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Meta-Analysis and Systematic Literature Review on Applications of Variational Quantum Algorithms (VQAs)

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Abstract

It is important that multidisciplinary community of scientists first investigate all the myriad potential directions that quantum machine learning might go to discover what it has to offer. Among these avenues, specified algorithms such as Variational Quantum Algorithms (VQAs) have been applied in different industries for simulation, optimization, and prediction purposes. The focus of this paper is to determine the principles associated with the use of VQAs in chemistry, machine leaning, and optimization, amongst many other developed algorithms. The key results indicated that VQAs can successfully be applied in the above-mentioned fields, with the goal to (1) find ground and excited energy states of different molecules in chemistry; (2) maximizing or minimizing an objective function under specified constraints in optimization; (3) developing trainable quantum models for accurate predictions of unknown and unseen datasets. After statistical analysis, it was discovered that the proportion of publications of VQAs for optimization, machine learning, and chemical purposes have been considerably high over the past 6 years. This is justified by the sparking attention that parametrized circuits have offered over the recent years. After comparing different size effects, it was discovered that the fields of application of VQAs are interconnected, since they presented a small effect size, with Cohen's d value being less than 0.2. From these observations, it can be concluded that the lessons developed from one application can serve as direction for others. The metallurgical industry as a field of chemistry can benefit from the methods developed in VQAs for optimization, simulation, and development of novel materials.

Keywords:

Quantum machine learning; optimization; metal extraction; algorithms; quantum circuit

Introduction

Global optimization algorithms provide a much better chance of finding the global or near global optimum than their local counterparts (Venter 2010). It is important to note that no algorithm can guarantee convergence on a global optimum in the general sense, and it may be more accurate to refer to these algorithms as having global properties. Global optimization algorithms may be classified as either evolutionary algorithms or deterministic algorithms, of which Quantum Machine Learning (QML) algorithms are a good example of.

An empirical methodology is what drives contemporary machine learning. While significant attempts are being made to develop theories, many of the phenomena seen in deep learning still lack a sufficient theoretical explanation. The strength of an algorithm is often tested by running practical benchmarks. Additionally, the computational complexity of a machine learning algorithm, the preferred tool in traditional quantum computing, does not always provide us with useful information because many of the issues that machine learning algorithms resolve, like non-convex optimization when training neural networks, are inherently computationally challenging (Schuld and Petruccione 2021).

Both near-term quantum computing technologies and fault-tolerant machine learning algorithms face difficulties as a result of this circumstance. Researchers developed two design choices in response to this dilemma, which on the one hand, is the rigorously constructed computational complexity analysis to evaluate the adoption of fault tolerance. On the other hand, near-term quantum computing enables a far more practical approach to quantum machine learning, which is one of the reasons it plays such a significant role in the area. However, even short-term viewpoints have issues. The designed solutions for the above-mentioned problems are: (1) hybrid quantum-classical algorithms which consider quick quantum calculations rather than outsourcing the entire machine learning pipeline to a quantum computer as constituents of more intricate classical ones. Thus, implementing the machine learning model as a quantum algorithm while leaving the training to a conventional co-processor is the most common division of labor. The second choice is (2) to research "quantum models" or general, hardware-tailored circuits as potential replacements for conventional models like neural networks or Gaussian processes.

According to Cerezo et al. (2021), variational circuits, also known as parameterized circuits or quantum neural networks in the context of machine learning, are a great match for these needs. In fact, variational circuits include a "template" of parametrized and fixed quantum gates that defines the architecture of the circuit, similar to how the layer structure determines the architecture of a neural network. The parameters may be optimized by minimizing a cost function, which customizes the gates and subsequently the circuit to a specific issue. Using a traditional feedback loop, optimization is carried out. To iteratively enhance the parameters, either a black-box assessment of the model is used, or gradient characteristics of the model landscape are queried.

VQAs, have become the most effective method for gaining a quantum advantage on Noisy Intermediate-Scale Quantum (NISQ) devices. An optimization-based or learning-based technique is required to account for all of the restrictions imposed by NISQ computers with a single approach, and this is exactly what VQAs do. In many ways, VQAs are the quantum equivalent of popular machine learning techniques like neural networks (Schuld and Petruccione 2021). Furthermore, as VQAs employ parametrized quantum circuits to be performed on the quantum computer and subsequently outsource the parameter optimization to a classical optimizer, they make use of the toolbox of classical optimization. In contrast to quantum algorithms created for the fault-tolerant period, this technique provides the additional benefit of maintaining a small quantum circuit depth and so reducing noise.

The fact that VQAs offer a broad framework that may be used to a number of challenges is one of its key benefits. Although this adaptability results in various algorithmic designs with various degrees of complexity, there are fundamental components that most (if not all) VQAs share. In this part, we go through the foundational elements of VQAs. These algorithms are mostly established on an architecture involving (1) a cost function, (2) Ansatzes, (3) gradients, and (4) optimizers, as per figure 1 below.

After identification of the problem at hand, the definition of the cost (loss) function becomes a salient step. The next step is developing an ansatz, or a quantum operation that depends on a collection of continuous or discrete parameters, which may be optimized. The optimization task is then trained in this approach using a hybrid quantum-classical loop. The main applications of VQAs include, however are not limited to:

1. Optimization, wherein they are used to solve classical and quantum-enhanced problems.
2. Chemistry, where their ability to estimate low-lying eigenstates and corresponding eigenvalues is applied for finding ground and excited energy states; and further applied for dynamic systems simulations.
3. Machine Learning, where their application focuses on learning patterns in quantum data with the goal of making accurate predictions on unknown, and unseen data.

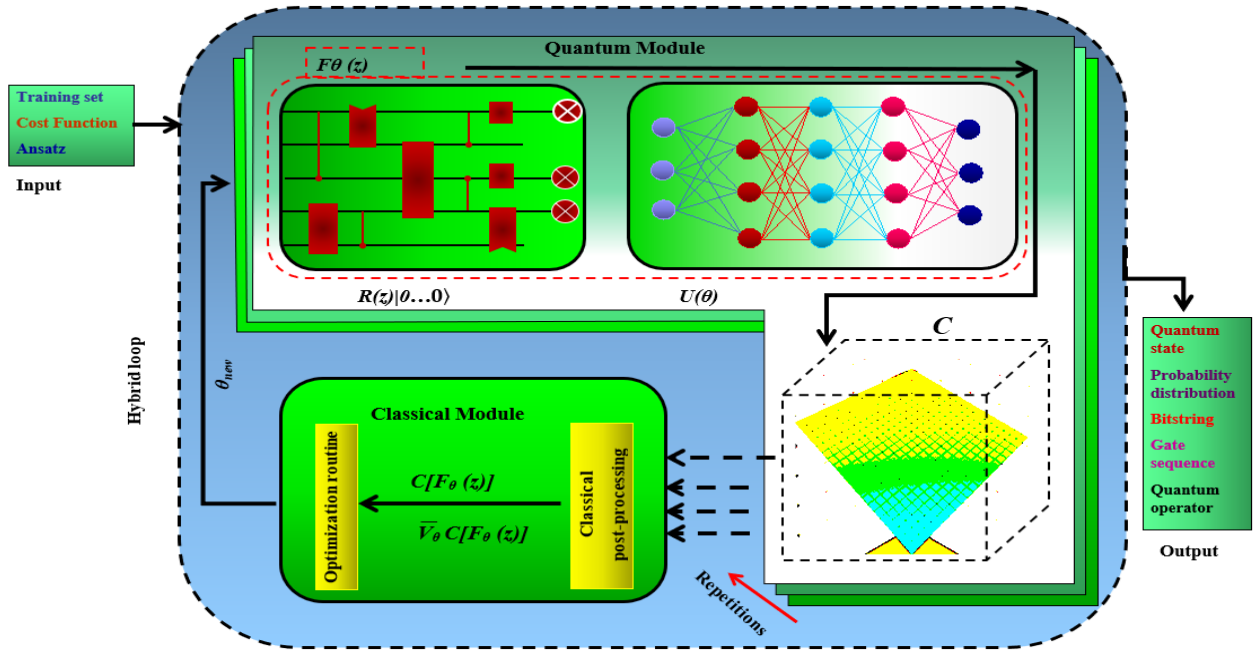

Figure 1. Variational Quantum Algorithm architecture.

