Vijayarangan Natarajan *Editor*

Quantum Artificial Intelligence

A Machine-Generated Literature Overview

Springer

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Preface

The field of quantum artificial intelligence (QAI) deals with solving academia and industrial challenges and improving the experience. This field involves multiple subjects like quantum information science, quantum computing, quantum programming, post-quantum cryptography, simulation, and quantum machine learning. It involves a lot of algorithms, computing methods, quantum spin, quantum particles, devices, and experiments toward analyzing the challenges.

This book, *Quantum Artificial Intelligence*, describes various research papers of QAI arising out of the challenges. It is a collection of research articles pertaining to QAI focusing on fundamental, programming, computational, and functional applications and challenges. There are six chapters presented in this book: Quantum information processing, Quantum programming, Post-quantum cryptography, Simulation of quantum and artificial systems, Quantum machine learning, and Applications. Each chapter is written based on theoretical and practical problems and solutions serving the unsolved problems related to academia and industry.

This book contains a variety of interdisciplinary academic fields and articles; the readers should have domain knowledge, including fundamentals of artificial intelligence, cryptography, programming, machine learning, mathematics, physics, mechanics and Computational, Artificial intelligence and Machine learning Systems (CAMS). This book is intended for graduate students, research scholars, academicians, and industry professionals.

The author of this book is grateful to God, family members, colleagues, friends, and publisher who encouraged a lot to investigate in a new era of QAI with a fathom of learning. This book is dedicated to them.

A special thanks to Shrutika Dasari of Springer Nature for editing the entire manuscript.

As written by the author: VIJAYARANGAN NATARAJAN

Dr. Vijayarangan Natarajan obtained his Ph.D. (Mathematics) in the year of 2001 at the Ramanujan Institute for Advanced Studies in Mathematics, University of Madras, Chennai. His doctoral research work was on Krein H*, J*-algebras, and triple systems. His research work includes mobile computing, Hilbert algebras, Jordan algebras, Lie algebras, number theory, elliptic curve cryptography, communication protocols, quantitative analysis, applications of real and complex analysis in image processing, artificial intelligence, machine learning predictions, stochastic computing, etc. He has also received the *Best Research Paper Award* given by the Ramanujan Mathematical Society in June 2000. He has a rich flavor of academic and industry experience around 30 years. He has presented his research work at several universities globally and published more than 100 articles, including papers, patents, and books. He is keen to focus on research areas like artificial intelligence, quantum computing, and stochastic process. He is fond of physical fitness too.

Chennai, Tamil Nadu, India — Vijayarangan Natarajan

About This Book

Auto-summaries can be generated by either an abstractive or extractive auto-summarization:

- An extraction-based summarizer identifies the most important sentences of a text and uses the original sentences to create the summary.
- An abstraction-based summarizer creates new text based on deep learning. New phrases are created to summarize the content.

The auto-summaries you will find in this book have been generated via an extractive summarization approach.

Each chapter was carefully edited by Dr. Vijayarangan Natarajan. The editors selected the papers which were then auto summarized. The editors have not edited the auto-summaries due to the extraction-based approach and have not changed the original sentences. You will find the editors' reviews and guidance on the auto-summaries in their chapter introductions.

In machine-generated books, editors are defined as those who curate the content for the book by selecting the papers to be auto-summarized and by organizing the output into a meaningful order. Next to the thoughtful curation of the papers, editors should guide the readers through the auto-summaries and make transparent why they selected the papers.

The ultimate goal is to provide a current literature review of Springer Nature publications on a given topic in order to support readers in overcoming information overload and to help them dive into a topic faster; to identify interdisciplinary overlaps; and to present papers which might not have been on the readers' radar.

Please note, that the selected papers are not used to train a LLM while the auto-summaries are created.

Introduction of the Book

The book *Quantum Artificial Intelligence* discusses the research on quantum information science, computational intelligence, quantum algorithms, machine learning, deep learning, artificial intelligence, and applications. This book covers quantum computing and quantum devices. To learn quantum artificial intelligence, it requires a variety of subjects like combinatorial optimization, soft computing, neural networks, learning algorithms, simulations, information science, and quantum mechanics.

Quantum computing is a growing subject which has an interrelationship with artificial intelligence, the computer science researchers explored. In this book, we provide the viability of practical applications in many domains. It is helpful to academia and industry to learn quickly about quantum artificial intelligence.

