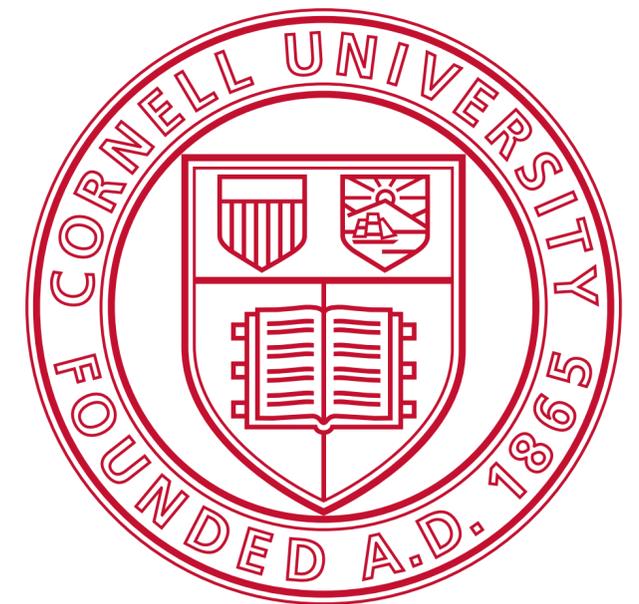
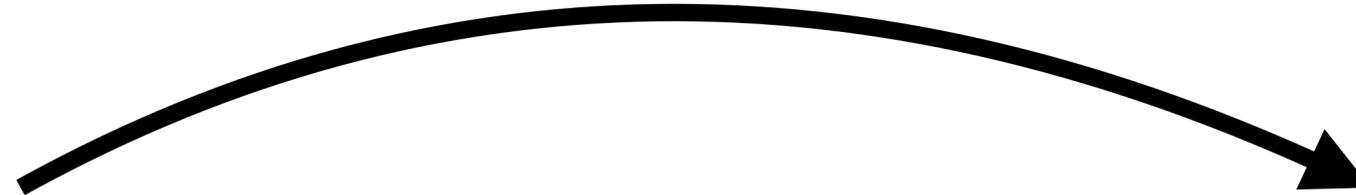


Cost-Based Query Optimization for Quantum Computation

Immanuel Trummer



Leverage For

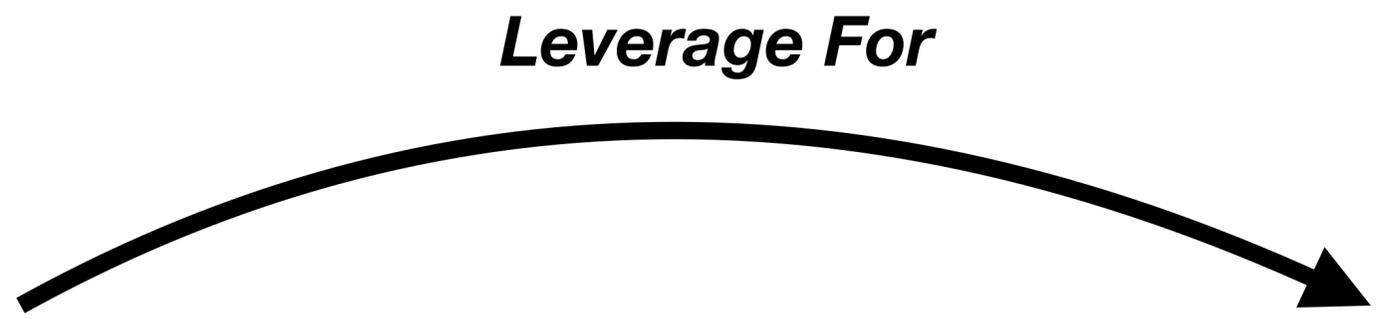


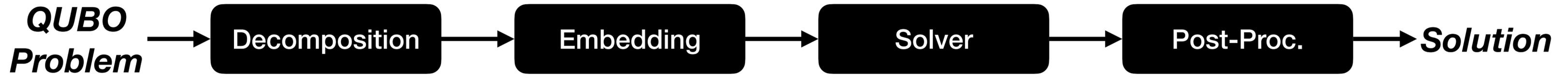
**Quantum
Computing**

**Query
Optimization**

**Quantum
Computing**

**Query
Optimization**





***QUBO
Problem***



Solution

Choice of Method

**QUBO
Problem**

Decomposition

Embedding

Solver

Post-Proc.

Solution

Choice of Method



QUBO Problem

Decomposition

Embedding

Solver

Post-Proc.