Objectives

Machine learning is the art and science of teaching computers to solve problems via data analysis rather than through explicit programming. In view of this, quantum computing refers to the information processing of devices based on the principles of quantum theory. It is only logical to wonder how machine learning and quantum computing may be synergically coupled given that both are anticipated to have an impact on how society manages information in the future. This paper, pertaining to variational quantum algorithms used for process optimization, quantum chemistry and machine learning is an emerging masterpiece that investigates this query. The application of the Variational Quantum Algorithms will be the major objective of the study, wherein the focus will be on developing a meta-analytic and systematic review of its applications in the above-mentioned application fields. The developed review will offer background information on the development of parametrized quantum circuits fit for its various applications. The potential challenges and opportunities associated with the use of such algorithms will be discussed and possible solutions will be suggested. Since to date, the field of quantum machine learning still faces predicaments related to understanding its architecture and future uses in the metallurgical field.

Methodology

"Scientists have known for centuries that a single study will not resolve a major issue. Indeed, a small sample study will not even resolve a minor issue. Thus, the foundation of science is the cumulation of knowledge from the results of many studies" (Hunter et al. 1986) . An important finding to emerge in this study is the understanding of the different applications of the VQAs in different fields and for the development of a potential use in metallurgy by assessing the challenges and opportunities related to the implementation of this young, yet rapidly growing discipline into the metal extraction industry. As a result, rises the need for a meta-analysis review incorporating a systematic review of the literature.

Meta-analysis literature review

According to Aguinis et al. (2011) and Kepes et al. (2013), in many scientific fields, meta-analysis is a key technique used for accumulating information. Its principle of operation revolves around an overview of a research question or field, much like a narrative review. A meta-analysis adds value by offering a quantitative evaluation of the relationship between two target variables or the efficacy of an intervention, going beyond a narrative description of important findings. Additionally, it may be used to test opposing theoretical hypotheses against one another or to pinpoint crucial moderators where the findings of various primary research diverge from one another. Meta-analysis, which has its roots in the 1970s synthesis of the efficacy of medical and psychological therapies, is now a standard technique in management research and related domains (Hansen et al. 2022).

Steps for conducting a meta-analysis.
As depicted in figure 1 below, the 8 main steps undertaken to generate a reliable and reputable meta-analysis involve the following points outlined in a study by Hansen et al. (2022), as per figure 2.

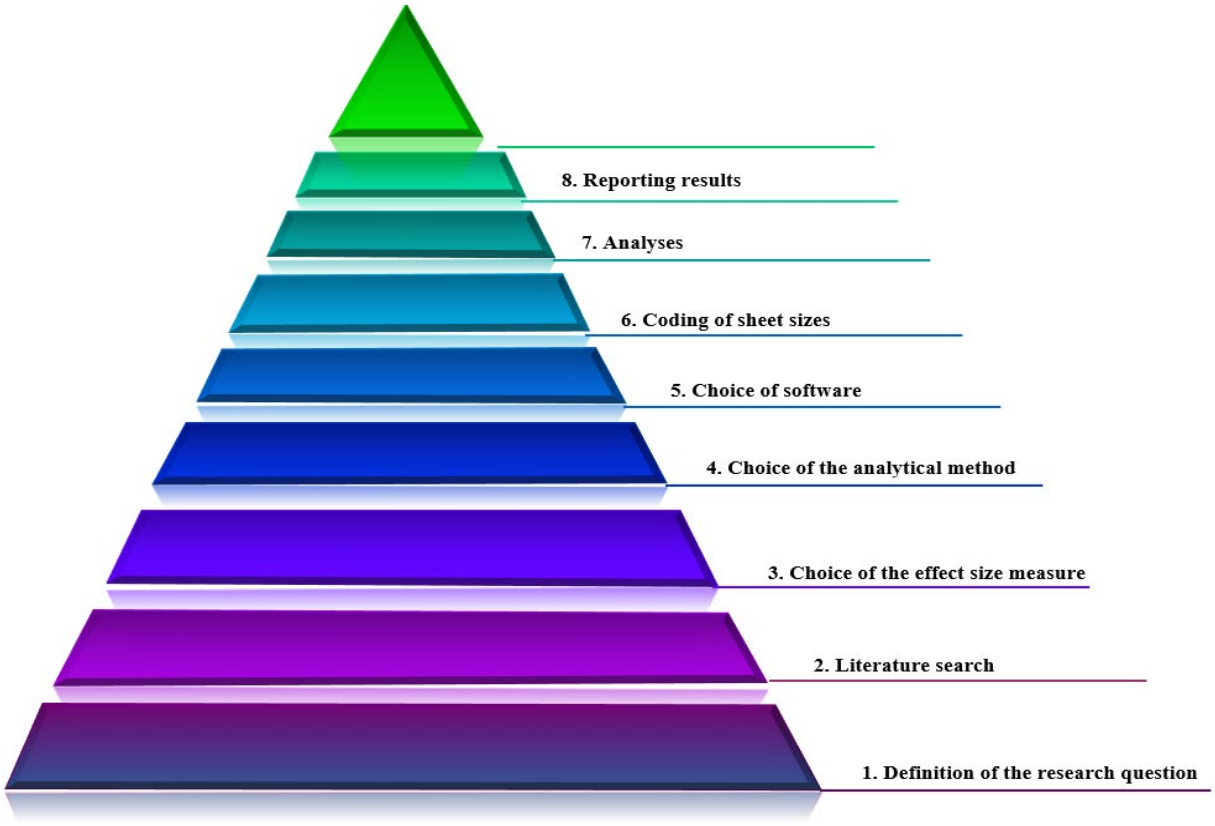

Figure 2. Summarized steps undertaken to compile and effectively develop a meta-analytic review.

Defining the research question: for this study, the definition and design of the research questions enabled the realm of the topic under investigation, thereby clarifying its scope.
The questions to be answered are as follows:

i. What are the main applications of Variational Quantum Algorithms, and what criteria characterize/ differentiate them?
ii. What specific methods or algorithms are used for each of the applications?
iii. What outcomes can be obtained from parameterized models to answer the problem at hand?
iv. What are the challenges and opportunities offered by VQAs?
v. How strong are the effects of choosing specific algorithms over the outcomes they offer?
vi. Does the choice of methods for VQAs relate to its applications?

The above questions will be answered by analyses and discussions derived from the current paper.

Literature Search: according to Hansen et al. (2022), the search procedure for a meta-analysis should be methodical, repeatable, and transparent, producing a sample that contains all pertinent papers.

Systematic techniques are used to gather, identify, and critically evaluate the research works that are already available such as articles, conference proceedings, books, and dissertations. A Systematic Literature Review provides the reader with the most recent research on a topic. Reviewing key areas of existing knowledge on a subject related to research questions is intended to identify areas that need additional investigation.