This book covers six chapters such as Quantum information processing, Quantum programming, Post-quantum cryptography, Simulation of quantum and artificial systems, Quantum machine learning, and Applications. Each chapter covers the in-depth knowledge of its domain. Chapter 3, Post-quantum cryptography, has some new crypto algorithms involving high-end computations. Finally, we have covered sufficient applications of quantum computing to gain a paramount of wisdom in this field.

Contents

Chapter 1
Quantum Information Processing

Introduction by the Editor

This chapter deals with an estimation theory of quantum particles and systems. The estimation of all parameters has been encoded in quantum state and processed through a quantum information matrix. The researchers have used the Born-Markov approximation for quantum estimation. Quantum mechanics has proven to be a valuable resource for the investigation of the behavior of complex networks. With the arrival of quantum computers, new algorithms have come out to do quantum chemistry, and importantly, atomic-like orbitals. Quantum compression algorithms help to develop the landscape of emerging IT technologies, IoT and Internet. Quantum Image processing (QIMP) has become a popular area of quantum research due to the ubiquity and primacy of digital image and video processing in modern life. In modeling noise in the quantum circuits, we assume a model by which each one- and two-qubit gates are followed by a depolarizing noise channel. Quantum computing (QC) potential use in High Energy Physics has led CERN, one of the top world users of large-scale distributed computing, to start programs such as the Quantum Technology Initiative (QTI) to further assess and explore the applications of QC. This chapter gives a survey on quantum cryptography in which quantum key distribution protocols are proven secure for industrial applications.

In this chapter, we outline a study involving quantum estimation and the dynamics of entangled qubits interacting with a bosonic environment. Then we cover up entangled qubits, bosonic bath interaction, Markovian master equation, quantum Fisher information and quantum correlation indicators. Further, we discuss the application of quantum-inspired measures for graph similarity to address challenges in graph comparison, which is relevant in various domains such as graph classification, outlier detection, and identifying interaction patterns in complex systems. This topic leads to highlight graph similarity and distinguishability, challenges in graph comparison, quantum-inspired measures for network similarity and experimental

V. Natarajan (ed.), *Quantum Artificial Intelligence*,
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evaluation. We bring out a procedure for defining virtual spaces and computing one-electron and two-electron integrals for plane-wave second quantized Hamiltonians in periodic systems. We cover up utilization of quantum computers through Microsoft Azure quantum service, correlation optimized virtual orbitals (COVOs), incorporation of first Brillouin zone integration and aperiodic systems.

In this chapter, we provide an overview of data compression algorithms within the context of edge computing, where processing is performed locally to minimize data transfer to centralized data centers. Edge computing addresses challenges associated with transferring large volumes of data generated remotely to centralized data centers efficiently.

We highlight the transformative potential of quantum technology and emphasize the importance of anticipating its future implications, including ethical, legal, social, and policy considerations. Then we describe the role of quantum computing (QC) in High Energy Physics, particularly at CERN, and report on the design and delivery of a series of lectures on quantum computing as part of the Quantum Technology Initiative (QTI).

Next, we focus on quantum renewable energy which shows the potential for quantum computing to address challenges in renewable energy, particularly in the context of the electrical grid.

In this chapter, we delve into the intersection of quantum information theory and relativistic quantum mechanics. The research demonstrates that in relativistic settings, the evolution of a massive spin-1/2 particle can contravene several standard assumptions of quantum information theory. Further, quantum physics explores the application of novel concepts surrounding uncommon quantum states to the physics of condensed matter, particularly focusing on solids within the framework of contemporary field theory. Also, we address the challenge of preserving entangled states in the presence of environmental effects, such as decoherence and dissipation, which can degrade the quantum information stored in a system. We introduce the concept of quantum programming, highlighting its interdisciplinary nature, drawing on principles from quantum mechanics, mathematics, and computer science. It sets the stage for understanding the significance of quantum programming languages in the context of quantum computing.

Quantum programming covers aspects such as support for quantum primitives and operations, quantum circuit construction, quantum algorithm implementation, and integration with classical programming languages.

The research survey exploits new ideas and methods in quantum states applied to condensed matter physics, especially solids, within contemporary field theory. It compares modern approaches with classical many-electron theory, focusing on ground states, excitations, quantum fluctuations, and phase transitions, with a particular emphasis on topological aspects and frustration effects. The survey covers variational methods, mean-field approximations, gauge field theory, and exotic states, alongside an overview of the theory of entangled topological states, spin liquids, and string networks.