Solution

Choice of Method

Decomposition Algorithms for Scalable Quantum Annealing

Elijah Pelofsky, Georg Hahn, Hristo Djidjev
Los Alamos National Laboratory, Los Alamos, NM 87545, USA
epelofsky@lanl.gov, ghahn@lanl.gov, djidjev@lanl.gov

CCS Concepts • Theory of computation → Quantum computation theory, Graph algorithms analysis

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1 INTRODUCTION
Commercial adiabatic quantum annealers such as D-Wave 2000Q, which is available at LAM, have the potential to solve important NP-hard optimization problems efficiently. However, one of the primary constraints of such devices is the limited number and connectivity of their qubits, which limits the size of the problem directly solvable on the machine to about 45 variables. This research presents two exact decomposition methods for the Maximum Clique and the Minimum Vertex Cover problem, two important and well-known NP-hard problems that allow solving problems of arbitrarily large size by splitting them up recursively into a series of relatively small subproblems. These subproblems are then solved exactly or approximately using any method of choice, which include a quantum annealer. Whereas some previous approaches are based on heuristics that do not guarantee optimality of their solutions, our decomposition algorithm uses the property that the optimal solution of the input problem can be reconstructed in polynomial time given all generated subproblems are solved optimally. We present a study of various heuristic and exact branch-and-bound reduction methods that help increase the scalability of our decomposition algorithms.

2 MAXIMUM CLIQUE PROBLEM
Given a graph G , the maximum clique (MC) problem asks to find a subset S of the vertices of G of maximum size such that there is an edge in G joining any two vertices of S . To solve the MC problem in case of a too large to fit in the annealer hardware, we use the MC partitioning method [15]. It divides the MC problem into two smaller subgraphs G_1 and G_2 , on which a MC should be found. We need to know the size of subgraphs G_1 and G_2 , that is, the number of vertices in each subgraph. We need to know the size of the largest clique in each subgraph G_1 and G_2 , that is, the maximum number of vertices in each subgraph that are all connected to each other. We apply the decomposition algorithm to recursively decompose the problem into smaller subproblems, until we reach a subproblem that can be solved exactly or approximately using any method of choice.

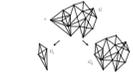


Figure 1: MC Decomposition

Moreover, finally, we use the solution for G_1 and G_2 to construct a solution for G .

In more detail, in order to compute subgraphs G_1 and G_2 , we choose an arbitrary vertex v of G and define G_1 as the subgraph of G induced by all neighbors of v that contain v itself and define G_2 as the graph resulting from G and all edges incident to v are removed from G . Intuitively, G_1 contains all cliques of G that contain v , and G_2 contains all cliques of G that do not contain v . Hence, a maximum clique of G will either be in G_1 or G_2 .

Since each of the subgraphs G_1 and G_2 contains at least one less vertex than G , the decomposition algorithm is guaranteed to complete in finite time, but the number of subgraphs generated might be exponential in the worst case. To reduce the number of subgraphs, we use upper and lower bounds on the solution contained by an generated subgraph with the aim of discarding them as well as reduction techniques. For instance, if in a currently considered subgraph G_i , we compute an upper bound u_i for G_i , meaning that the size of the MC for G_i is not greater than u_i , and the lower bound l_i for G_i is not smaller than l_i , then G_i can be ignored. This technique widely used in branch-and-bound algorithms to combinatorial optimization, can lead to a dramatic decrease in the number of subgraphs that are generated.

We also compare the effectiveness of several upper bound techniques. We use a greedy search heuristic to find an upper bound on the chromatic number of the graph, which is the same number of colors needed to color each vertex of G such that no edge connects two vertices of the same color. Since each vertex in a clique must have a distinct color, the chromatic number is an upper bound on the clique number [7]. Although computing the chromatic number is NP-hard, there are much better heuristics for its approximation compared with the case for the clique number. Therefore, a greedy search heuristic for the chromatic number provides an easily computable bound to compare against the clique number. We use the heuristic function `greedy_color` of the NetworkX package [6], which is applied to the complement \bar{G} of G . The `greedy_color`

Decomposition Algorithms for Solving NP-hard Problems on a Quantum Annealer

Elijah Pelofsky*, Georg Hahn*, Hristo Djidjev*

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Abstract
NP-hard problems such as the maximum clique or minimum vertex cover problem, two of Karp's 21 NP-hard problems, have several applications in computational chemistry, biochemistry and computer network security. Adiabatic quantum annealers can search for the optimum value of such NP-hard optimization problems, given the problem can be embedded on their hardware. However, this is often not possible due to certain limitations of the hardware connectivity structure of the annealer. This paper studies a general framework for a decomposition algorithm for NP-hard graph problems aiming to identify an optimal set of vertices. Our generic algorithm allows us to recursively divide an instance until the generated subproblems can be embedded on the quantum annealer hardware and subsequently solved. The framework is applied to the maximum clique and minimum vertex cover problems, and we propose several pruning and reduction techniques to speed up the recursive decomposition. The performance of both algorithms is assessed in a detailed simulation study.

