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Application

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Title of the project: **Harmonic oscillator-inspired Particle Swarm Optimization applied to the Variational Quantum Eigensolver**

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Annotation - English version

The quantum computer is a promising emerging technology but has drawbacks in its current application due to the hardware limitations of a purely-quantum computer. As a result, current research in attempting to apply quantum computers to specific physical problems/systems relies on a quantum-classical hybrid of algorithms. One such powerful algorithm is The Variational Quantum Eigensolver (VQE), whose strong potential as an application has garnered growing attention in the quantum computing industry (in the current NISQ era). This algorithm works to find the lowest energy eigenvalues for physical systems, and it therefore can, for obvious reasons, be a very useful tool in industries and research institutes that work in the fields of condensed matter physics and chemistry, where determining the energy levels of a physical-chemical system accurately is crucial and necessary. The VQE algorithm, being a hybrid algorithm, contains a quantum part and a classical part (refer to attachment image). The quantum part uses the quantum computer to find the lowest energy eigenvalue for a Hamiltonian that represents some physical system using a trial wavefunction. The classical part of the algorithm uses a classical optimization technique to parametrize the wave function such that the expectation value of the Hamiltonian is minimized. The entire algorithm can be visualized in the figure [see separate attachment figure. In our previous work of applying a non-gradient population-based optimization method known as Particle Swarm Optimization (PSO), we were able to develop a more refined version of this classical optimization technique that is based on physics-intuition, calling it Harmonic-oscillator Particle Swarm Optimization (HOPSO). The advantage of this algorithm is that it allows for more fine-tuning of its parameters and does not encounter an issue with explosions in the system due to its physics-based foundation (see the submitted manuscript here: https://bit.ly/4g8qs5W). We now seek to apply this newly developed optimization technique onto a quantum computer.

Anotácia - Slovenská verzia

Kvantový počítač je sľubná vznikajúca technológia, ale má nevýhody vo svojej súčasnej aplikácii kvôli hardvérovým obmedzeniam čisto kvantového počítača. Výsledkom je, že súčasný výskum v snahe aplikovať kvantové počítače na špecifické fyzikálne problémy/systémy sa spolieha na kvantovo-klasický hybrid algoritmov. Jedným z takýchto výkonných algoritmov je The Variational Quantum Eigensolver (VQE), ktorého silný potenciál ako aplikácie si získal rastúcu pozornosť v odvetví kvantovej výpočtovej techniky (v súčasnej dobe NISQ). Tento algoritmus pracuje na nájdení najnižších vlastných hodnôt energie pre fyzikálne systémy, a preto môže byť zo zrejmých dôvodov veľmi užitočným nástrojom v priemyselných odvetviach a výskumných ústavoch, ktoré pracujú v oblasti fyziky a chémie kondenzovaných látok, kde sa určujú úrovne energie fyzikálno-chemický systém presne je rozhodujúci a nevyhnutný. Algoritmus VQE, ktorý je hybridným algoritmom, obsahuje kvantovú časť a klasickú časť (pozri obrázok v prílohe). Kvantová časť využíva kvantový počítač na nájdenie najnižšej vlastnej hodnoty energie pre hamiltonián, ktorý predstavuje nejaký fyzikálny systém pomocou skúšobnej vlnovej funkcie. Klasická časť algoritmu využíva klasickú optimalizačnú techniku na parametrizáciu funkcie wav tak, aby sa minimalizovala očakávaná hodnota hamiltoniánu. Celý algoritmus je možné znázorniť na obrázku [pozri samostatnú prílohu obrázok 1a]. V našej predchádzajúcej práci na aplikovaní negradientovej populačnej optimalizačnej metódy, známej ako Particle Swarm Optimization (PSO), sme dokázali vyvinúť prepracovanejšiu verziu tejto klasickej optimalizačnej techniky, ktorá je založená na fyzike-intuícii a nazývame ju harmonická- oscilátor Particle Swarm Optimization (HOPSO). Výhodou tohto algoritmu je, že umožňuje viac dolaďovať svoje parametre a vďaka svojmu fyzikálnemu základu nenaráža na problém s výbuchmi v systéme (pozri odovzdaný rukopis tu: https://drive.google. com/file/d/107MNIZYkXkdXugoYTsAsC-egMrSqbZO7/view?usp=drive_link). Teraz sa snažíme aplikovať túto novo vyvinutú optimalizačnú techniku na kvantový počítač.