In this chapter, we present how physical implementations of cryptographic algorithms can leak information, making them susceptible to side-channel attacks. The concept of secure computation amid such leakage is termed leakage resilience. An innovative research brings out leakage resilience with fault-tolerant quantum computation, demonstrating that a noise model ensuring fault tolerance also implies leakage resilience. For fault-tolerant implementation at the quantum gate, the researchers apply Toffoli gate in order to perform quantum classical translation. Further, the researchers have shown that leakage-resilient gadgets construction in the quantum circuits will be executed through fault-tolerant implementation.

The research work "Stationary States of a Dissipative Two-Qubit Quantum Channel and Their Applications for Quantum Machine Learning" describes the behavior of two-qubit systems under dissipation. It shows how stationary states can be harnessed for quantum machine learning or deep learning applications. The research study illustrates that by managing dissipation, it is possible to stabilize entangled states, which are crucial for quantum computing and machine learning algorithms.

The authors explore various methods to control and utilize dissipative processes to maintain coherence and entanglement in two-qubit systems. These methods are applied to create robust quantum states that can be used in quantum machine learning tasks, providing a foundation for developing more efficient quantum algorithms and improving the reliability of quantum computations in the presence of environmental interactions. The recent research work describes how to manage these adverse effects to provide stationary entangled states for quantum machine learning (QML). Further, the research brings out that the channel can determine if an initial quantum state will result in a stationary entangled state. This algorithm is applied to propose a theoretical framework for quantum neural networks (QNNs) using variational quantum circuits. Then these circuits encode data in the continuous variables (CVs) of the two-qubit states. Subsequently, linear, and nonlinear transformations in the QNN are implemented using the stationary states of the two-qubit channel and the measurement process, respectively. The model's effectiveness is tested on supervised binary classification tasks, demonstrating that integrating non-unitary transformations and parallel-processed neural computing in such a channel meets the requirements for a meaningful QNN. This CV-QNN model, with enough layers, could execute any algorithm feasible on a universal CV quantum computer. Nowadays, a lot of research programs fulfill the challenges in qubit channels and the measurement process through QML.

At the end of Chap. 1, we bring out a significant connection between two important areas of research: leakage resilience in cryptographic algorithms and fault-tolerant quantum computation. By leveraging techniques from quantum error correction and fault tolerance, the research provides insights into how cryptographic schemes can be made resilient to leakage.

Machine Generated Summaries

Disclaimer: The summaries in this chapter were generated from Springer Nature publications using extractive AI auto-summarization: An extraction-based summarizer aims to identify the most important sentences of a text using an algorithm and uses those original sentences to create the auto-summary (unlike generative AI). As the constituted sentences are machine selected, they may not fully reflect the body of the work, so we strongly advise that the original content is read and cited. The auto generated summaries were curated by the editor to meet Springer Nature publication standards. To cite this content, please refer to the original papers.

Machine generated keywords: spin, theory, initial state, edge, topological, survey, material, interaction, article, mathematical, electronic, basis, quantum compute, ground state, series.

Multiparameter Estimation for a Two-Qubit System Coupled to Independent Reservoirs Using Quantum Fisher Information [1]

This is a machine-generated summary of:

Bukbech, S.; El Anouz, K.; El Allali, Z.; Metwally, N.; El Allati, A.: Multiparameter estimation for a two-qubit system coupled to independent reservoirs using quantum Fisher information [1].

Published in: Quantum Studies: Mathematics and Foundations (2023).

Link to original: https://doi.org/10.1007/s40509-023-00303-6

If you want to cite the papers, please refer to the original.

For technical reasons we could not place the page where the original quote is coming from.

Abstract-Summary

"The quantum Fisher information is used as an estimator of the phase damping of the initial state settings and the interaction damping parameter."

"It is exhibited that the initial state settings play a role as a controller of the precision of the estimation degree of these parameters."

"We classified the state that could be used to estimate the phase damping with high accuracy."

"The constant behavior of the variances of the estimated parameters shows that the optimal estimation could be achieved for small values of the damping parameter."

Introduction

"Various outstanding results in statistical theory and quantum information theory have been explained according to the concept of quantum measurement, which gives rise to many substantial theories, including quantum metrology, quantum estimation theory and so on. The major goal of quantum estimation theory is to perform robust precision measurements for parameters included in quantum systems."

"In this spirit, improvements in precision limits can be fulfilled with the simultaneous quantum estimation of all parameters encoded in the quantum state [2–4]."