Study inclusion criteria and sample composition are employed when the choice of studies to include in the meta-analysis must then be made by researchers. To assure the quality of the findings, several recommendations for literature reviews advise restricting the sample to research published in reputable academic publications. For the literature review, inclusion and exclusion tables are used, coupled with Preferred Reporting Items for Systematic review and Meta-Analysis (PRISMA) diagrams for the justification of literature selection (Moher et al. 2009; Page et al. 2021).

Choice of the effect size measure: standardized mean differences and (z-transformed) correlation coefficients serve as the study's two main indicators of meta-analytical impact magnitude. Once the principal effect size measure for the meta-analysis has been established, it can be essential in the subsequent coding procedure to translate research results that are reported in effect sizes that differ from the primary effect size that was selected. The **Cohen's d** method of size effects is the tool to be applied in the current study (Aguinis, Dalton, et al., 2011; Geyskens et al., 2009).

Choice of the analytical method used:
the meta-analysis research topic directly affects the choice of meta-analytical methodology (Stanley and Jarrell, 1989; Wasserman et al., 1988; Wilson, 1999). In meta-analyses, research questions may address a general link between variables or the effect of an intervention, or they may concentrate on moderating or mediating influence. For this paper, the focus will be meta-regression, which will focus on establishing statistical correlations between the algorithm's applications and its main outcomes. As a result, it seeks to test several putative modifiers at once to evaluate the heterogeneity between observed effect sizes. The dependent variable in meta-regression is the coded effect size, which is regressed on a set of moderator variables.

Choice of software:
software options for performing meta-analyses range from commercial to open-source, from built-in features to additional statistical software packages, then landing on software specifically designed for the task (Cheung and Vijayakumar, 2016). However, in addition to individual preferences, the complexity of the methods utilized and the dataset itself determines which software is best. Minitab version 21 and Excel will be used as the software for the meta-regression and statistical effect size tasks, respectively.

Coding of Sheet Sizes: the coding sheet's design is the initial stage in the coding procedure. Because the design of the coding sheet relies on the techniques employed, the applicable software, and the complexity of the study design, there is no universal template. In its most basic form, the coding sheet would have columns for the research name or identifier, the effect size coded from the main study, and the study sample size when examining a correlational relationship between two variables using the univariate technique (Hansen et al., 2022).

Analyses: the robustness of the meta-analytical conclusions should be ensured by doing some preliminary sensitivity studies prior to the principal analysis (Rudolph et al., 2020). First, if there are a small number of overall effect sizes, significant outlier observations may unintentionally influence the observed results. The primary analysis is the next stage in meta-analysis after controlling and correcting for the potential presence of influential outliers or publication bias. Here, meta-analysts must choose between two different types of models that are based on two different assumptions: random effects and fixed effects.

Reporting Results:
reporting the findings of a meta-analysis is the last stage in the process. Most importantly, the reader should be able to understand all actions and methodological choices (Appelbaum et al., 2018; DeSimone et al. 2021; Levitt et al. 2018; Page et al 2021).

The PRISMA flow diagram (Fig. 3) is a tool used to clearly demonstrate how a researcher traveled from the databases searched to the publications they would discuss and to document distinct phases of the literature search process across many resources. It is a specific kind of flowchart that is utilized to present systematic reviews and meta-analyses. Through reporting on choices made at various phases of the systematic review, the PRISMA flow diagram clearly highlights the screening procedure and creates transparency in the selection process.

Any form of research that investigates traits of a certain subset of a population must define inclusion and exclusion criteria. This aids in the constant, trustworthy, and impartial identification of the study population by researchers. Participants in the study are therefore more likely to possess the qualities necessary to adequately address the research issue. The major factors that influenced the choice of this decision-making tool involve the language, and publication content as a result of strict keyword search. The choice of search database was developed to ensure the reliability of the obtained information, thereby including publications from renowned journals. Given the young and relatively unclear growth of quantum machine learning, the choice of the publication years has been restricted to 24 years, from all authors of different geographical locations. The resulting inclusion table (see table 1), whose opposite is an exclusion table is displayed below.

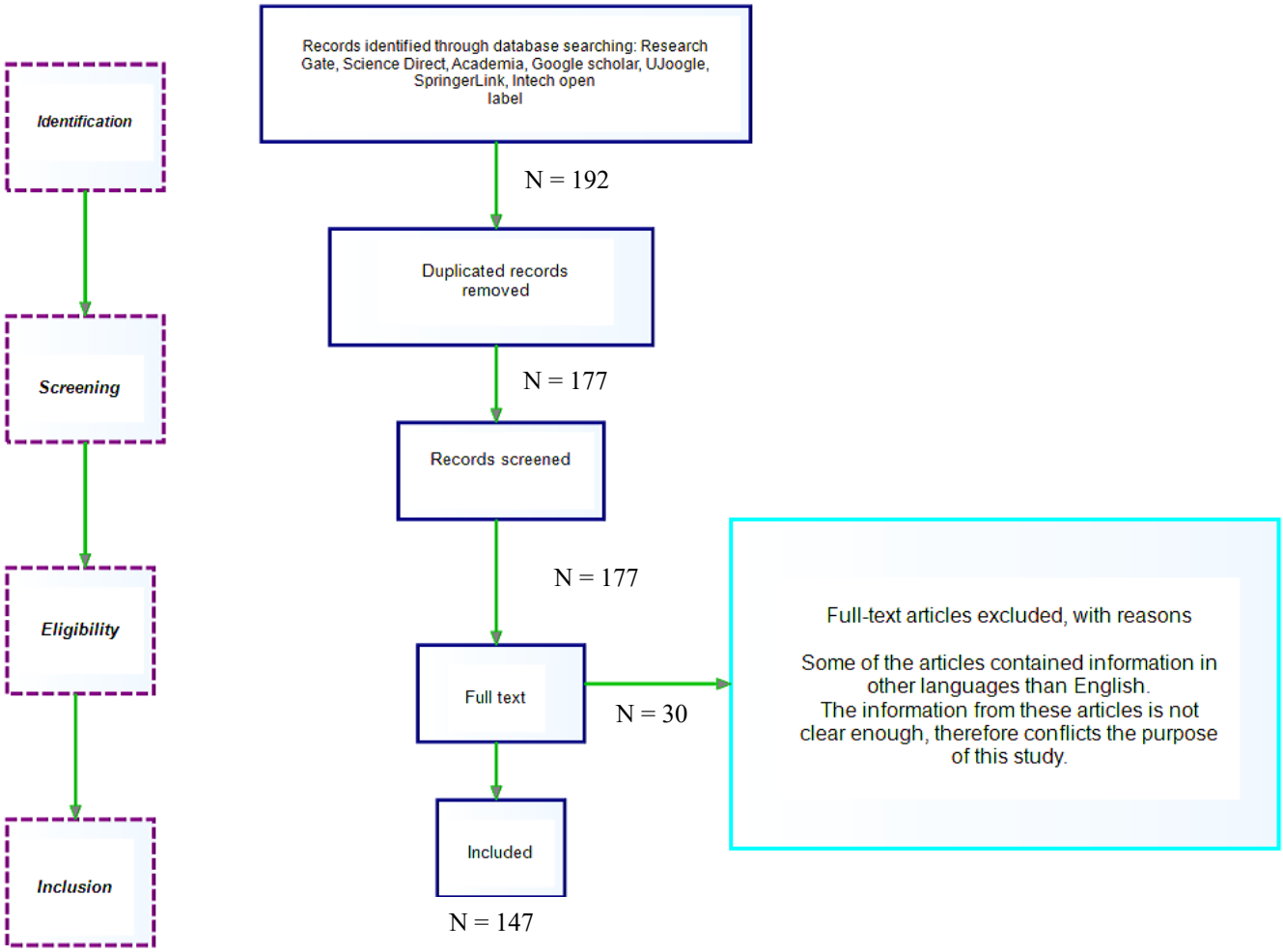

Figure 3. PRISMA diagram showing the number of articles that were included in the study.

