18-819F: Introduction to Quantum Computing
47-779/47-785: Quantum Integer Programming & Quantum Machine Learning

Course Overview

Lecture 00

2021.08.31.

Electrical & Computer ENGINEERING
TEPPER
USRA Universities Space Research Association

Agenda

- Lecturers
- Objectives
- Expectations
- Pre-requisites
- Tentative Course Outline Mini I & II
  - Teasers of new content to be learned
- Grading Policy
  - Project choices and examples
- Course Policy
- Videos and extra resources
- USRA Collaboration

Lecturers

- Prof. Sridhar Tayur
  - Ford Distinguished Research Chair; University Professor of Operations Management; Tepper School of Business CMU
  - Academic Capitalist

- Prof. Elias Towe
  - Professor of Electrical and Computer Engineering

- Dr. Davide Venturelli
  - Associate Director for Quantum Computing of the Research Institute of Advanced Computer Science (RIACS) at the USRA.
  - Senior Scientist NASA Quantum AI Laboratory (QuAIL)

- Dr. David E. Bernal
  - Associate Scientist in Quantum Computing at USRA-RIACS and NASA QuAIL
  - 2019 awardee of USRA Feynman Quantum Academy Program at NASA Ames Research Center

- Maximiliano Stock
  - Civil Engineer. Researcher at INCAE Business School. Visitor at Tepper School of Business, CMU.
  - Finalist at the Airbus Quantum Computing Challenge 2019.

Objectives

This course covers recent developments in **Quantum Computing** for the solution of **combinatorial optimization problems** and **machine learning (ML)**. We will cover mathematical programming and machine learning, their non-quantum (classical) solution methods and concepts that **take advantage** of **near-term quantum** and **quantum-inspired computing**. The **annealing** and **circuit model of quantum computing** that are currently implemented in various hardware architectures will be discussed.

We will explore how these machines can potentially be used for **hardware-tailored ML** algorithms to **solve problems that classical computers struggle with**.

The course contains a series of lectures and practical exercises using quantum resources such as quantum annealing and gate-based computers to gain exposure to these novel computational models, all through the **cloud-based Quantum Computing** access platform Amazon Braket.

The course main deliverable is a **final group project** that allows the students to familiarize themselves with a problem of their interest and apply classical and unconventional computing tools towards addressing these applications.

Expectations

- This course is not going to focus on the following topics:
  - Computational complexity theory
    - 15-651 Algorithm Design and Analysis in CS
  - Quantum Information Theory
    - 33-658 Quantum computation and Info theory in Physics
  - Analysis of speedup using differential geometry, algebraic topology, etc.
    - 21-752 Algebraic Topology or 21-759 Differential Geometry in Mathematics

Pre-requisites

- No explicit pre-requisites are listed but we recommend:
  - An **undergraduate-level** understanding of **probability, calculus, statistics, graph theory, algorithms,** and **linear algebra** is assumed.
  - Knowledge of **linear and integer programming will be useful**.
  - **Programming skills** are **strongly recommended** (Python preferred)
  - **Basic** concepts in **physics** are **recommended** but lack of prior knowledge is not an issue as pertinent ones will be covered in the lectures.
  - **No particular knowledge in quantum mechanics** or algebraic geometry **is required**.

Tentative Course Outline First Half / Mini 1

- Introduction to Linear Algebra for Quantum Mechanics and Machine Learning:
  - Complex numbers, vectors and vector spaces, functions as vectors, inner product, norms, projections, Hilbert spaces, basis vectors, matrices, Hermitian operators, and special matrices
- Introduction to Mathematical Programming methods:
  - Linear Programming; Integer Programming; Nonlinear Programming; Mixed-Integer Nonlinear Programming; Introduction to computational complexity.
- Basic classical machine learning:
  - Support vector machine model; Deep learning neural networks; Running classical machine learning algorithms on computing systems with accelerators; Challenges of running machine learning algorithms on current state-of-the-art classical computing hardware
- Ising, Quadratic Unconstrained Binary Optimization (QUBO)
  - Ising model basics; Simulated Annealing, Markov-chain Monte Carlo methods, benchmarking classical methods, Formulating combinatorial problems as QUBOs.
- Introduction to Test Sets
  - Groebner basis; Graver basis; GAMA: Graver Augmented Multiseed algorithm; Applications: Portfolio Optimization, Cancer Genomics
- Physics-Inspired Hardware for solving Ising/QUBO
  - Graphical Processing Units; Tensor Processing Units; Complementary metal-oxide-semiconductors (CMOS); Digital Annealers; Oscillator Based Computing; Coherent Ising Machines