Scientific Objectives

Our scientific aim is to apply this newly developed optimization technique, HOPSO (see the submitted manuscript here: https://drive.google.com/file/d/107MNIZYkXkdXugoYTsAsC-egMrSqbZO7/view?usp=drive_link), on the Variational Quantum Eigensolver, and then proceed to analyze its performance on a real quantum computer. In doing so, we not only introduce a new physics-based non-gradient optimization method to the optimization world, but we also seek to explore the possible potentials and drawbacks in the VQE framework, including comparing the currently-popular gradient based methods to a new physics-inspired non-gradient population optimization method. HOPSO's introduction is expected to improve the accuracy and efficiency of quantum computations, facilitating more precise energy level determinations in complex molecular systems. Through integrating HOPSO, we anticipate setting new benchmarks in the optimization capabilities of hybrid quantum systems. Furthermore, in our research we expect to be able to fight one of the main drawbacks of current VQEs, namely the inability to find a minimum in the situation of waste Barren plateaus, i.e. areas of parameter values with equal energy level. Finally, we aspire for this research project to enable the application of quantum computational techniques to a broader range of physical problems, potentially revolutionizing fields that depend on precise energy calculations. The project aims to demonstrate the scalability and applicability of HOPSO in real-world quantum tasks, potentially leading to significant advancements in both theoretical and applied quantum computing. In conclusion, the new results, in both the theoretical- and the practical (application), will serve to both the growing quantum computing field as well as to the (classical) computation and optimization community.

State of the Art

The Variational Quantum Algorithm was first developed in 2014 in the paper titled “A variational eigenvalue solver on a photonic quantum processor” by Alberto Peruzzo et al. Since then, many papers have been published and a concise review of the methods and practices can be found in the recently published “The Variational Quantum Eigensolver: A review of methods and best practices” (Tilly et al., 2022; doi: 10.1016/j.physrep.2022.08.003). The Particle Swarm Optimization algorithm was first developed by James Kennedy and Russel Eberhart in 1995 with the paper “Particle Swarm Optimization” (doi: 10.1109/ICNN.1995.488968). Since then, various forms of PSO and its application have emerged in notable published works such as “A Modified Particle Swarm Optimizer” (Y. Shi and R. Eberhart, 1998; doi: 10.1109/ICEC.1998.699146) and “Recent advances in particle swarm” (Xiaohui Hu et al., 2004; doi: 10.1109/CEC.2004.1330842). “A Comprehensive Survey on Particle Swarm Optimization Algorithm and Its Applications” (Zhang, Y., Wang, S., & Ji, G., 2015; doi: 10.1155/2015/931256) provides a comprehensive survey of various PSO algorithms, covering both traditional and recent developments. Our current paper is titled “Harmonic Oscillator based Particle Swarm Optimization”. This is a newly-invented optimization algorithm that is rooted in the Particle Swarm Optimization (PSO) algorithm in the fact that they both consider a particle’s position (i.e. candidate-solution to the problem) and velocity, however, the two differ in how they apply these quantities in the iterative process. Namely, the velocity of the PSO algorithm is directly influenced by the linear sum of the “cognitive” influence and a “social” influence. These terms represent the individual particle’s best result in its personal history, and the best result found in the history of the entire collective swarm, respectively. The new velocity then directly influences the position to get a (potentially) better solution of the individual particle with each iteration. In other words, the particles collectively converge to an optimal value. The HOPSO algorithm, however, takes a new term called the “attractor” which is a weighted sum representing the balance between the “cognitive” and “social” influences. Since the harmonic oscillator equation is well known in physics, we use this equation (specifically, the damping oscillation) as our position equation, and its derivative as the velocity equation. It is possible to know the initial position and velocity given time is set to zero initially, from which we can then derive the initial amplitude. Since the attractor term is some vector, we include this into the equation for the amplitude, thereby creating a model in which the particles will periodically oscillate around this attractor term, damping overtime. The amplitude equation also includes the position, the velocity, the damping parameter, angular frequency and a phase (the latter three serve as tuning parameters). These are all derived from the logic of the harmonic oscillator. The amplitude determines how, and where the particle searches the space. The particle travels in oscillatory motion, and when an improved global or personal position is found, the attractor term will change, which then reset the position, velocity, and amplitude thereby allowing the particle to search in some new area corresponding to where the better position was found. The manuscript is currently being reviewed in its final stages of completion and is anticipating publication (see the submitted manuscript here: https://bit.ly/4g8qs5W).