Table 1. Inclusion table for literature search.

	Inclusions
Years	24-year scale of studies (1999-2023)
Language	English only
Sector	All sectors (both private and public)
Countries	Any country
Authors	Any Author
Publication	All research articles that are published, journals, books, and conference articles
Content	The focus of articles include: ✓ Quantum computing ✓ Quantum Machine Learning algorithms ✓ Optimization algorithms ✓ Quantum chemistry and physics ✓ Variational Quantum Algorithms (VQAs)

Results and Discussion

According to Biamonte (2021), task-oriented programming is made possible by the VQA paradigm, which is one of its key benefits. In other words, VQAs offer a framework that can be used for a variety of activities. In fact, it has been demonstrated that VQAs enable universal quantum computing, leading to the proposal of VQAs for nearly all applications envisioned for quantum computers.

Chemistry applications

In the beginning, variational algorithms were recommended as a method for locating the ground states, or lowest energy eigenstates, of quantum systems. According to the variational principle of quantum mechanics, the ground state $|\psi\rangle$ minimizes the expectation $\langle\psi|H|\psi\rangle$ of the system's Hamiltonian H. Variational Quantum Eigensolvers (VQEs) are designed to create a state where $|\psi(\theta)\rangle = W(\theta)$ using a parametrized ansatz $W(\theta)$.

Instead of locating the ground state $|\psi\rangle$, we locate the parameters that reduce the aforementioned expectation, resulting in the energy of the system. In other words, the cost is determined by the Hamiltonian's anticipation in a VQA, where $C(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$

Given an ansatz $|\psi(\theta)\rangle$, the ground state $|\psi(\theta^*)\rangle$ can be best approximated by minimising the expectation over all possible parameter configurations.

The quantum computer is used to estimate $C(\theta)$ for successively improved candidate parameters θ in most variations of quantum eigensolvers. On a traditional processor, iterative optimization may be carried out using different training methods.

Types of VQE approaches

- Orthogonality constrained VQE
- Subspace expansion method
- Subspace VQE
- Multistate contracted VQE
- Adiabatically assisted VQE
- Accelerated VQE

Variational Quantum Algorithms further found applications in chemistry wherein they were set for dynamical quantum simulation of chemical systems. According to Nielsen and Chuang (2011), this application of VQAs has been developed since traditional quantum Hamiltonian simulation techniques often discretize time into tiny time steps and mimic each time evolution with a quantum circuit, such as the Trotter-Suzuki product formula. As a result, the circuit depth often grows polynomially as the system size and simulation duration rise. The cumulative hardware faults for such deep quantum circuits might be too great due to the noise present in NISQ devices. VQAs for dynamical quantum simulation only employ a shallow depth circuit as a solution to this problem, greatly minimising the effect of hardware noise.

The developed algorithms (methods) to achieve the above-mentioned task are:

- Iterative approach
- Subspace approach
- Variational fast forwarding
- Simulating open systems

Optimisation Applications

The Quantum Approximative Optimisation Algorithm (QAOA), the most well-known VQA for quantum-enhanced optimisation, was first developed by Farhi et al. (2014) to roughly tackle combinatorial issues like Constraint-Satisfaction (SAT) and Max-Cut problems, as per the further findings by Lin and Zhu, (2016); and Wang et al., (2018).

Farhi et al. (2014) alluded that combinatorial optimisation problems are usually defined by n bits and m clauses. These clauses are a restriction on a subset of the bits that is met by some assignments of those bits but not by others. The goal function is the number of fulfilled or satisfied clauses, defined on n bit strings, as per the equation below.

$$\mathbf{C}(\mathbf{z}) = \sum_{\alpha=1}^{\mathbf{m}} \mathbf{C}_{\alpha}(\mathbf{z}) \qquad \textbf{\textit{Equation 1}}$$

where $z = z_1 z_2 \ldots z_n$ is the bit string and $C_\alpha(z) = 1$ if z satisfies clause α and 0 otherwise.
Usually, just a small subset of the n bits is needed for C. A string must satisfy each requirement for satisfiability to exist. A string that maximizes the goal function is what MaxSat requests.
A string z is needed for approximate optimization if C (z) is near to the C maximum. By boosting each classical variable s_j to a Pauli spin -1/2 operator σ_j^z, QAOA encodes the objective function in a quantum Hamiltonian H_P with the intention of setting up the ground state of H_P. The quantum adiabatic algorithm served as the inspiration for QAOA, which substitutes adiabatic evolution with p rounds of alternate time propagation between the problem Hamiltonian H_P and a suitable mixer Hamiltonian H_M.

According to Shaydulin et al. (2019), finding the best values of the cost function is a challenging challenge since the QAOA optimization landscape is non-convex and has a large number of local optima. Therefore, significant work has gone into developing a good classical optimizer that uses the quantum computer as little as feasible.

To provide a satisfactory performance for the QAOA, gradient-based, as per studies by Crooks (2018) and Romero et al., (2019); and derivative-free, as indicated by Wecker et al., (2016) and Yang et al. (2017) and reinforcement learning approaches were examined (Khairy et al. 2020) . This area of research is continuing to be active today (Cerezo, Arrasmith, et al. 2021).

Although the qubit-and-gate circuit model is by far the most popular formalism, we wish to quickly highlight a few different computational models. There are now efficient translations between these that have been demonstrated to be equal up to a polynomial overhead.

A method known as quantum annealing, which may be thought of as a heuristic to adiabatic quantum computing stated in the context of QAOA, was prominent in the early years of quantum machine learning literature. Adiabatic quantum computing, first outlined by Farhi et al. (2000), may be thought of as an analog form of quantum computing, where the answer to a computation issue is stored in the ground state of a Hamiltonian that governs the dynamics of a system of n qubits (Das and Chakrabarti 2008).

Starting with a quantum system that is relatively easy to realize in the context of a specific experimental setup and gradually changing it to be regulated by the required Hamiltonian assures that the system is ultimately discovered in the ground state.

It turns out that for many problems, maintaining the system's ground state during the adjustment (the annealing schedule) necessitates a very gradual evolution from one Hamiltonian to the next and frequently requires a time scale that is exponential in the size of the problem. This confirms once more that nature appears to have established some general bounds for computation (Schuld and Petruccione 2021).

A heuristic for the adiabatic method, whose dynamics closely resemble simulated annealing in computer science, is quantum annealing. The primary distinction between classical and quantum annealing is the substitution of quantum fluctuations for thermal fluctuations, allowing the system to tunnel through both thick and thin energy barriers.Although it is independent of the barrier's height, the likelihood of quantum tunneling diminishes exponentially with barrier width. As a result, issues with an objective function that is extremely ragged are particularly well-suited for quantum annealing.