"Exhaustively, the process of estimating various parameters at the same time provides more robust precision than estimating them individually via Quantum Fisher Information Matrix (QFIM)."

"As we have already pointed out, the QFIM is the key quantity representing the precision limit for multiparameter quantum estimation because of its applications in different domains [5–12]."

From Classical to Quantum Estimation Theory

"One of the most significant approaches to multiple parameter estimation is to perform individual measurements for each parameter."

"Estimating all parameters simultaneously provides robust precision bounds [4]."

"We examine some preliminaries of the multi-parameter quantum estimation theory, where we shall investigate the QFIM and construct the corresponding QCRB."

"The QFIM is a fundamental tool on which multiparameter quantum estimation is built."

"The estimation precision bound is determined by the quantum multiparameter QCRB."

"Saturating the QCRB is a critical issue in quantum estimation."

"For quantum single-parameter estimation, the QCRB in principle can be reached all the times [4]."

"The problem arises in multi-parametric quantum estimation, because quantum measurements are not always commutative."

"The non-existence of an optimal common measurement for the estimation of all parameters."

Proposed Model

“In the context of the Born–Markov approximation, the bath correlation is important in determining how the system evolves over time.”

“In this inspiration, we should mention that in the above calculations, we have used the Born–Markov approximation as a good assumption that simplifies the derivation of the master equation by assuming that the environment relaxes to its equilibrium state after being perturbed by the system.”

“We intend to verify whether we have an optimal estimation using the proposed model.”

[Section 1]

“This indicates that the estimation of the phase parameter depends on the initial state settings, whether it is partially/maximally entangled.”

“This means that the initial state is prepared in a maximally entangled state of the Bell type (MES).”

“The initial state settings have a major role in governing the decay rate, where those prepared in MES are the most sensitive to the damping parameter.”

“The increasing rate depends on the initial state settings, whether it is a maximally or partially entangled state.”

“This confirms that the initial state settings could be used as a controller on the precision of estimation.”

“The ability to estimate the damping parameter, however, is dependent on whether the initial qubit system is prepared in a MES or a PES.”

Conclusion

“The possibility of estimating the phase of the initial state and the damping parameters of the environment is discussed, where we estimate these parameters individually and simultaneously by using the quantum Fisher information (QFI) as an estimator.”

“At a later time, where the initial state turns into a partially entangled state (PES), the estimation process of the phase parameter increases.”

“The decay rate of QFI as an estimator of the phase parameter that is depicted for maximally entangled states is larger than the one displayed for partially entangled states.”

“The sensitivity of the estimation degree to large values of the damping parameter is discussed for different initial state settings.”

“The behavior of the minimum variance of the damping parameter shows that, one can estimate it with high precision if the initial system is prepared in a partially entangled state.”

Quantum-Inspired Measures of Network Distinguishability [13]

This is a machine-generated summary of:

Polychronopoulou, Athanasia; Alshehri, Jumanah; Obradovic, Zoran: Quantum-inspired measures of network distinguishability [13].

Published in: Social Network Analysis and Mining (2023).

Link to original: https://doi.org/10.1007/s13278-023-01069-w

If you want to cite the papers, please refer to the original.

For technical reasons we could not place the page where the original quote is coming from.

Abstract-Summary

"The recent emergence of information physics as a theoretical foundation for complex networks has inspired the utilization of measures, initially developed for use with quantum mechanical systems, for the solution of graph theory research problems."

"A network similarity measure is required for any data mining application on graphs, such as graph clustering, classification, or outlier detection."

"A natural starting point for the identification of such a network similarity measure is information physics, offering a series of measures typically used to quantify the distance of quantum states."

Introduction

"A variety of network theoretic tools are used for the analysis of these complex systems (Bunke et al. [14]), and the question of graph distinguishability or graph similarity is often a central aspect of study."

"Quantum mechanics has proven to be a valuable resource for the investigation of the behavior of complex networks (Biamonte et al. [15])."

"Quantum gases have been used to describe network evolution, and the emergence of different structures in complex networks has been represented in terms of a quantum-classical transition for quantum gases (Javarone et al. [16])."

"These quantum-inspired methods offer a mathematical method of graph comparison, they satisfy the mathematical properties of a metric, offer intelligible results with high interpretability, and were shown in Polychronopoulou et al. [17] to satisfy intuitive graph similarity properties for monoplex networks."

Methods

"This formulation allows multiplex networks to be compared using the distance measures introduced for single layer graphs, with the supra-adjacency matrix substituting the monoplex adjacency."