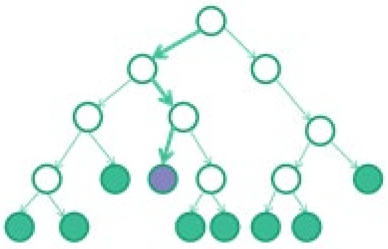
Mathematical Programming – Discrete Optimization

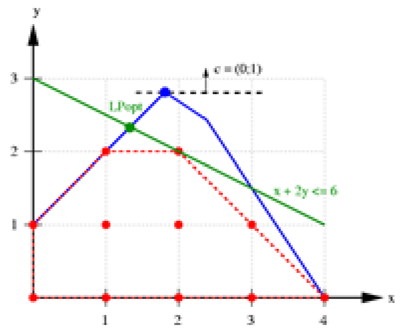
Current status and perspectives

Classical methods

Methods based on divide-and-conquer

- Branch-and-Bound algorithms
- Harness advances in polyhedral theory
- With global optimality guarantees
- Very efficient codes available
- Exponential complexity

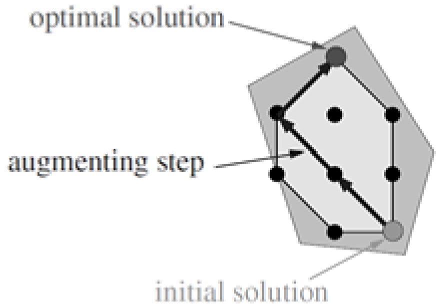




Not very popular classical methods

Methods based on test-sets

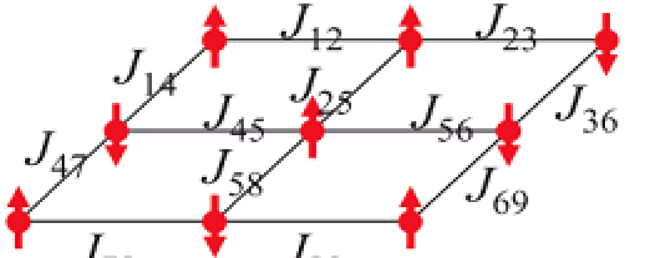
- Algorithms based on “augmentation”
- Use tools from algebraic geometry
- Global convergence guarantees
- Very few implementations out there
- Polynomial **oracle** complexity **once we have test-set**



[1] https://de.wikipedia.org/wiki/Branch-and-Cut
[2] Algebraic And geometric ideas in the theory of discrete optimization. De Loera, Hemmecke, Köppe. 2012

Ising Model, QUBO

Mental model and applications



$$H = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j - \sum_j h_j\sigma_j$$

$$\sum_{s_1=0}^{1}\sum_{s_2=0}^{1}\cdots\sum_{s_n=0}^{1}$$

$$H = -J\sum_{i=1}^{N} s_i s_{i+1} - H\sum_{i=1}^{N} s_i$$

$$H = -\sum_{i=1}^{N}\left[J s_i s_{i+1} + H\frac{s_i+s_{i+1}}{2}\right]$$

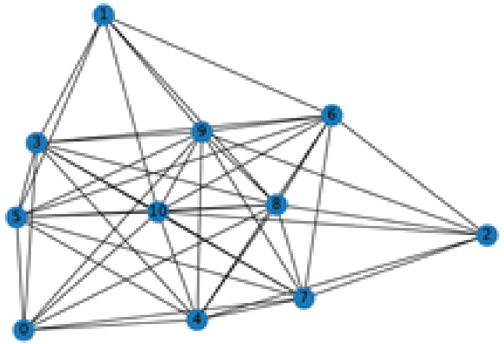
$$Z = e^{\Psi} = \sum_j e^{-\beta H(\mathbf{x}_j,\mathbf{p}_j)}$$

$$z(x) = \begin{cases} -1 & \text{if } x = 0 \\ +1 & \text{if } x = 1 \\ 0 & \text{otherwise} \end{cases}$$

$$Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1}\cdots\sum_{s_n=0}^{1}\exp\left(\beta\sum_{i=1}^{N}\left[Jz(s_i)z(s_{i+1}) + H\frac{z(s_i)+z(s_{i+1})}{2}\right]\right)$$