Keywords Decomposition algorithm; D-Wave; Maximum clique; Minimum vertex cover; NP-hard; Optimization

1 Introduction
Novel computing technologies allow one to search for solutions of NP-hard graph problems that are very hard to solve classically [11]. One such device is the quantum annealer of D-Wave Systems, Inc. [20], which can propose approximate solutions of quadratic unconstrained binary optimization (QUBO) and Ising problems given by the minimum of a function of the form

$$H(x_1, \dots, x_n) = \sum_{i=1}^n w_i x_i + \sum_{1 \leq i < j \leq n} w_{ij} x_i x_j. \quad (1)$$

where $x_i \in \{0, 1\}$ and $w_i, w_{ij} \in \mathbb{R}$ for $i, j \in \{1, \dots, n\}$ are linear weights and $w_{ij} \in \mathbb{R}$ for $i, j \in \{1, \dots, n\}$ are quadratic weights. The problem in Eq. 1 is called a QUBO problem if $w_{ij} \in \{0, 1\}$ and an Ising problem if $w_{ij} \in \{-1, 1\}$ for all i, j . The function in Eq. 1 is often called a QUBO or Ising function, respectively. The formulation in Eq. 1 is general enough to allow all NP-hard problems to be formalized as minimizations of such a function [7]. Both QUBO and Ising formulations are equivalent [1, 12, 21, 22]. The D-Wave quantum annealer aims to find a minimum of the function in Eq. 1 by mapping it to a physical quantum system, from which a solution is read off after hardware-implemented annealing is completed. In such a mapping, linear weights are mapped onto qubits and quadratic weights are mapped onto links between qubits called couplers. Moreover, if w_{ij} and w_{ji} are mapped onto qubits q_i and q_j , then w_{ij} is mapped onto the coupler connecting q_i and q_j .

However, directly computing a minimum of a given function of the type given in Eq. 1 on a quantum annealer is often not possible due to a variety of reasons. First, there is a limitation on the input problem size that can fit on the quantum hardware due to the finite number of available qubits (up to roughly 2000 qubits for the recent D-Wave 2000Q⁺ computer). Second, even if the number of qubits exceeds the number of variables, the current D-Wave technology provides only limited qubit connectivity

Integer programming techniques for minor-embedding in quantum annealers

David E. Bernal^{1,2}, Kyle E. C. Booth¹, Ronald Dreier³, Hediost Alghamdi⁴, Stihler Taylor⁵, and Davide Venturelli^{1,2,3}

¹ Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh PA 15213, USA
² Department of Mechanical & Industrial Engineering, University of Toronto, Toronto ON M5S 3G5, Canada
³ Department of Mechanical & Industrial Engineering, University of Toronto, Toronto ON M5S 3G5, Canada
⁴ Tripper School of Business, Carnegie Mellon University, Pittsburgh PA 15213, USA
⁵ Quantam, AI Lab (QAIL), NANSI, Ames Research Center, Moffett Field CA 94035, USA
⁶ UNIS, H2020, Maastricht University, Maastricht, The Netherlands
d.venturelli@utoronto.ca

Abstract. A major limitation of current generations of quantum annealers is the sparse connectivity of manufactured qubits in the hardware graph. This technological limitation has generated considerable interest, motivating efforts to design efficient and robust minor-embedding procedures that bypass sparsity constraints. In this paper, starting from a previous equational formulation for Dreier et al. (arXiv:1903.04481), we propose integer programming (IP) techniques for solving the minor-embedding problem. The first approach involves a direct translation from the previous equational formulation to IP, while the second decomposes the problem into an assignment master problem and filter condition checking subproblems. The proposed methods are able to detect infeasibility and provide bounds on solution quality, capabilities not offered by currently employed heuristic methods. We demonstrate the efficacy of our methods with an extensive computational assessment involving three different families of random graphs of varying sizes and densities. The direct translation as a monolithic IP model can be solved with existing commercial solvers yielding valid minor-embeddings; however, its performance is degraded by the decomposition approach. Our results demonstrate the promise of a methods for the embedded hardware, highlighting the advantages of using IP technology for minor-embedding problems.

Keywords: Graph minors • Quantum annealer • Integer programming • Decomposition • Algebraic geometry

1 Introduction
Graph minor theory (GMT), the central theme of this work, is prominent across many fields. In quantum computing, GMT is employed to extend the scope of problems that can be represented on current quantum computing hardware [5, 19]. Mapping a dense problem (target) graph T to a sparse (target) graph X can be achieved by constructing connected subgraphs of the target graph X from the high degree logical vertices y . The resulting mapping is called a minor-embedding of T into X .

Numerous heuristics for finding minor-embeddings have been proposed [1, 4, 20]. While these approaches are generally fast, they do not provide guarantees on the quality of the produced minor-embeddings nor can they prove the nonexistence of a minor-embedding for infeasible problems. An approach that attempts to address these shortcomings was recently introduced in Dreier et al. [9]. This approach uses tools from algebraic geometry and produces an equational formulation (as opposed to a purely combinatorial approach) to the minor-embedding problem.

