quantum-inspired Evolutionary Algorithms" (QEAs) to solve redundancy allocations problems as an approach to increase the reliability of an engineering system. Also focused on the redundancy allocation problem, but presenting a numerical case study, our second recommended reference is Paramanik et al. (Paramanik et al., 2023), which proposes the use of "Quantum Particle Sward Optimization" (QPSO) to find near optimal solutions in order to enhance the overall reliability of a given system.

4. Quantum-based probabilistic inference

Here, we pose another question: why probabilistic inference and sampling tasks can be solved using a quantum compute?

As shown in Section 2, a quantum computer can be understood as a machine that transforms probability distributions over a discrete set of elements. As such, they represent ideal playgrounds to implement probabilistic models such as Bayesian networks. Moreover, by encoding a particular probabilistic model into a quantum computer, they can be extended with the attributes of additional quantum algorithms. As we will see in this section, this interconnectivity between traditional probability models and quantum algorithms results in very rich interactions that can hold benefits for inference and sampling tasks.

First, it is necessary to briefly review how probabilistic models are encoded into a quantum computer. Currently, the main encoding approach is the one given by Borujeni et al. (2021), where it is proposed an algorithmic process to translate a Bayesian network over categorical variables into a unitary operation. However, this approach has two main limitations. First, it is not suited for encoding random variables representing continuous probability distributions. This is a relevant drawback as many operational variables in risk and reliability applications are modelled as Normal, Log-Normal, or Weibull distributions. Second, the number of qubits required to encode a Bayesian network scales at least linearly with the number of random variables in the model. This requires relatively large quantum computers to encode practically relevant models.

When the probability model is encoded into the quantum computer, each measurement of the final quantum state is equivalent to computing one forward pass of the Bayesian network. While interesting from a theoretical point of view, this approach on its own would not be conducive to any advantages over traditional computers. For that reason, the encoding of Bayesian networks as a unitary operation is usually combined with a protocol called the Quantum Amplitude Amplification Algorithm (QAAA), proposed originally by Low et al. (Low et al., 2014). The QAAA is capable of increasing the likelihood of sampling from a particular subset of states. In probabilistic terms, this is equivalent to increasing the likelihood of sampling from a conditional probability distribution $P(Q|E=e)$, where Q is a set of query variables and E is a set of evidence states. Therefore, this operation can produce immense benefits for risk and reliability applications, particularly in terms of characterization of low-probability, high-consequence scenarios.

For example, San Martin and Lopez Droguett (San Martín Silva and López Droguett, 2023) presented an approach that combines the Bayesian network encoding process and the QAAA to explore more efficiently the failure space given by the probabilistic model. Experimental results obtained from a small case study show that the proposed quantum approach can obtain an advantage over traditional rejection sampling using Monte Carlo simulation for obtaining more accurate estimates of the conditional failure probability using the same number of samples. In a similar fashion, Nikmehr and Zhang (N2023) used the Quantum Amplitude Estimation (QAE) algorithm to perform a reliability assessment of several power systems varying in their complexity.

An alternative application of quantum computing to study risk and reliability related models is presented by San Martin et al. (San Martin et al., 2022). In their paper, they describe how a fault tree model can be encoded into a unitary operation. Results from a case study concerning a Dynamic Positioning System (DSP) show that the execution of this unitary operation is equivalent to performing a Monte Carlo simulation over the original fault tree. On a final example, Zio (Zio, 2023) proposes the use of quantum-based probability theory to analyze the reliability of a wireless network system. This is done through the framework of Bayesian networks and their quantum counterpart. The final result is a reliability measure dependent on a term denoted as the *interference*. This term comes from considering the probabilities of events as complex numbers, and therefore from the interaction of their phases. In practical terms, this extra parameter can be used to incorporated operational data into the quantum model.

5. Concluding remarks and future research

This paper attempts to close the relevant gap that currently exists between quantum computing and the exploration of practical applications in the field of risk and reliability. For this, a math-based introduction of the theory behind quantum computing was presented to the reader, followed by the presentation of two relevant applications: quantum-based combinatorial optimization, and quantum-based inference and sampling enhancement. In each section, a curated set of references were included to introduce the reader into the development of this field.

Based on the past discussion, we highlight four key research paths that we believe hold great promise for the field of risk and reliability in the near future. First, in relation to quantum-based combinatorial optimization, a major challenge to solve is in relation to the restrictions placed upon the objective functions that can be tackled using the QAOA. As explained in Section 3, the QAOA is only suited for solving QUBO problems. For this reason, research in the area should focus on developing methods to transform the most relevant optimization problems in the field of risk and reliability towards QUBO formulation.

Concerning quantum-based probabilistic inference and sampling, significant challenges remain in enhancing the flexibility and efficiency of encoding methods for Bayesian networks. A notable unresolved issue is the integration of Bayesian networks containing continuous variables into quantum algorithms. Similarly, the quantum encoding of systems with practical relevance currently requires many times more qubits than what is available in modern quantum computers. As such, developing approaches that can make better use of quantum resources while increases the range of random variables that can be encoded into the system appears to be the logical trajectory for further advancement.

Finally, our expectation is for this paper to pave the way for extensive exploration of quantum-based algorithms in the field of risk and reliability applications. Quantum computing is currently undergoing exciting advancements, presenting opportunities across all disciplines. The early testing of these approaches will reveal crucial for researchers and practitioners alike in welcoming these new capabilities.

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