Schuld and Petruccione, (2021), outlined the fact that an annealing device was the first piece of commercially viable quantum computing hardware has led to the community of quantum machine learning's intense interest in quantum annealing. A procedure called quantum annealing (QA) uses quantum fluctuations to determine the global minimum of an objective function over a range of potential solutions (candidate states). The D-Wave quantum annealer has been used for machine learning demonstrations as early as 2009 (Neven et al. 2009). The only issue types that can currently be solved by quantum annealers are what are known as quadratic unconstrained binary optimization problems. Although the advantages of the quantum schemes have been shown in the literature mentioned above, measuring the performance of quantum annealing in comparison to classical annealing schemes is a challenging problem (Heim et al., 2015; Santoro and Tosatti 2006). Additionally, general statements about speedups and actual quantum behavior are still debatable. Further algorithms related to optimization such as gradient based optimization and linear systems optimization are discussed by (Ambainis 2012; Berry et al. 2017; Scherer et al. 2017; Subaşl et al. 2019). The interested reader is referred to these textbooks for additional references.

Machine Learning (ML) Applications

Biamonte et al. (2017) explained that generally, "quantum machine learning" is the process of employing a quantum computer to identify patterns in quantum data in order to make precise predictions about yet-to-be-observed data. For the purpose of the current paper, the few tasks that will be focused on are related to classification, autoencoding, and quantum neural networks. This relationship between VQAs and (typical) QML applications demonstrates how lessons learnt in one area may be very helpful in another, thereby fostering a close relationship between these two disciplines (Cerezo, Arrasmith, et al. 2021).

In machine learning, the categorization of data is a common problem. The objective is to train a classifier to correctly predict the label of each input given training data of the form $\{x^{(i)}; y^{(i)}\}$, where $x^{(i)}$ are inputs and $y^{(i)}$ are labels. Since the non-linearity of classical neural networks is essential to their effectiveness, one might anticipate that a quantum classifier will likewise exhibit this characteristic. As demonstrated by Schuld et al. (2020), parametrized quantum circuits may enable linear transformations, and non-linearity can be accessed via a quantum system's tensor product structure.

Here, a parametrized quantum circuit $U(\theta)\, V(x)\, |\psi_0\rangle$ is used to conduct a linear transformation after embedding the input data x into the quantum state. The difference between the expected value of a readily measurably observable and the real label is then used to establish the cost function. This method has been applied to classification and generalization tasks (Mitarai et al., 2018; Schuld et al., 2020). The discussion of various methods of embedding classical data into quantum states (such as data re-uploading) has been thoroughly explained by Lloyd et al., (2020); Mitarai et al., (2018); Pérez-Salinas et al., (2020); and Schuld et al., (2021). Furthermore, (Havlíček et al., 2019) provides an example of variational classification in practice to deepen the understanding associated with the application of VQAs in machine learning classification through Supervised learning with quantum-enhanced feature spaces.

An autoencoder is traditionally a particular type of artificial neural network (ANN) architecture that has been taught to return its input as its output while undergoing a critical degree-of-freedom funneling process (Heaton, 2018).

Through this funneling procedure, data points that are a member of a certain set of data are produced as compressed representations. The autoencoder for data compression is a crucial machine learning component. The goal is to push data through a bottleneck while preserving its ability to be recovered. (Romero et al., 2017) presented a VQA for quantum autoencoding as a quantum analogue with the intention of compressing quantum data. (For alternate strategies for quantum autoencoders), as per findings from Verdon et al., (2018); and Wan et al., (2017).

According to Cerezo, Arrasmith, et al., (2021), the input to the algorithm is an ensemble of pure quantum states $\{p_\mu|\psi_\mu\rangle\}$ on a bipartite system AB, where $p_\mu$are real and positive coefficients such that $\sum_\mu;\ p_\mu = 1$. The objective is to train a given ansatz U (θ) to compress this ensemble into the A subsystem, such that one can recover each state $|\psi_\mu\rangle$ with high fidelity from subsystem A, with the B subsystem being discarded and thus being thought of as the "trash". Evidence from (Romero et al., 2017) explain that the cost function is based on the overlap between the output state on B and a predetermined pure state due to the strong relationship between data compression and decoupling.

Studies by Beer et al., (2020); Diep, (2020); Farhi and Neven (2018) revealed that there have been several suggested Quantum Neural Network (QNN) designs, including perceptron based QNNs. Each node of the neural network in these topologies represents a qubit, and the connections between them are provided by parameterized unitaries operating on the input states in the form of $U(\theta) = U_L(\theta_L) \ldots U_2(\theta_2)U_1(\theta_1)$; where U($\theta$) can be generically expressed as the product of L sequentially applied unitaries. In addition, Quantum Convolutional Neural Networks (QCNNs) were introduced by Cong et al., (2019) and have been applied to image identification, error correction, and the discrimination of quantum states belonging to various topological phases. Furthermore, Pesah et al., (2021) Zhang et al., 2021) have been demonstrated that QCNNs and QNNs with tree tensor network designs do not have barren plateaus (which will be described later), making them potentially a trainable architecture that may be used for large-scale implementations.

One of the further objectives of the current paper is to identify the potential link of the applications to fit purposes in the extraction metallurgy and mineral processing field. In addition to the applications outlined in the previous lines, the metallurgy industry may further benefit of VQAs in the following points:

1.Molecular structure determination: there have been significant advancements in the traditional treatment of the structure of molecular systems during the last several decades. Among these are techniques that are approximate, like Hartree-Fock or density functional theory (DFT), or approaches that are intimately related to quantum information, such the density matrix renormalization group approach that makes use of matrix product states as an ansatz. The works by Chan and Sharma, (2011), and White, (1992) can be considered precursors of the suggested application in extractive metallurgy, wherein the determination of molecular structures play a crucial role.

2.Material sciences applications: when dealing with weakly correlated materials, traditional approaches for materials simulations often combine density-functional theory with approximation techniques, such as the local density approximation (Jung et al. 2006). However, many effects resulting from highly coupled systems are not amenable to such conventional techniques. These are outside the purview of near-term devices since long-term methods for material modelling need phase estimation, as mentioned by Babbush et al. (2018); Bauer et al. (2016) and Berry et al.(2018). In contrast, near-term VQAs for strong correlation issue analysis work to minimize the circuit depth through the use of clever initializations (Dallaire-Demers et al. 2019) or by circuit structure optimization (Grimsley et al. 2019; Tang et al. 2021).

The ability to process voluminous datasets while ensuring the most reliable and quickest solution to a given set of objective functions from a larger set of candidate solutions subjected to constraints has made the application of quantum machine learning concepts and related algorithms adequate for mineral processing and metal extraction processes. Furthermore, quantum machine learning algorithms have been advertised as capable of solving the global minimum of combinatorial problems such as discrete search space optimization wherein the objective function outcomes many local minima. This is made possible using peculiar quantum properties such as superposition, entanglement, teleportation, and speedup. The development and practical applicability of basic quantum circuits with numerous quantum gates integrated with machine learning algorithms and related postulates for different possible process optimization avenues therefore make VQAs a tool of outstanding performance in the metallurgy and minerals industry. The design and development of novel materials for chemistry-related applications is now being investigated by employing quantum algorithms to optimize and simulate.

After thorough understanding of the different methods (algorithms) parented by VQAs, the diagram below summarizes the applications of VQAs, and the respective algorithms developed and considered fit for their applications. The results are displayed in figure 4 below.