"Alternative representations have been proposed for multiplex networks, typically constructing a monoplex network by aggregating the various layers."

"The authors of Sánchez-García et al. [18] introduced the notion of graph quotients and an aggregate network that summarizes the connections of nodes among the different layers, normalised by the multiplexity degrees of the nodes."

"If the monoplex aggregate is seen as the network describing the absolute connection between nodes, and the layers are seen as evidence of this connection, then the extension for use with multiplex networks is natural."

"The aggregate monoplex describes the reliability of connections between nodes, as affected by multiple sources of information, the layers of the multiplex network."

Evaluation on Artificial Data

"In the simple case of repeated node removals, the monotonically increasing behavior of the distance measures is evident and confirms that they all act as measures of graph distinguishability."

"With the exception of Bures distance, the measures have identified that the removal of one node is more crucial for smaller networks, as is evident by the slope of the curves."

"All distances are sensitive to distinguishing targeted from random operations, both for the case of continuous edge removals targeting popular nodes, and continuous edge removals targeting edges of higher weights."

"Each network is then continuously modified, applying at each step one elementary graph edit operation, and the distance between the modified and original network is calculated."

"To the case of monoplex networks, quantum distances satisfy intuitive similarity aspects: they continuously increase as the networks are further modified and this applies to most multiplex representations and all types of data."

Applications on Real Data

"As a first application, we evaluate the effectiveness of the distance measures on classification problems with real world single layer networks."

"Following this motivation, we evaluate the effectiveness of the quantum-inspired graph distance measures in the problem of computing pairwise similarities between layers, and then performing hierarchical clustering of structurally similar layers in multiplex networks."

"The plot indicates that most of the distances are able to achieve an accurate classification when two or more layers are used, with an F1 score that is increasing with the addition of more layers."

"What is evident is that traditional methods, and the baselines, such as DELTACON, as well as quantum distances are increasing their accuracy with the addition of more layers."

"For many of the multiplex representations the accuracy is starting to drop after the addition of a given number of layers, defining a point at which the complexity of the problem increases, more evidently for the edge-weight and trace distances."

Discussion

"These measures are well-established mathematical methods that incorporate the intrinsic structure of the entire network and have high interpretability."

"Quantum and information physics undoubtedly compose a rich resource of mathematically established and interpretable measures, used for the evaluation or comparison of natural systems."

"Many of these measures have been translated into meaningful complex network tools, in this work and previous ones (Biamonte et al. [15])."

"In the case of multiplex networks, quantum states separability can be seen as layer separability as well possible measure of the layers' informative power."

Periodic Plane-Wave Electronic Structure Calculations on Quantum Computers [19]

This is a machine-generated summary of:

Song, Duo; Bauman, Nicholas P.; Prawiroatmodjo, Guen; Peng, Bo; Granade, Cassandra; Rosso, Kevin M.; Low, Guang Hao; Roetteler, Martin; Kowalski, Karol; Bylaska, Eric J.: Periodic plane-wave electronic structure calculations on quantum computers [19].

Published in: Materials Theory (2023).

Link to original: https://doi.org/10.1186/s41313-022-00049-5

If you want to cite the papers, please refer to the original.

For technical reasons we could not place the page where the original quote is coming from.

Abstract-Summary

"A procedure for defining virtual spaces, and the periodic one-electron and two-electron integrals, for plane-wave second quantized Hamiltonians has been developed, and it was validated using full configuration interaction (FCI) calculations, as well as executions of variational quantum eigensolver (VQE) circuits on Quantinuum's ion trap quantum computers accessed through Microsoft's Azure Quantum service."

"This work is an extension to periodic systems of a new class of algorithms in which the virtual spaces were generated by optimizing orbitals from small pairwise CI Hamiltonians, which we term as correlation optimized virtual orbitals with the abbreviation COVOs."

"With these procedures, we have been able to derive virtual spaces, containing only a few orbitals, that were able to capture a significant amount of correlation."

"Calculations performed on the Quantinuum H1–1 quantum computer produced surprisingly good energies, in which the error mitigation played a small role in the quantum hardware calculations and the (noisy) quantum simulator results."

Introduction

"With the arrival of quantum computers, researchers are actively developing new algorithms to carry out quantum chemistry calculations on these platforms, in particular for calculations containing strong electron-electron correlations (aka high-level quantum chemistry methods)."