$$\min c\mathbf{x} \quad A\mathbf{x} = b \quad \mathbf{x} \in \{0,1\}^n$$

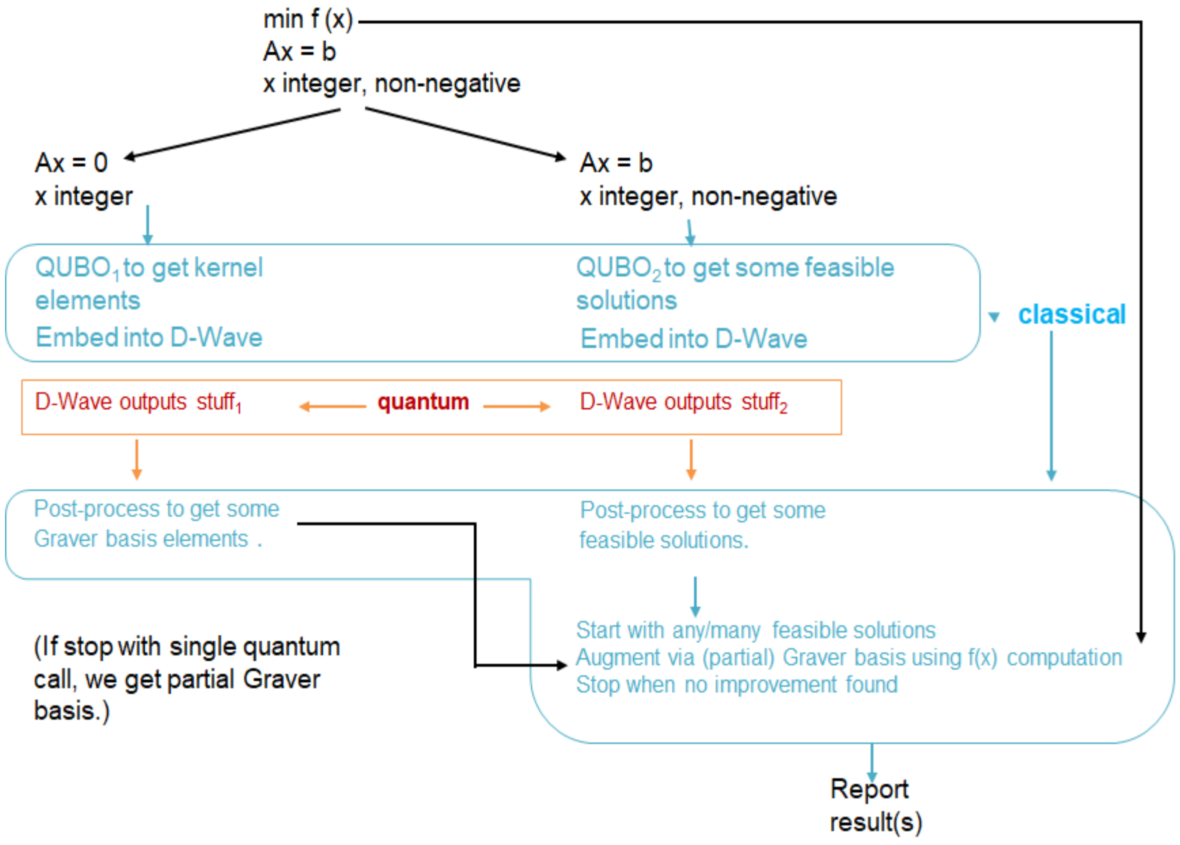
$$\Rightarrow \min_{\mathbf{x}} c\mathbf{x} + \rho(A\mathbf{x}-b)^T(A\mathbf{x}-b), \quad \mathbf{x} \in \{0,1\}^n \; = \; \min_{\mathbf{x}} \mathbf{x}^T Q\mathbf{x} + c, \quad \mathbf{x} \in \{0,1\}^n \Rightarrow$$



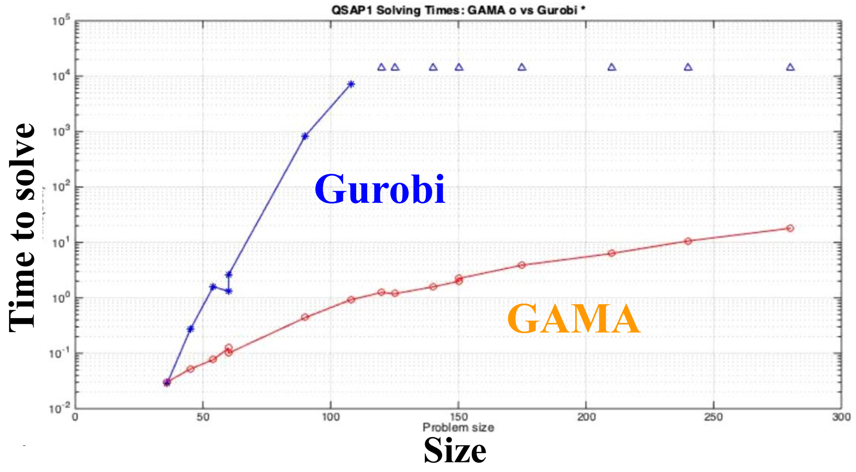
[1] https://en.wikipedia.org/wiki/Ising_model