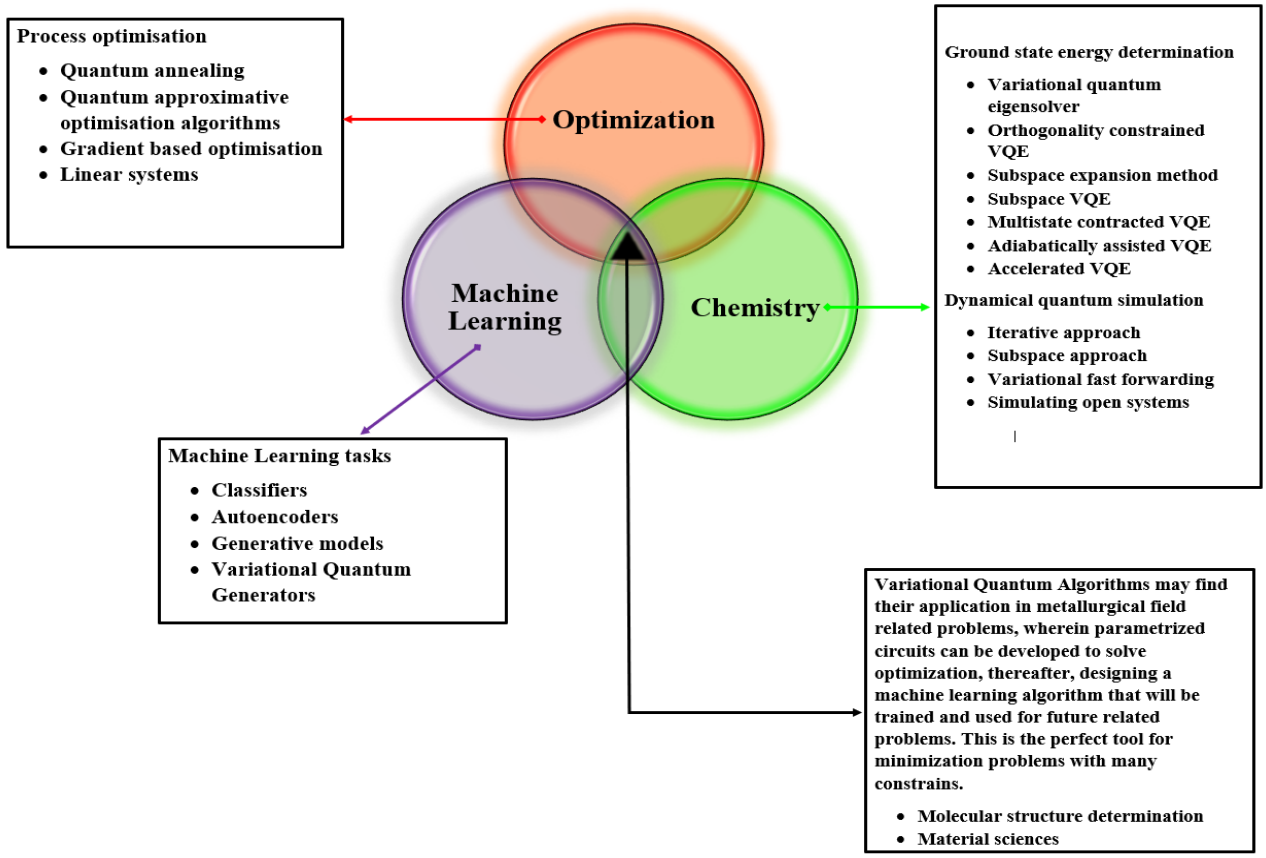

Figure 4. Summary of the various applications of VQAs and their potential point of contact for suggested applications in the metallurgy field.

Potential Opportunities and Challenges for VQAs :
Although it is still a relatively new field of study, quantum machine learning has made significant progress. It is moving in an exciting but also difficult place, as we have noted throughout this book. The primary driver behind this is the intention to show that certain approaches work better than others, even if we now only have limited practical access to them. Other aspects of quantum computing may not be hampered by this since computational complexity theory is a potent tool that researchers have perfected. However, because machine learning is a mathematical abstraction of challenging real-world issues, theoretical research is made much more difficult. The use of data in machine learning provides highly specific difficulties, even when contrasted to other near-term applications like optimization and quantum chemistry (Schuld and Petruccione, 2021).

The following may be considered as a few potential challenges that VQAs are facing and some of the suggested solutions.

Table 2. The different challenges of VQAs and their explanations, with a set of suggested solutions.

Challenge	Description	Suggested Solution
Efficiency	The ability to estimate expectation values (and more generic cost functions) efficiently is a prerequisite for VQAs to offer a quantum advantage. As noted in the section on BPs, the presence of BPs might exponentially raise the precision requirements necessary for the optimisation phase of VQAs, but even in the absence of such BPs, these expectation value estimations are not certain to be efficient (Cerezo, Arrasmith, et al., 2021).	The plausible solutions: ▪ Commuting sets of operators ▪ Optimized sampling ▪ Classical shadows ▪ Neural network tomography
Trainability	The high expressibility of the quantum ansatz U is necessary to ensure that the variational quantum algorithm (VQA) result is sufficiently near to the precise solution for the target issue. To boost expressibility, we may theoretically add more quantum gates and training parameters to the PQC, or we can use post-processing modules for neural networks. The trainability is a significant consideration for VQAs using actual quantum hardware. Unfortunately, there is a trade-off between expressibility and trainability in VQA, and optimisation problems such barren plateaus, which may be brought on by entanglement in the quantum circuit and noise on NISQ devices, significantly restrict the performance of VQAs (Liu et al., 2023).	▪ Barren plateaus ▪ Ansatz and initialization strategies
Accuracy	The ability to put NISQ devices to work practically is one of the key objectives of VQAs. VQAs, which may be able to reduce quantum circuit depth, offer a method to deal with hardware noise to achieve this aim. Furthermore, as will be covered below, VQAs can be used with error mitigation techniques to further boost accuracy. However, the question of how hardware noise may affect a VQA's accuracy remains (Cerezo, Arrasmith, et al., 2021).	▪ Impact of hardware noise ▪ Noise resilience ▪ Error mitigation

The publications that were used and the primary goals of the study that was reported in the articles are summarized in table 3 below. This table also demonstrates how the articles were organized as a function of applications.

Table 3. Applications of VQAs in different fields suggested with findings and publication details.

Application	**Author, Year**	**Purpose of study and algorithm (methods) used**
Chemistry	(AI Quantum, 2020; Babbush et al., 2018; Bakulin et al., 2013; Bauer et al., 2016; Benedetti et al., 2019; Berry et al., 2018; Bravo-Prieto et al., 2019; Bravyi et al., 2020; Cao et al., 2019; Carolan et al., 2020; Chen et al., 2020; Cong et al., 2019; Coyle et al., 2020; Dallaire-Demers et al., 2019; Du et al., 2020; Farhi et al., 2014; Franken and Georgiev, 2020; Hastings, 2019; Heya et al., 2018; Jones et al., 2019; Khatri et al., 2019; Küchlin and Sinz, 2000; Liu and Wang, 2018; Lubasch et al., 2020; McArdle et al., 2019, 2020; McClean et al., 2017; O'Brien et al., 2019; Outeiral et al., 2021; Peruzzo et al., 2014; Romero and Aspuru-Guzik, 2021; Sharma et al., 2020, 2022; Subaşl et al., 2019; Wang et al., 2019; Wang, Koh, et al., 2021a, 2021b; Weinberg et al., 2012; White, 1992; Xu et al., 2021; Yang et al., 2017; Zhou et al., 2020)	The papers here outlined focused on developing specified algorithms that can used for either determining the ground energy state of particles/ molecules or in dynamic simulation of chemical systems. The main algorithms applied are Variational *Quantum Eigensolvers* (VQEs) in various forms, and *simulation approaches*