In this paper, starting from this equational formulation, we propose integer programming (IP) techniques for tackling the embedding problem. Our proposed approaches differ from the computationally demanding (Greedy) based approaches used previously and are aimed at more efficiently computing embeddings while retaining the interesting properties that arise from the equational formulation of the problem. Our first approach, detailed in Section 3, directly translates the previous equational formulation to IP, while our second approach decomposes the problem into an assignment master problem and filter condition checking

CHARME: A chain-based reinforcement learning approach for the minor embedding problem

HOANG M. NGO¹, Department of Computer and Information Science and Engineering, University of Florida, USA
NGUYEN H. K. DO², Department of Computer Science, Posts and Telecommunications Institute of Technology, Vietnam
MINH N. VU³, Department of Computer and Information Science and Engineering, University of Florida, USA
TAMER KAHVECI⁴, Department of Computer and Information Science and Engineering, University of Florida, USA
MY T. THAI⁵, Department of Computer and Information Science and Engineering, University of Florida, USA

Quantum Annealing (QA) holds great potential for solving combinatorial optimization problems efficiently. However, the effectiveness of QA algorithms heavily relies on the embedding of problem instances, represented as logical graphs, into the quantum unit processing (QUP) whose topology is in form of a limited connectivity graph, known as the minor embedding problem. Existing methods for the minor embedding problem suffer from scalability issues when confronted with larger problem sizes. In this paper, we propose a novel approach utilizing Reinforcement Learning (RL) techniques to address the minor embedding problem, named CHARME. CHARME includes three key components: a Graph Neural Network (GNN) architecture for policy modeling, a state transition algorithm ensuring solution validity, and an order exploration strategy for effective training. Through comprehensive experiments on synthetic and real-world instances, we demonstrate that the efficiency of our proposed order exploration strategy as well as our proposed RL framework, CHARME. In detail, CHARME yields superior solutions compared to fast embedding methods such as Minorminer and ATOM. Moreover, our method surpasses the OCT-based approach, known for its slower runtime but high-quality solutions, in several cases. In addition, our proposed exploration enhances the efficiency of the training of the CHARME framework by providing better solutions compared to the greedy strategy.

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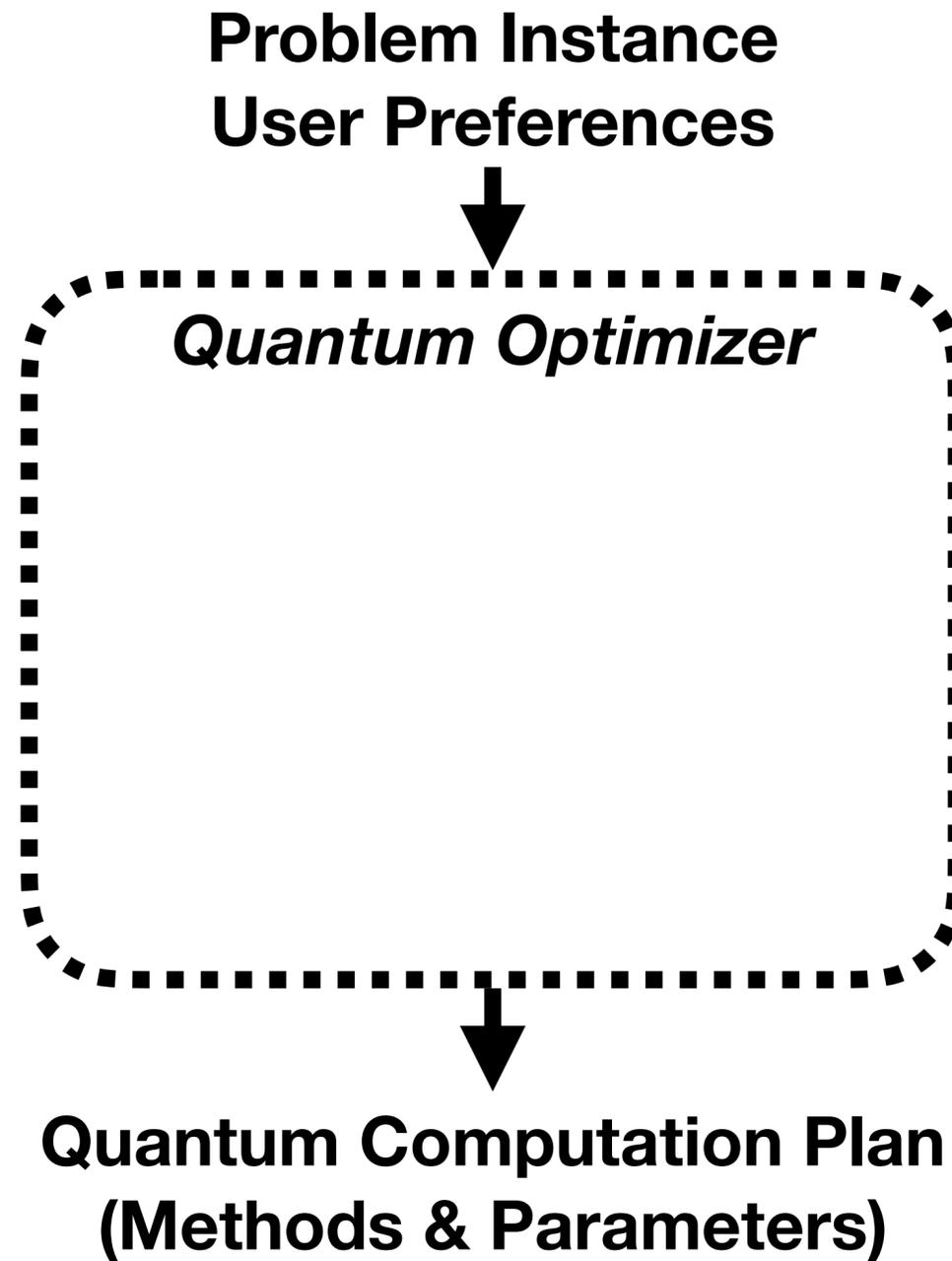
Authors' addresses: Hoang M. Ngo, Department of Computer and Information Science and Engineering, University of Florida, Gainesville, Florida, USA; Nguyen H. K. Do, Department of Computer Science, Posts and Telecommunications Institute of Technology, Hanoi, Vietnam; Minh N. Vu, Department of Computer and Information Science and Engineering, University of Florida, Gainesville, Florida, USA; Tamer Kahveci, Department of Computer and Information Science and Engineering, University of Florida, Gainesville, Florida, USA; My T. Thai, Department of Computer and Information Science and Engineering, University of Florida, Gainesville, Florida, USA

