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Editorial: Experience with quantum annealing computation

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Editorial on the Research Topic
Experience with quantum annealing computation

This *Frontiers Research Topic* comprises 13 peer-reviewed papers published in the period August 2023 through June 2024. These papers are cross-listed with *Frontiers in Computer Science*.

The call for submissions invited papers that address all aspects of empirical experience with annealing-based quantum computers, including: best practices in performance tuning; new approaches to hybrid computation (combining classical and quantum methods); estimation of resource usage; new application areas; and software tools and infrastructures. Original research papers as well as tutorials and surveys are within scope.

The submitting authors stepped up to the challenge, submitting works that cover a broad variety of Research Topics and formats. Here is a brief synopsis of each paper.

Early steps toward practical subsurface computations with quantum computing: Greer and O'Malley describe an application of quantum annealing to the problem of seismic inverse analysis, which arises in subsurface hydrology (geoscience). They show how to formulate the problem as a QUBO and present demonstration of the method using two real-world problems. They observe that the approach works well on low-contrast inputs but is challenged by higher precision requirements in problem representation for high-contrast inputs.

Tutorial: calibration refinement in quantum annealing: Chern et al. present a tutorial for calibration refinement, also known as *shimming*, to improve performance of quantum annealers, which are susceptible to crosstalk, device variation, and environmental noise. Explanations and code are supplied showing how to find symmetries for suppressing bias in outputs. Examples are provided for finding small subgraphs in the connectivity graph and finding symmetries of an Ising model via generalized graph automorphism. Other methods, implementations, and limitations are discussed.

Posiform planting: generating QUBO instances for benchmarking: Hahn et al. use planted-solution techniques to develop input generators to be used for benchmarking quantum annealers. Using a technique called posiform planting, they demonstrate that it is possible to construct large QUBO problems with known optimal solutions, thus allowing an evaluation of success probability on large problems. These instances are run on D-Wave quantum annealers to test performance.

Quantum image denoising: a framework via Boltzmann machines, QUBO, and quantum annealing: Kerger and Miyazaki examine applications relating to image de-noising for Boltzmann machines. This work is interesting because it presents two steps where annealers can potentially be used: in the training of the network, and in a separate de-noising step that is formulated as a QUBO. In experimental tests with D-Wave platforms these methods were indeed found to be successful in reducing the noise in images.

Individual subject evaluated difficulty of adjustable mazes generated using quantum annealing: Ishikawa et al. consider the application of quantum annealing to the problem of generating maze puzzles that are difficult for humans to solve. They develop a cost function Q_{update} that scores problem difficulty for a given individual, and show how to formulate the cost function as a QUBO. They present an analysis of computation time, and describe empirical comparisons to a standard classical approach and a hybrid solver. The quantum annealer is efficient at generating mazes with difficulty tailored to individuals.

Benchmarking quantum annealing with maximum cardinality matching problems: Vert et al. aim to tackle the Maximum Cardinality Matching problem with both quantum and simulated annealing. There exist classical algorithms for this problem that can solve it efficiently, although the authors show that the problem is challenging for both simulated and quantum annealing.

Exploring performance on both original inputs and embedded inputs (after compilation onto the connection topology of the quantum annealer), the authors look at the effects of various parameters such as chain strength and annealing time on performance. These experiments are replicated for quantum annealers with both the Pegasus and Zephyr topologies, highlighting their differences.

Moreover, small-scale classical simulations of the quantum annealing process by solving the Schrodinger equation are used to present the ideal behavior of the quantum processing units. As an interesting observation, the authors note that classical algorithms exhibited worse scaling performance in the embedded version of the problems than the quantum annealer. They show that although this is a native limitation of the quantum hardware, it has less impact on quantum performance than on other solution methods.

Exploration of new chemical materials using black-box optimization with the D-Wave quantum annealer: Doi et al. address an application in screening materials using black-box optimization, which describes cases where a subset of constraints or objectives in an optimization problem cannot be fully encoded as part of the model and must be accessed by an oracle.

One way to address these problems is via Bayesian optimization, where samples are drawn iteratively from a solution space aiming to balance exploration of the black-box function and exploitation toward an optimal solution given by an objective. To balance these two goals and determine which point to sample next, an *acquisition function* is proposed such that the function maximum indicates where to draw the next sample.

The authors apply this approach to the problem of exploring a discrete space of chemical materials to find the binding of substituents to specific sites of the molecular frame as the composition of chemical materials. The objective function is considered black-box as it encodes a Density-Functional Theory (DFT) computation. The authors formulate the acquisition function as a QUBO and tackle it using quantum annealing. Their experiments show how the proposed method varies with respect to the variance of the probability distribution represented by the acquisition function, which aims to represent the exploration-exploitation trade-off.

Software techiques for training restricted Boltzmann machines on size-constrained quantum annealing hardware: Salmenperä and Nurminen study software techniques to train restricted Boltzmann machines using quantum annealers. The main focus of this work is how to make use of hardware with limited size. They describe dropout techniques that allow the annealer to be applied to a subnetwork, and an approach to processing multiple small networks in parallel on the same chip. The authors present results of empirical tests of these methods.

Pneumonia detection by binary classification: classical, quantum, and hybrid approaches for support vector machine (SVM): Guddanti et al. develop a machine learning tool that can accurately classify chest X-ray images as belonging to normal or pneumonia-infected individuals. Classical, quantum (D-Wave), and hybrid annealing methods are explored. The results of these methods are compared and contrasted.

Quantum annealing research at CMU: algorithms, hardware, applications: Tayur and Tenneti present a mini-review of quantum annealing research at Carnegie Mellon University. A highlight of this work is the study of Graver-basis-based hybrid optimization methods using quantum annealers. Other work includes developments of efficient minor-embedding strategies and development of photonic Ising machines. This work includes studies on more abstract benchmark-related problems like Max Cut, as well as real-world problems in cancer genomics.

Adiabatic quantum computing impact on transport optimization in the last-mile scenario: Sales and Araos apply a hybrid quantum-classical approach to transport optimization in the ever-evolving landscape of global trade and supply chain management. They look at the Vehicle Routing Problem (VRP) which is to find an optimal set of routes for multiple vehicles to service a given set of customers. The VRP implementation uses a 2-phase approach: first clustering (grouping the customers), and then finding the optimal routes inside each cluster. This research offers contributions to logistics optimization techniques and their potential for enhancing supply chain efficiency.

Experimenting with D-Wave quantum annealers on prime factorization problems: Ding et al. present a detailed report of experimental decisions that led to the largest prime number factorization (8,219,999 = 32,749 * 251) performed with a pure quantum computational approach reported in the literature to date (doi: 10.1038/s41598-024-53708-7). The authors describe their experiences and experimental results, to develop guidelines for best-use of D-Wave quantum annealers. They address tradeoffs arising in algorithmic questions such as minor-embedding and handling of flux biases. This report provides guidance to other practitioners about improving performance for their own applications.

ILP-based resource optimization realized by quantum annealing for optical wide-area communication networks: Witt et al. apply D-Wave quantum annealers to the problem of resource allocation within communication networks. This work focuses on developing a framework that uses neural networks to refine the solutions returned by the quantum annealer; the authors also perform a detailed study of parameter setting. They observe that improvements using the network were possible in some cases, but not in others.

We are pleased to report that this broad collection of contributions to better understanding of quantum annealing processors is now available to the research community.

Author contributions

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Conflict of interest

CM was employed by D-Wave Systems at the time this Research Topic was developed.

The remaining authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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