		relying on *variation or iterations.*
Optimisation	(Acar et al. 2021; Amaro et al., 2022; Ambainis, 2012; Barthelemy and Haftka, 1993; Berry et al., 2017; Biamonte, 2021; Cao and Wang, 2021; Cerezo, Arrasmith, et al., 2021; Cerezo, Sone, et al., 2021; Cincio et al., 2018; Cîrstoiu et al., 2020; Crooks, 2018; Das and Chakrabarti, 2008; "Design Optimization", 2007; Du et al., 2022; Endo et al., 2020; Fontalvo, 2019; Friedrich and Maziero, 2023; Garcia-Saez and Latorre, 2018; Gibbs et al., 2021; Glos et al., 2022; Grimsley et al., 2019; Havlíček et al., 2019; Heim et al., 2015; Higgott et al., 2019; Huang et al., 2021; Innocenti et al., 2022; Kandala et al., 2019; Khairy et al., 2020; Li and Benjamin, 2017; Lin and Zhu, 2016; McClean et al., 2018, 2021; Moll et al., 2018; Morales et al., 2020; Nakanishi et al., 2019; Neven et al., 2009; Parrish et al., 2019; Pérez-Salinas et al., 2020; Peruzzo et al., 2014; Peters et al., 2021; Rattew et al., 2019; Romero et al., 2017, 2019; Saleem et al., 2023; Santoro and Tosatti, 2006; Scherer et al., 2017; Schuld et al., 2019, 2020; Schuld and Killoran, 2019; Shaydulin et al., 2019; Sim et al., 2019; Steinbrecher et al., 2019; Stoudenmire and Schwab, 2016; Tang et al., 2021; Verdon et al., 2018; Wan et al., 2017; Wang, Fontana, et al., 2021; Wang et al., 2022, 2018; Wecker et al., 2016; Yuan et al., 2019; Zhou et al., 2020)	From this set of applications of VQAs, the main purpose of the study is to optimise different processes using specified sets of algorithms such as *Quantum Annealing, Quantum Approximative Optimisation, gradient, and linear methods*. The optimisation task is achieved by developing a parametrised circuit, where the objective function is set to constraints. This approach has been found successful in the minimisation of many functions, thereby resolving the problem at hand.
Machine Learning	(Abrams and Lloyd, 1999; Ban et al., 2021; Beer et al., 2020; Biamonte, 2021; Biamonte et al., 2017; Cao and Wang, 2021; Cerezo, Arrasmith, et al., 2021; Cincio et al., 2018; Cîrstoiu et al., 2020; Crooks, 2018; Diep, 2020; Endo et al., 2020; Farhi and Neven, 2018; Fontalvo, 2019; Friedrich and Maziero, 2023; Gibbs et al., 2021; Glos et al., 2022; Hansen et al., 2022; Havlíček et al., 2019; Huang et al., 2021; Innocenti et al., 2022; Kandala et al., 2019; Khairy et al., 2020; Kusumoto et al., 2019; Li and Benjamin, 2017; Lloyd et al., 2020; McClean et al., 2018, 2021; Mitarai et al., 2018; Moll et al., 2018; Nakaji and Yamamoto, 2021; Nielsen and Chuang, 2011; Pérez-Salinas et al., 2020; Pesah et al., 2021; Peters et al., 2021; Rattew et al., 2019; Romero et al., 2017, 2019; Saleem et al., 2023; Schuld et al., 2019, 2020, 2021; Schuld and Killoran, 2019; Shaydulin et al., 2019; Sim et al., 2019; Steinbrecher et al., 2019; Stoudenmire and Schwab, 2016; Verdon et al., 2018; Wan et al., 2017; Wang, Fontana, et al., 2021; Wecker et al., 2016; Zhang et al., 2021)	The use of machine learning methods such as *Classification Autoencoding, Generative modelling, Variational Quantum Generation*, has been taken into advantage for the development of robust, accurate and reliable machine learning algorithms that can be trained, validated, and tested for future purposes.

Statistical analysis

The meta-analysis related to the collected results from the different sources is assessed in this section of the paper. Table 4 below presents the number of articles as per the different applications as a function of time. From these results, it is observed that VQAs have a relatively low existence (less than 24 years). This is because the application of quantum machine learning for these purposes' dates to recent years. It is further observed that the number of articles increases as a function of time for all three areas of application of VQAs, thereby indicating a spark of interest in the application of these algorithms in the different fields.

According to Cerezo et al. (2021), the connection between VQAs and (typical) QML applications shows that the lessons learned in one field can be of great use in the other, hence providing a close connection between these two fields. This correlation is observed in the results depicted in table 4.

Table 4. Increasing application of VQAs in the targeted field over the years.

	Years under study			
Application of VQAs	1999 - 2004	2005 - 2010	2011 - 2016	2017 - 2023
Optimization	1	4	5	44
Machine Learning	1	0	2	51
Chemistry	2	0	4	38

The graphical representation of the relationship between the different algorithms governed by the number as a function of time shows that more interest has been given to VQAs over the recent years (see figure 4). This is attributed to the observations made by Schuld and Petruccione (2021), stating that there are high hopes for quantum machine learning algorithms because of its parent fields (quantum mechanics and machine learning). On the one hand, there is a burgeoning commercial interest in quantum technology, which is beyond the sphere of a purely academic interest and is approaching the key point of becoming available for the implementation of quantum algorithms. On the other side, machine learning and artificial intelligence are promoted as a key (if not the key) future technology that businesses must invest in to stay competitive. When these two worlds collide, there is typically a tremendous amount of interest in quantum machine learning from the IT sector. However, this excitement is not necessarily matched by the scientific difficulties that academics are only now starting to investigate.