"Most high-level quantum chemistry methods in use today (e.g., full configuration interaction (FCI) (Szabo and Ostlund [20]; Ross [21]; Gan et al. [22]; McArdle et al. [23]; Tubman et al. [24]; Sugisaki et al. [25]; Kawashima et al. [26]), coupled cluster (CC) (Coester [27]; Coester and Kummel [28]; Čížek [29]; Paldus et al. [30]; Mukherjee et al. [31]; Purvis and Bartlett [32]; Bishop and Kümmel [33]; Paldus and Li [34]; Crawford and Schaefer [35]; Bartlett and Musiał [36]; Peng et al. [37]), and Green's function (GF) (Green [38, 39]; Feynman [40, 41]; Martin and Schwinger [42]; Baym and Kadanoff [43]; Peng et al. [37]) approaches) are based on second-quantized Hamiltonians, which are written in terms of the creation and annihilation operators of the Fermion orbitals along with the one-electron and two-electron integrals for the system."

"One of the first, and still popular, class of basis sets used in quantum chemistry methods are atomic-like orbitals or the linear combination of atomic orbitals (LCAO) basis set."

"We have recently developed new methods for generating optimized orbital basis sets, called COVOs (Bylaska et al. [44])."

Pseudopotential Plane-Wave Second-Quantized Hamiltonian

"A standard way to remove this issue in plane-wave calculations is to replace these singular potentials by pseudopotentials."

"For methods that utilize linear combinations of atomic orbitals (LCAO) as the basis, the size of the basis set and subsequently generated Hartree-Fock orbitals is fairly small."

"Many of the periodic forms presented in the following sections are written in terms of Fourier space using periodic plane-wave basis sets, rather than real space."

"Descriptions of the plane-wave methods used in this work can be found in the following references (Bylaska et al. [45, 46]; Bylaska [47]; Bylaska and Rosso [48]; Bylaska et al. [49]; Pickett [50]; Ihm et al. [51]; Car and Parrinello [52]; Payne et al. [53]; Remler and Madden [54]; Kresse and Furthmüller [55]; Marx and Hutter [56]; Martin [57]; Valiev et al. [58]; Chen et al. [59])."

Algorithm for Defining a Virtual Space with a Small CI Hamiltonian

"These new types of orbitals are able to capture significantly more correlation energy than with virtual orbitals coming from Hartee-Fock (Bylaska et al. [44])."

"The above formulas can be generalized to work beyond two electron systems by using corresponding orbitals techniques (King et al. [60]; Bylaska and Rosso [48])."

"We also note the COVOs approach is similar in spirit to the optimized virtual orbital space (OVOS) approach developed over 30 years ago by Adamowicz and Bartlett Adamowicz and Bartlett [61]; Adamowicz et al. [62]."

"The corresponding orbital transformation (King et al. [60]) can be used to generalize for different orthonormal sets."

"In cases, where the two-electron matrix elements of the spin-orbitals have a double noncoincidence (King et al. [60]) the matrix elements are again block diagonal, otherwise the matrix elements can be represented as a sum of periodic Coulomb and exact exchange energies, where the Filon integration strategy (Bylaska et al. [49]) can be used to fold in the first Brillouin zone integration present in the exact exchange energies."

Results for the Ground State of the LiH Molecule Using Periodic Boundary Conditions

"The NWChem program package (Kendall et al. [63]; Valiev et al. [64]; Bylaska et al. [45]; Bylaska [47]; Apra et al. [65]) was used for all calculations in this study, except for the FCI calculations, which used the TINYMRCC suite by Jiří Pittner."

"The average difference error for the 1, 4, 8, and 12 COVOs calculations from the 18 COVOs calculation is 12.9 kcal/mol, 2.7 kcal/mol, 1.0 kcal/mol, and 0.4 kcal/mol respectively."

"The energy for large R should be the same as the combined energy of the isolated H and Li atoms."

"At large R a significant difference between aperiodic and periodic calculations can be observed."

Quantum Computer Calculations for the Ground State of the LiH Molecule Using Periodic Boundary Conditions

"To computing ground-state energies at different bond lengths on a quantum computer, we also wanted to measure the effects of noise on the corresponding circuit evaluations."

"The VQE method is a hybrid quantum-classical approach in which energies are evaluated on quantum hardware or simulators, and classical computers perform the algorithm to optimize the variational parameters."

"Proposals for robust quantum error correction require qubit numbers and performance that are not yet available via Cloud-based NISQ devices today (Shor [66]; Cory et al. [67]; Reed et al. [68]), so before executing the circuits on the H1–1 quantum computer, we wanted to ensure that noise played a manageable role in computing the ground-state energies."