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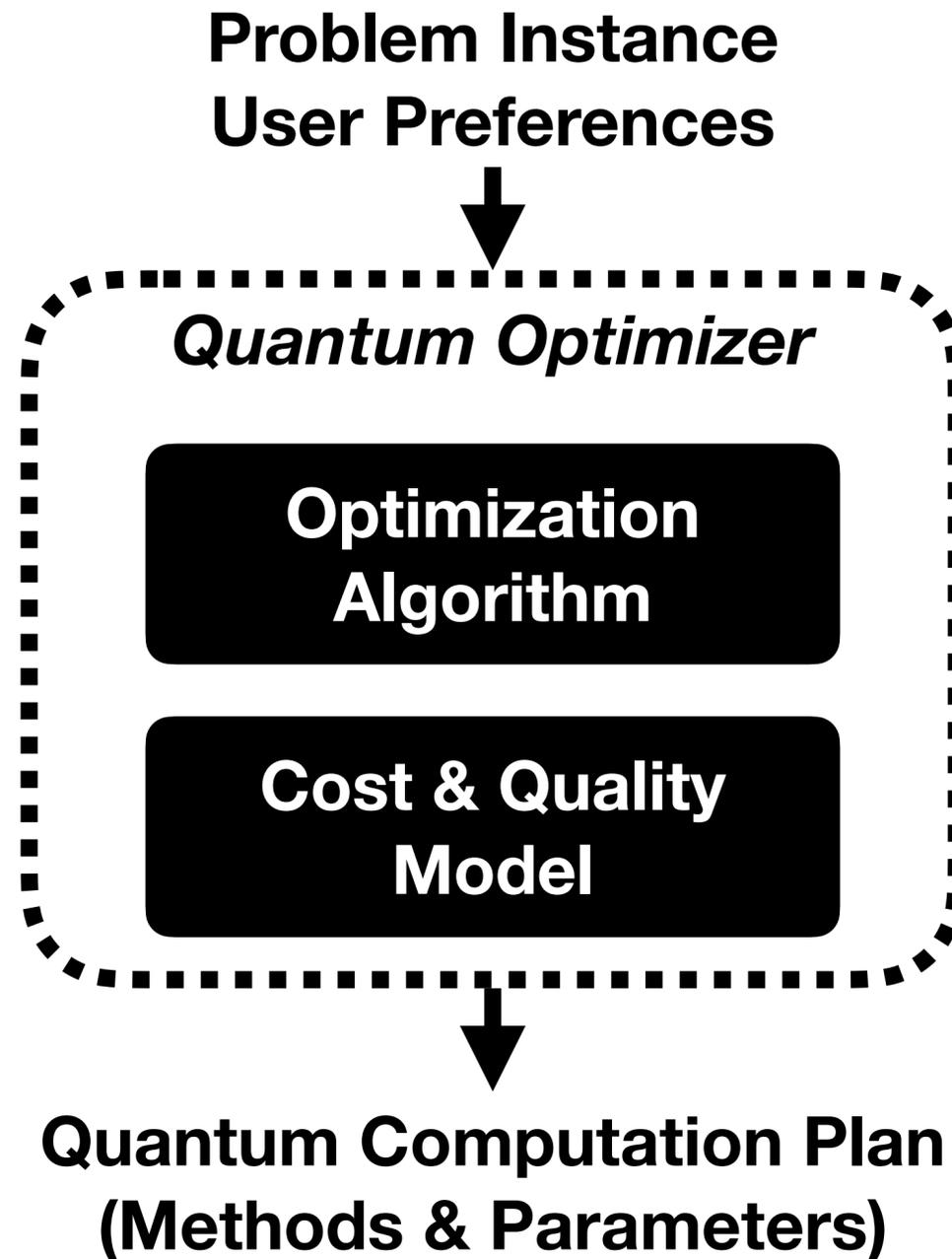
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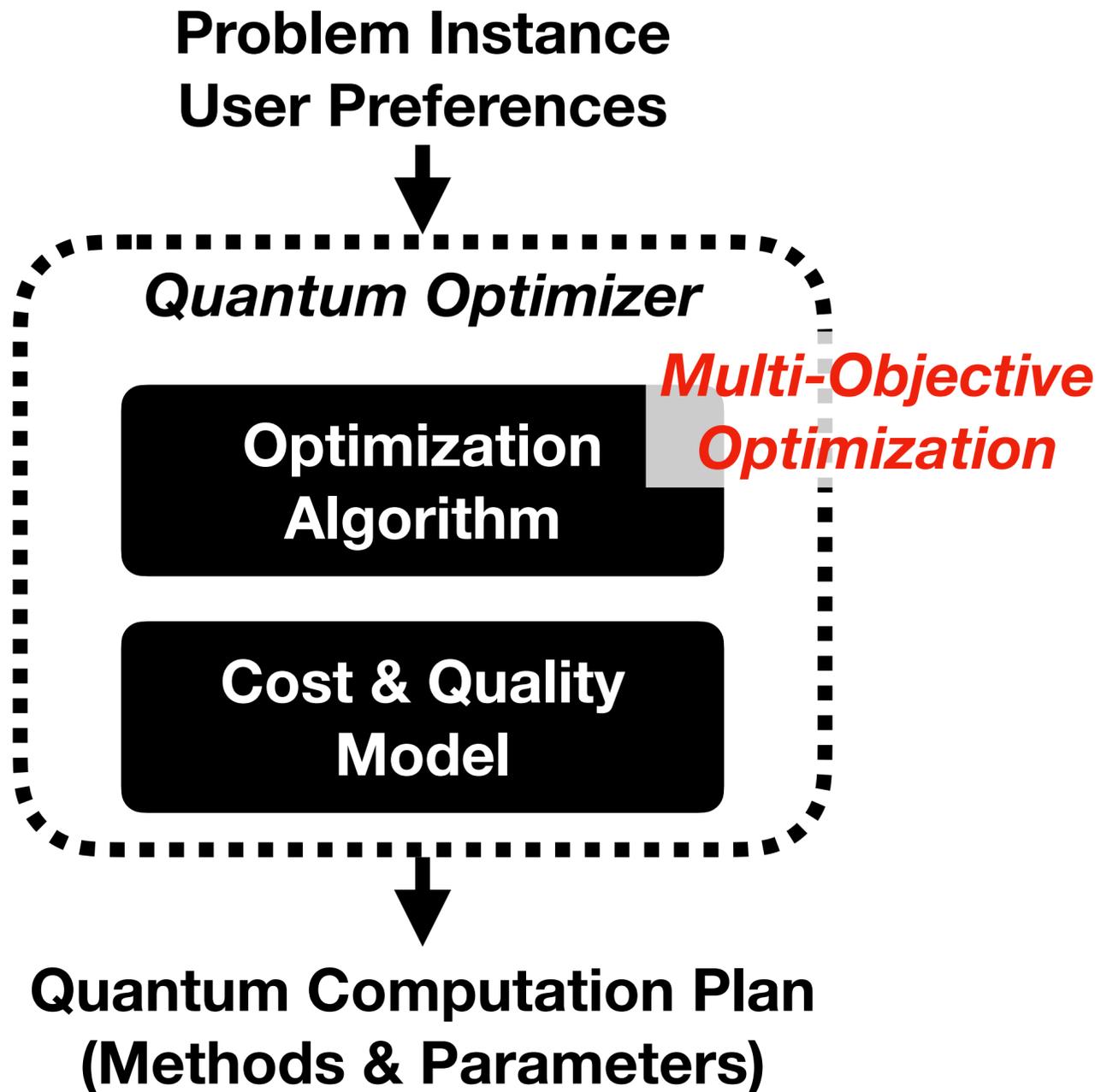
"Query Optimization" for Quantum Computing