Graver Augmented, Multiseed Algorithm GAMA

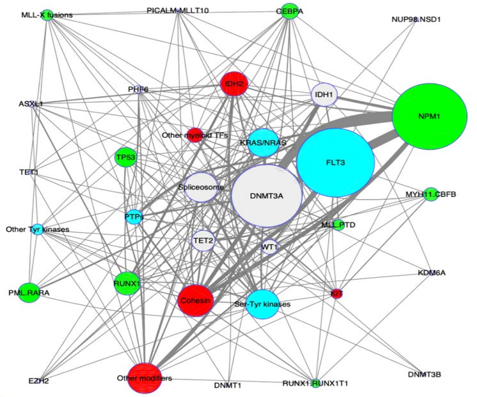
Mental model and applications



Cardinality Constrained Quadratic Optim



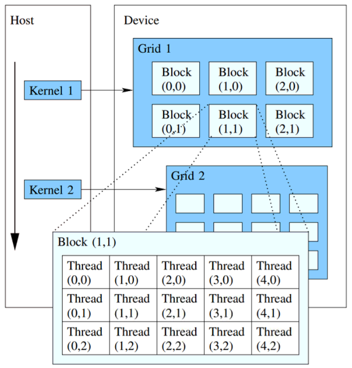
Cancer Genomics

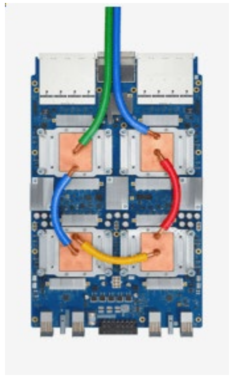


[1] https://arxiv.org/pdf/1902.04215.pdf
[2] https://arxiv.org/pdf/1907.10930.pdf
[3]https://www.biorxiv.org/content/10.1101/845719v1.full.pdf

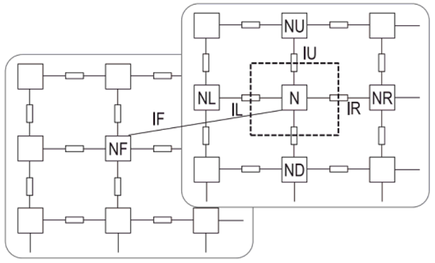
Specialized hardware for solving Ising/QUBO

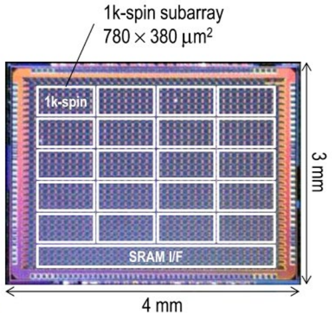
GPUs and TPUs





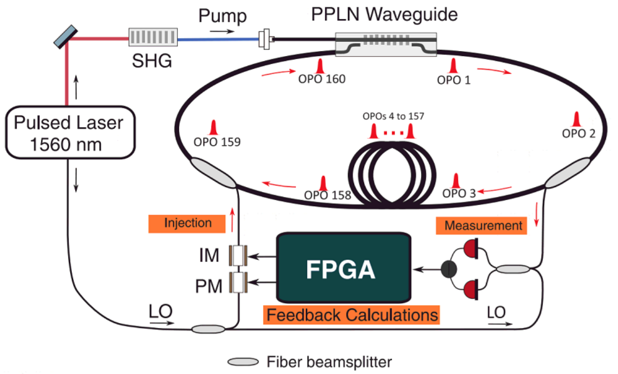
Complementary metal-oxide semiconductors (CMOS)





Digital annealers

Coherent Ising Machines (CIM)