"After convincing evidence that the error from the noise for this circuit can be well tempered, we performed the last stage of the calculations, where the same energy evaluation and error mitigation technique was performed for 500 runs on the Quantinuum H1–1 quantum computer."

Conclusion

"For an (N + 1)-state Hamiltonian, the method is based on optimizing the virtual orbitals to minimize a small select CI Hamiltonian (i.e., COVOs) that contains configurations containing all N filled RHF orbitals and the one virtual orbital to be optimized."

"The method was applied to the simple, but non-trivial, LiH molecule in a periodic system, and we were able to obtain good agreement between the total energies from aperioidic and periodic plane-wave FCI calculations."

"Subsequent calculations showed that the correlation energy converged steadily as more virtual orbitals were included in the calculation."

"With 18 virtual orbitals the correlation energies were found to be converged to less than 1 kcal/mol."

"That the energies obtained using the H1–1 quantum computer were able to reproduce the FCI values to less than 11 milliHartree (6.9 kcal/mol) with a modest number of 500 shots performed; slightly less when corrected for noise."

Classical and Quantum Compression for Edge Computing: The Ubiquitous Data Dimensionality Reduction [69]

This is a machine-generated summary of:

Bagherian, Maryam; Chehade, Sarah; Whitney, Ben; Passian, Ali: Classical and quantum compression for edge computing: the ubiquitous data dimensionality reduction [69].

Published in: Computing (2023).

Link to original: https://doi.org/10.1007/s00607-023-01154-0

If you want to cite the papers, please refer to the original.

For technical reasons we could not place the page where the original quote is coming from.

Abstract-Summary

"Edge computing aims to address the challenges associated with communicating and transferring large amounts of data generated remotely to a data center in a timely and efficient manner."

"A survey of data compression algorithms with a focus on edge computing."

"Not all compression algorithms can accommodate the data type heterogeneity, tight processing and communication time constraints, or energy efficiency requirement characteristics of edge computing."

"We discuss specific examples of compression algorithms that are being explored in the context of edge computing."

Introduction

"Identification, as well as the development of data compression algorithms for EC devices is important for the implementation of EC."

"Given the heterogeneity of EC data types, volumes, processing, and communication time sensitivities, and resource constraint severities, it stands to reason to employ or devise compression algorithms that are tailored to such highly dynamic EC environments."

"We review existing data compression algorithms with an emphasis on their suitability for EC."

"We discuss the characteristics of a given data compression technique that may render it more suitable for EC than other techniques."

"With recent efforts to make use of quantum computing, "new" data types are being created, which may require quantum compression algorithms."

"We end with the quantum perspective of information theory with an introduction and a survey of quantum algorithms to compress quantum data."

Data at the Edge

"This section concerns recent work on compression algorithms designed for data at the edge."

"Before discussing data compression in the context of edge computing, we give a brief overview of the function of compression algorithms and the reasons that users may turn to them."

"If holding the entirety of the decompressed data in memory is impossible in this scenario, the user will require an algorithm whose output supports partial decompression or even computations performed directly on the compressed representation."

"Much of the data encountered on the edge is of a structured type (image data, for example) that has been previously studied and its compression algorithms are already available."

"One emergent theme in the literature is the design of new compression algorithms to handle novel edge data types."

"Beyond new compression algorithms, successful management of edge data requires an understanding of the relative strengths and weaknesses of existing, competing methods."

Compression at the Edge

"What makes data compression at the edge different than compression applied to data elsewhere on the network is the characteristic features of edge computing applications."

"At the edge, data compression improves not only the storage and latency but also the computation offloading."

"In the context of fog computing, such an optimization problem was recently reported in the work by Nguyen et al. [70], where studies with compression, first only at the mobile edge sensor, and then, at both the sensor and the fog server, showed that high levels of reduction in energy and delay cost can be obtained."

"Efficient data compression at the edge with minimized loss of information is a key to reducing energy consumption and enabling edge applications."

"Deepu et al. [71], aimed to reduce power consumption for IoT devices and investigated a data transmission method based on lossy and lossless data compression for wireless sensors."

Classical Compression Algorithms

"The original input data is approximated by Chebyshev polynomials, achieving very high compression ratios on serial data streams with minimal loss of scientific information."

"Power-efficient acquisition, processing, and storage, and time-efficient transmission of healthcare data at the edge is an active area in which enabling compression techniques are needed."