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"Query Optimization" for Quantum Computing

Problem Instance
User Preferences



Quantum Optimizer

**Optimization
Algorithm**

**Multi-Objective
Optimization**

**Cost & Quality
Model**



**Quantum Computation Plan
(Methods & Parameters)**

Multiobjective Query Optimization
(Extended Abstract)

Christos H. Papadimitriou
Division of Computer Science
U. C. Berkeley
Berkeley CA 94720
christos@cs.berkeley.edu

Mihalis Yannakakis
Bell Laboratories
Lucent Technologies
Murray Hill, NJ 07974
mihalis@research.bell-labs.com

Abstract

The optimization of queries in distributed database systems is known to be subject to delicate tradeoffs. For example, the Mariposa database system allows users to specify a desired delay-cost tradeoff (that is, to supply a decreasing function $w(d)$, specifying how much the user is willing to pay in order to receive the query results within time d). Mariposa divides a query graph into horizontal "strides," analyzes each stride, and uses a greedy heuristic to find the "best" plan for all strides. We show that Mariposa's greedy heuristic can be arbitrarily far from the desired optimum. Applying a recent approach in multiobjective optimization algorithms to this problem, we show that the optimum cost-delay tradeoff (Pareto) curve via Mariposa's framework can be approximated best within any desired accuracy. We also present a polynomial algorithm for the general multiobjective query optimization problem, which approximates arbitrarily well the optimum cost-delay tradeoff (without the restriction of Mariposa's heuristic stride subdivision).