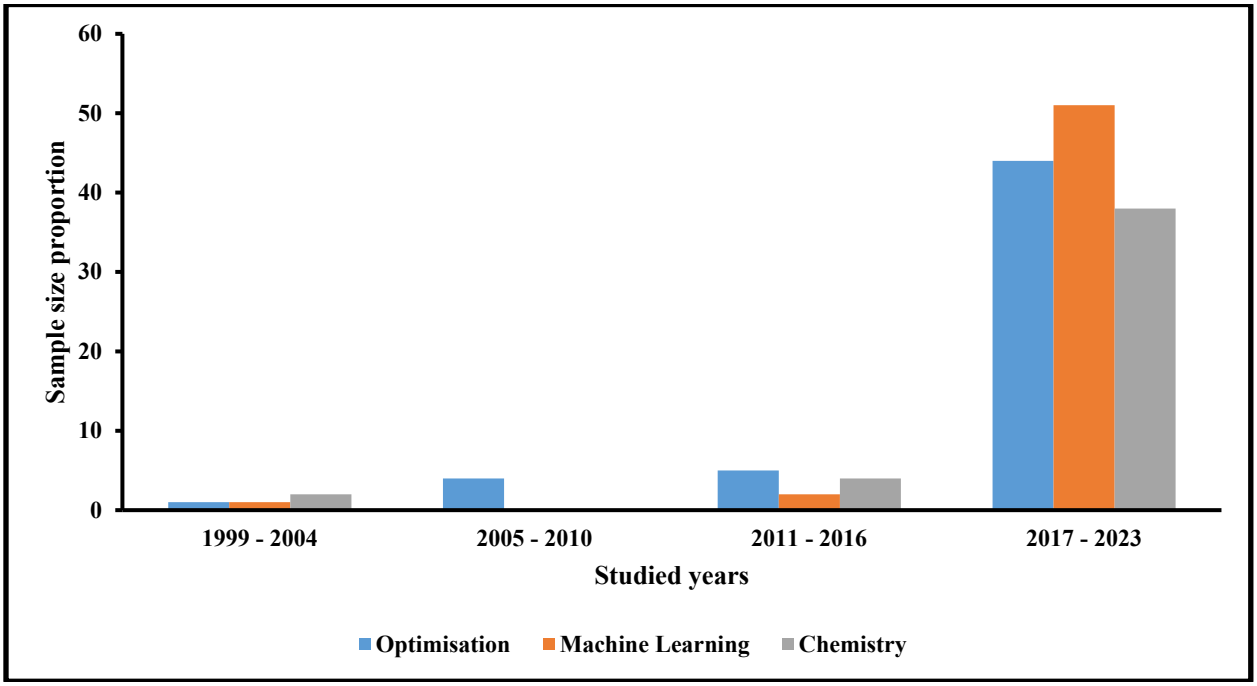

Figure 5. Publication proportions of VQAs, showing interest in the recent years in the targeted fields.

The nature of many statistical tests makes it possible for researchers to alter findings, whether consciously or accidentally, hence effect sizes are valuable to report on. Many people would view more samples when thinking about data analysis as good. However, it can be simple to distort the truth of the relationships in the data since many statistical tests are biased towards bigger samples, meaning larger samples are more likely to provide statistically significant findings. As effect sizes seek to quantify and conceptualize the links that this statistical significance is testing, they become crucial at this point (King 2019).

As a result of the above, Cohen's d standardized effect size values are reported in table 5 below. From table 5, it is observed that the values of Cohen's d were varying between 0.27 and 0.36, thereby indicating a small size effect between the different applications of VQAs. The rule of thumb related to Cohen's d results is mainly associated with the following size effect interpretations

Table 5. Statistical effect size calculated for Cohen's d values of the different applications of VQAs.

:Small effect, d = 0.2

- Medium Effect, d = 0.5
- Large Effect, d = 0.8

Application	Lower confidence Limit	Cohen's d value	Upper confidence Limit
Chemistry	0.10	0.27	0.24
Machine Learning	0.14	0.32	0.34
Optimisation	0.18	0.36	0.42

The observations from the figure above may be explained by the fact that the applications emanate from the same mother algorithm known as VQA. Furthermore, the information from table 1 can further explain the proportions observed in terms of an evenly distributed interest for the development of these algorithms**.**

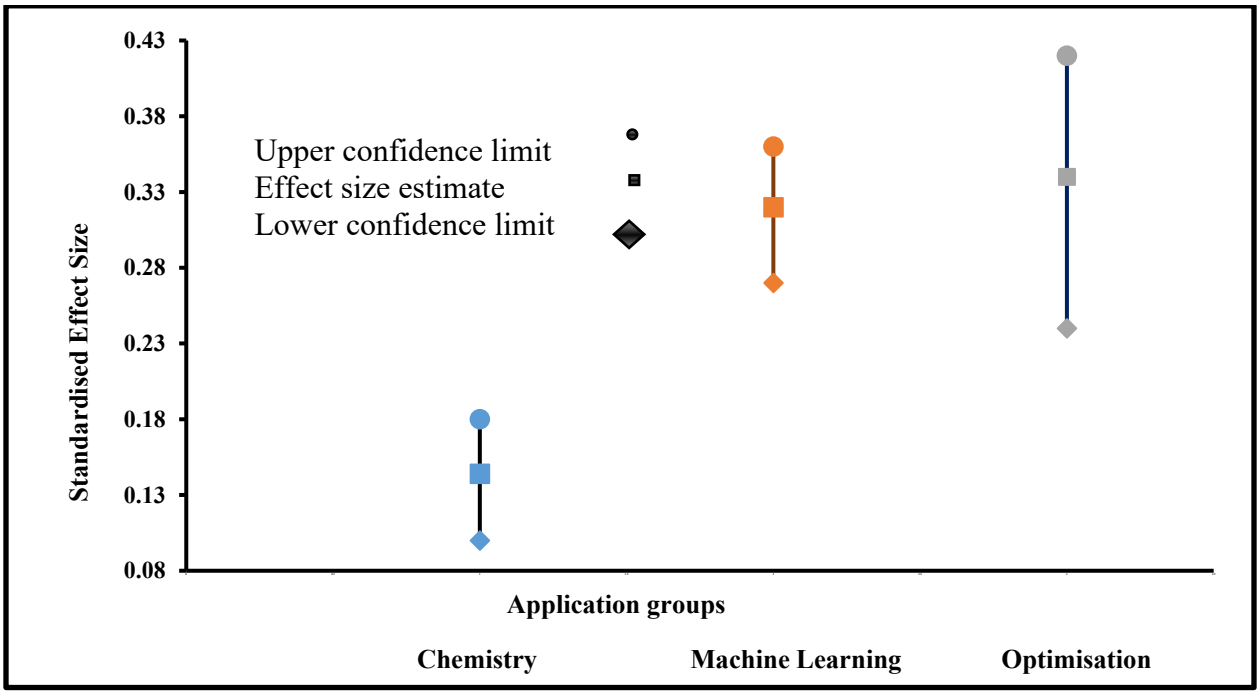

Figure 6. Standardized effect sizes of the different VQA applications.

The measured effect sizes may carry a further explanation related to the explanation problem, wherein the main question asked is associated to whether the effect is big enough to mean something. The answer to this question is yes, when looking at the proportion of data collected from this study, although VQAs can find further applications in other fields.

4. Conclusions

The current paper focused on systematically reviewing the application of VQAs in chosen study fields. The motivation towards this was as a result of the attention that these algorithms attract in many fields. To ensure reliability and avoiding biases, the obtained results were meta analytically analyzed, and the following were drawn as conclusions:

VQAs can be applied in the chemistry field for finding energy states and simulating dynamic chemical systems with VQEs being the most applied algorithm applied in different methods, such that provided an ansatz $|\psi(\theta)\rangle$, the

ground state $|\psi(\theta^*)\rangle$ can be best approximated by minimising the expectation over all possible parameter configurations.

Applications in optimization rely on maximizing or minimizing an objective hybrid quantum-classical function set to specified constraints, with QAOA being the algorithm with the most effect. The primary goal of the objective function is the number of fulfilled or satisfied clauses, defined on n bit strings.

In the machine learning field, VQAs have been of thorough application for development of models that can be trained and optimized for further applications, where quantum classifiers and quantum neural networks are the most used. The goal is to train a classifier to accurately predict each input's label using training data with input and labels. One may assume that a quantum classifier will also have this property as the non-linearity of conventional neural networks is crucial to their success.

In the metallurgy industry, as a branch of chemistry and in need of optimization, there may be a need to bring together all the above-mentioned applications, to develop, optimize, and simulate accurate models which can be used to better explain metallurgical scenarios. The rising need for design and development of novel materials for chemistry-related applications is already upon us, and therefore should employ quantum algorithms to optimize and simulate them.

The statistical analysis shows relationship amongst the different methods used in VQAs for various applications, thereby revealing a small effect size. There has been a skyrocketing increase in terms of the development and implementation of VQAs in the last 6 years as compared to any time before this time, thereby showing an increase in publications related to the chemistry, optimization, and machine learning fields.

The Cohen's d value indicates a small effect size amongst the different applications of VQAs, which is attributed to the proportion of publications observed over the assessed time period.

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