[1]https://arxiv.org/pdf/1807.10750.pdf
[2]https://arxiv.org/pdf/1903.11714.pdf
[3]https://arxiv.org/pdf/1806.08815.pdf
[4]https://spectrum.ieee.org/tech-talk/computing/hardware/fujitsus-cmos-digital-annealer-produces-quantum-computer-speeds
[5]https://science.sciencemag.org/content/sci/354/6312/614.full.pdf

Tentative Course Outline Second Half / Mini 2

- Axioms of Quantum Mechanics
  - Postulates of quantum mechanics, review of classical bits (cbits), the single quantum state and the quantum bit (qubit); Quantum measurement, quantum operations; Multiple quantum states, observables
- Qubit Gate model of quantum computing
  - Reversible operations on qubits, logic gates and quantum circuits; Qubits for information processing; general quantum computation process; Example of the power of quantum computing, Deutsch's problem
- Quantum methods for solving Ising/QUBO in the NISQ Era
  - Adiabatic Quantum Computing, Quantum Annealing and D-Wave; QAOA: Quantum Alternating (Approximate) Optimization Ansatz (Algorithm); Exercises on Amazon Braket
- Quantum Algorithms for future quantum processors
  - HHL Algorithms for solving a system of linear equations ($Ax = b$); Factorizing large numbers; period finding; quantum Fourier Transform; Quantum shell game; Grover's search algorithm
- Noise in quantum computing and quantum error correction
  - Review of classical error correction methods; quantum error correction

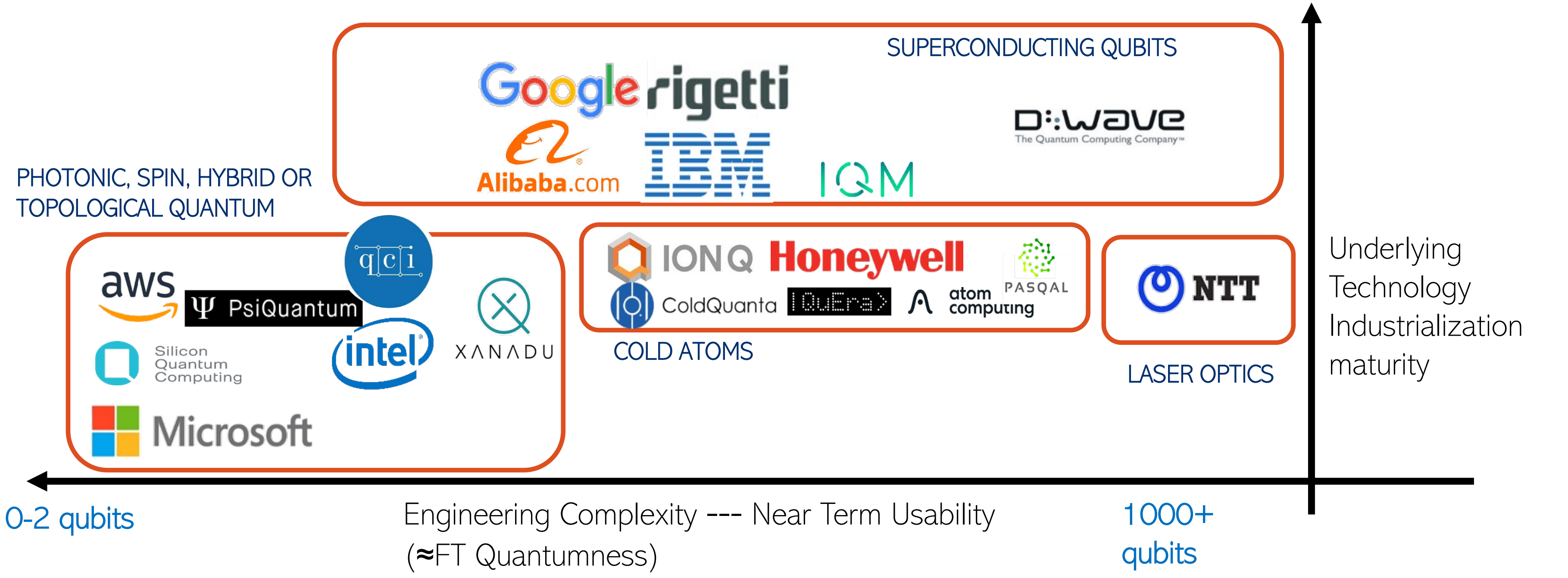
Unconventional Computing

Three Strategies, Multiple Technologies

FAULT-TOLERANT QUANTUM:
- Phase Estimation
- Amplitude Amplification/Estim.
- Sampling