1 Introduction

In Computer Science we have always been interested in trade-offs between various resources for the solution of computational problems: however, it was only very recently that tradeoffs have begun to be considered as computational problems in their own right—probably the result of the advent of the Internet and the ensuing increasingly complex socio-economic context of

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¹At the recent FOCS conference, there was a session devoted almost exclusively to multi-objective optimization, the *benefit*, and the relationship between the two [FOCS].

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Approximation
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Multiobjective Query Optimization
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Abstract
The optimization of queries in distributed database systems is known to be subject to delicate tradeoffs. For example, the MapReduce database system allows users to specify a desired delay-cost tradeoff (that is, to supply a decreasing function $w(d)$, specifying how much the user is willing to pay in order to receive the query results within time d). MapReduce divides a query graph into horizontal "strikes," analyzes each strike, and uses a greedy heuristic to find the "best" plan for all strikes. We show that MapReduce's greedy heuristic can be arbitrarily far from the desired optimum. Applying a recent approach in multiobjective optimization algorithms to this problem, we show that the optimum cost-delay tradeoff (Pareto) curve via MapReduce's framework can be approximated best within any desired accuracy. We also present a polynomial algorithm for the general multiobjective query optimization problem, which approximates arbitrarily well the optimum cost-delay tradeoff (without the restriction of MapReduce's heuristic strike subdivision).

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Approximation
Algorithms

Neo: A Learned Query Optimizer

Ryan Marcus¹, Parimarjan Negi², Hongzi Mao³, Chi Zhang¹,
Mohammad Alizadeh⁴, Tim Kraska⁴, Olga Papaemmanouil¹, Nesime Tatbul^{1,5}
¹Brandeis University ²MIT ³Intel Labs
⁴{ryan, chi, olga}@cs.brandeis.edu ⁵{pnegi, hongzi, alizadeh, kraska, tatbul}@mit.edu

ABSTRACT
Query optimization is one of the most challenging problems in database systems. Despite the progress made over the past decades, query optimizers remain extremely complex components that require a great deal of hand-tuning for specific workloads and datasets. Motivated by this shortcoming and inspired by recent advances in applying machine learning to data management challenges, we introduce *Neo (Neural Optimizer)*, a novel learning-based query optimizer that relies on deep neural networks to generate query execution plans. Neo bootstraps its query optimization model from existing optimizers and continues to learn from incoming queries, building upon its successes and learning from its failures. Furthermore, Neo naturally adapts to underlying data patterns and is robust to estimation errors. Experimental results demonstrate that Neo, even when bootstrapped from a simple optimizer like PostgreSQL, can learn a model that offers similar performance to state-of-the-art commercial optimizers, and in some cases even surpasses them.

1. INTRODUCTION
In the face of a deluge of machine learning success stories, every database researcher has likely wondered if it is possible to *learn* a query optimizer. Query optimizers are key to achieving good performance in database systems, and can speed up query execution by orders of magnitude. However, building a good optimizer today takes thousands of person-engineering-hours, and is an art only a few experts fully master. Even worse, query optimizers need to be tediously maintained, especially as the system's execution and storage engines evolve. As a result, none of the freely available open-source query optimizers come close to the performance of commercial optimizers offered by IBM, Oracle, or Microsoft.

Due to the heuristic-based nature of query optimization, there have been many attempts to apply learning to query optimizers. For example, almost two decades ago, Leo, DB2's Learning Optimizer, was proposed [53]. Leo learns from its mistakes by adjusting its cardinality estimations over time. However, Leo still requires a human-engineered cost model, a hand-picked search strategy, and a lot of developer-tuned heuristics. Importantly, Leo only improves its cardinality estimation model, and cannot further optimize its search strategy based on data (e.g., to account for uncertainty in cardinality estimates for join order selection).

More recently, the database community has started to explore how neural networks can be used to improve query optimizers [36, 60]. The majority of this work has focused on replacing a component of the optimizer with learned models. For example, DQ [25] and ReJOIN [35] use reinforcement learning combined with traditional human-engineered cost models to automatically learn search strategies and explore the space of possible join orderings. These papers show that learned search strategies can outperform conventional heuristics on a given cost model. Moreover, in addition to the cost model, these systems still rely on heuristics for cardinality estimation, physical operator selection, and index selection.