"The discrete transform, used in data compression, returns a vector of the same length as the input vector."

"With the steady increase in the processing power, Karhunen–Loeve transform (KLT) has been gaining increasing attention in signal and data processing for denoising and compression."

"For cases when the data matrix S is sparse (i.e., not dense) or can be represented in a domain in which the signal matrix has many zero or near zero components, compressed sensing can use the information about the sparsity in S to reconstruct the signal with a smaller sampling rate than permissible by (but without violating) the sampling theorem."

Quantum Compression Algorithms

"By invoking quantum computing at the edge where better sensors that can operate faster and generate more complete datasets, new data compression techniques and algorithms are necessary."

"The notion of an edge quantum computing device was recently introduced and described in the form of a realization of quantum sensors that generate quantum state data to be processed by quantum processors and quantum algorithms and communicated through quantum internet [72]."

"Several papers in the literature address this problem using different algorithms or schemes, quantum—classical data, quantum ensembles, state projection, etc. In

[73], a protocol for which an ensemble of qubits, storing all information about the quantum state, can in theory be perfectly compressed into exponentially fewer physical qubits is proposed."

"In [74], the authors consider the problem of One-Shot classical data compression while using quantum side information."

Conclusion

"The presented survey puts forth the ubiquity of data compression in the landscape of emerging IT technologies and IoT, as well as in relation to near-future visions of the quantum internet and the quantum IoT. It specifically emphasizes the need for efficient data compression for resource-constrained edge applications."

"As can be summarised from the presented material, the diversity in both the number of algorithms of potential for compression at the edge and in the edge computing use cases means that the unification of the pertinent concepts and approaches will be challenging."

"From a methodological point of view and future work directions, one may seek to explore new integral transforms of potential for data compression and examine their efficiency as the compression method of choice for edge computing."

"An interesting case could be that an index transform such as the Mehler–Fock transform, or Kontorovich–Lebedev transform which may find potential application in data compression."

Toward Implementing Efficient Image Processing Algorithms on Quantum Computers [75]

This is a machine-generated summary of:

Yan, Fei; Venegas-Andraca, Salvador E.; Hirota, Kaoru: Toward implementing efficient image processing algorithms on quantum computers [75].

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For technical reasons we could not place the page where the original quote is coming from.

Abstract-Summary

"Quantum information science is an interdisciplinary subject spanning physics, mathematics, and computer science."

"To promoting its mathematical and physical foundations, scientists and engineers have increasingly begun studying cross-disciplinary fields in quantum information processing, such as quantum machine learning, quantum neural networks, and quantum image processing (QIMP)."

"These issues include enhancing current models of quantum image representations, designing quantum algorithms for solving sophisticated operations, and developing physical equipment and software architecture for capturing and manipulating quantum images."

Introduction

"The expectation is that harnessing the properties of quantum-mechanical systems in QIMP (e.g., computational parallelism) will result in the realization of advanced technologies that will outperform, enhance, or complement existing and upcoming digital technologies for image and video processing tasks."

"QIMP has become a popular area of quantum research due to the ubiquity and primacy of digital image and video processing in modern life (Yan and Venegas-Andraca [76])."

"Different from all the previous works, the present paper seeks to arouse the interest of scientific and engineering communities toward the greater realization of QIMP-based technologies by identifying and discussing three primary issues using a few simulation experiments, the development of which will be most helpful for advancing the field of QIMP: improving current models of quantum-image representations, core level of designing quantum algorithms for solving sophisticated operations, and developing hardware (physical equipment) and software architectures (a new genre of blueprints) for capturing and manipulating quantum images."

Storage and Retrieval of Images in Quantum Systems

"We now analyze the FRQI representation model in order to quantify the amount of resources needed to store and retrieve information contained in quantum images."

"Current models of quantum image representation require extensive improvement to integrate and take full advantage of quantum-mechanical properties, as well as to design efficient strategies for image retrieval."

"Steps in QIMP research programs must include quantum-state tomography techniques (Banaszek et al. [77]) that, possibly combined with advanced computational paradigms such as machine learning (Youssry et al. [78]), would potentially lead to optimized quantum image retrieval processes [4]. A potential fruitful area for further development of QIMP is to test upcoming quantum image representation models, algorithms, and information retrieval techniques in fields in which images are likely to play a key role."

"A promising research avenue would be to design quantum image storage and retrieval methods suitable for use as input to algorithms from the emergent fields of

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