Methodology and Work Plan

In the paper by Tilly et al. (2022) (referenced in the “state of the art” section), the Variational Quantum Eigensolver (VQE) pipeline is presented as an intricate iterative process that integrates quantum and classical computing to optimize the Hamiltonian’s minimum eigenvalue. Initially, the pipeline begins with the problem setup where the Hamiltonian defining the system's total energy is specified. Subsequently, an ansatz, a parameterized quantum circuit hypothesized to approximate the ground state, is chosen. This ansatz is then applied to an initialized quantum state on a quantum processor, followed by measurements to estimate the Hamiltonian's expectation value. Classical optimization algorithms come into play afterwards, where they adjust the quantum circuit parameters based on the measurement outputs to minimize the expectation value. This process of measurement and optimization is repeated iteratively until convergence is achieved. The final assessment ensures that the estimated minimum eigenvalue accurately and appropriately represents the system’s ground state. With this, error mitigation strategies are employed throughout the VQE algorithm to counteract potential quantum decoherence and operational errors, thereby enhancing the accuracy of the computational result. Following this outlined pipeline, we present and explain what aspects we have already completed, and which require further research and/or modification.

The Hamiltonian that we are working with is one that represents the Lithium Hydrite molecule system—a step up from the commonly-studied hydrogen molecule. It is a significantly more complex Hamiltonian requiring more parameters and an extensively larger search space.

We currently have access to the supercomputer "Devana" at the Slovak Academy of Sciences, however we also require access to the IBM quantum computer as well, which will require financial support.

The use of the supercomputer is necessary for the classical part of the VQE algorithm–our newly invented optimization method, HOPSO. Our algorithm has already demonstrated preliminary success when applied to a set of standard benchmark test optimization functions when compared to other non-gradient methods such as PSO, Differential Evolution (DE) and COBYLA. Particularly, HOPSO’s iterative search procedure not only reaches the optimal value quickly and efficiently, but also offers a strong advantage against the other optimization methods, such as the traditional PSO algorithm, in the fact that it prevents explosions and has better tuning features. That is, it is less sensitive to the tuning parameters and offers more control over them hence, unlike the PSO, converging to a value is done in a more controlled manner with more flexibility and with less likeliness in premature convergence (getting stuck in a local minima). However, applying HOPSO to the VQE algorithm necessitates the use of a supercomputer, given the exceptionally large datasets and expansive search space involved, along with the numerous parameters that must be managed in this complex problem, as outlined earlier.

One new feature we will present and apply is the periodic operation feature. In optimization, particularly within quantum circuits where cost functions are naturally periodic, addressing the challenges associated with periodicity is

crucial. Specifically, in our HOPSO algorithm, we apply a modulo operation to the best positions—rather than to all positions—to ensure that the evaluations of the cost function remain within the intended bounds. This approach effectively prevents the misuse of distances, which can lead to large errors or "explosions" in the search space.This refinement is particularly important for optimizing periodic functions because it addresses the potential issues that arise from ignoring the periodic nature of the problem. For example, by modulating the best position, we ensure that the distance calculations between personal and global best positions are correctly handled, avoiding excessive jumps across the search space that could otherwise disrupt the optimization process. Our preliminary results on small systems, such as the hydrogen molecule, have demonstrated the efficacy of this approach, leading to accurate and efficient convergence. Given these promising results, we plan to extend the application of this technique to more complex systems, such as lithium hydride, within the VQE framework using quantum circuits.

Attached image