Other approaches demonstrate how machine learning can be used to achieve better cardinality estimates [22, 28, 43, 44]. However, none demonstrate that their improved cardinality estimations *actually lead to better query plans*. It is relatively easy to improve the average error of cardinality estimates, but much harder to improve estimations for the cases that actually improve query plans [27]. Furthermore, unlike join order selection, selecting join operators (e.g., hash join, merge join) and choosing indexes cannot be entirely reduced to cardinality estimation. SkemerDB [56], showed that adaptive query processing strategies can benefit from reinforcement learning, but it requires a specialized (adaptive) query execution engine and cannot benefit from operator pipelining.

In this paper, we present *Neo (Neural Optimizer)*, a learned query optimizer that achieves similar or improved performance compared to state-of-the-art commercial optimizers (Oracle and Microsoft) on *their own query execution engines*. Given a set of query rewrite rules to ensure semantic correctness, Neo learns to make decisions about join order, operator, and index selection. Neo optimizes these decisions using reinforcement learning, tailoring itself to the user's database instance and basing its decision on actual query latency.

Neo's design blurs the boundaries between the main components of a traditional query optimizer: cardinality estimation, the cost model, and the plan search algorithm. Neo does not explicitly estimate cardinalities or rely on hand-crafted cost models. Neo combines these two functions in a *value network*, a neural network that takes a partial query plan and *predicts* the best expected runtime that could result from completing this partial plan. Guided by the value network, Neo performs a simple search over the query plan space to make decisions. As Neo discovers better query plans,

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"Query Optimization" for Quantum Computing

Problem Instance
User Preferences



Quantum Optimizer

Multi-Objective
Optimization

Optimization
Algorithm

Cost & Quality
Model

No Analytical
Formulas

Learned
Optimization

Quantum Computation Plan
(Methods & Parameters)

Approximation
Algorithms

Multiobjective Query Optimization
(Extended Abstract)

Christos H. Papadimitriou, Mihalis Yannakakis
Division of Computer Science, Bell Laboratories
1, C. Berkeley, Laurent Technologies
Berkeley CA 94720, Murray Hill, NJ 07974
christos@cs.berkeley.edu, mihalis@research.bell-labs.com

Abstract
The optimization of queries in distributed database systems is known to be subject to delicate tradeoffs. For example, the Mariposa database system allows users to specify a desired delay-cost tradeoff (that is, to supply a decreasing function $w(d)$, specifying how much the user is willing to pay in order to receive the query results within time d). Mariposa divides a query graph into horizontal "strikes," analyzes each strike, and uses a greedy heuristic to find the "best" plan for all strikes. We show that Mariposa's greedy heuristic can be arbitrarily far from the desired optimum. Applying a recent approximation in multiobjective optimization algorithms to this problem, we show that the optimum cost-delay tradeoff (Pareto) curve via Mariposa's framework can be approximated best within any desired accuracy. We also present a polynomial algorithm for the general multiobjective query optimization problem, which approximates arbitrarily well the optimum cost-delay tradeoff (without the restriction of Mariposa's heuristic strike subdivision).

1. Introduction
In Computer Science we have always been interested in trade-offs between various resources for the solution of computational problems. However, it was only recently that tradeoffs have begun to be considered as computational problems in their own right—probably the result of the advent of the Internet and the ensuing increasingly complex socio-economic context of computation.¹

Consider the query optimization problem, for example, arguably the most important and complex problem in databases. Tradeoffs between parallelism and communication in query optimization have been studied in [CHM, HM], and elsewhere. The Mariposa wide-area database system [SAP+] was architected to make such tradeoffs explicit in an advantageous way. Mariposa assumes that a subquery can be executed in many diverse database sites, and each site submits a "bid" for the query, specifying a delay for delivering the result, and an associated cost. The query optimizer then chooses these bids to a user-specified cost-delay tradeoff (a non-increasing function $w(d)$, specifying for each value d of the delay the amount of money the user is willing to pay in order to receive the query's results within time d), and attempts to determine the combination of subquery executions that maximizes the savings from this user-specified curve. Mariposa's algorithm for this involves subdividing a query graph (obtained from a single-site optimizer) into horizontal "strikes" that can (independent subqueries, compiling a cost-delay tradeoff for each strike from the bids for those subqueries, and then examining the strike tradeoffs by a greedy heuristic.

Expecting a user to submit a desired tradeoff curve seems to us a little unrealistic. A much better user interface would be, instead, presenting to the user the costs and delays of several query plans, for his/her choice. Obviously, we really need to process query plans that are *undominated*, in that each has the property that no other plan is better in terms of both cost and delay. The set of all undominated solutions is called in the field of multiobjective (or multicriteria) optimization a *Pareto curve*—it captures the informal concept of a tradeoff. Obviously, presenting to the user such a set of solutions to choose from is far superior to requiring a user-specified tradeoff and returning a solution that is in some rather arbitrary sense "most advantageous."

¹At the recent FOCS conference, there was a session devoted almost exclusively to multi-objective optimization, the benefit, and the relationship between the two [FCS].

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Summary

- Use **query optimization ideas** for multi-step quantum computation
 - Approximate multi-objective optimization
 - Learned cost and quality models