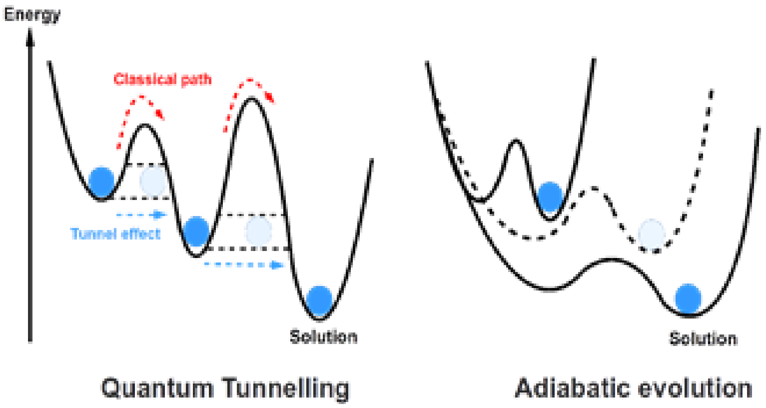
GATE-MODEL NISQ:
- Quantum Approximate Optimization
- Quantum Alternate Operator Ansatz
- Variational Quantum Eigensover
- Quantum Neural Networks

ANALOG:
- Quantum Annealing
- Coherent (Optical) Ising Machines
- Oscillator-based Computing
- Quantum-Inspired Digital Annealers

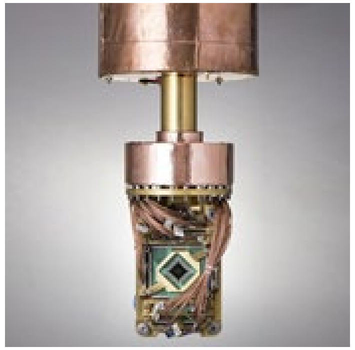


Quantum methods for solving Ising/QUBO

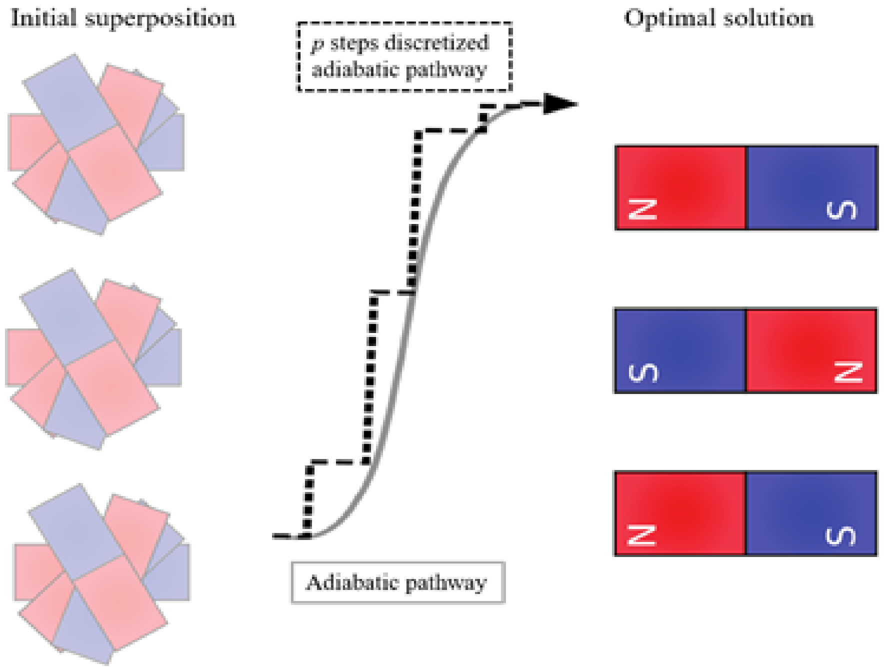
Adiabatic Quantum Computation



Gate-based computers and Quantum Annealers



Quantum Annealing and QAOA



[1]https://miro.medium.com/max/2420/1*n0wMIZVftp8cVLW8Mn6_Ew.png
[2]https://www.ibm.com/blogs/research/2017/11/the-future-is-quantum/
[3]https://www.dwavesys.com/press-releases/d-wave-makes-new-lower-noise-quantum-processor-available-leap

Recent Results: QA

Recent applied, advanced use (paused annealing, reverse annealing):

Ferromagnetically shifting the power of pausing

Zoe Gonzalez Izquierdo,[1,2,3] Shon Grabbe,[2] Stuart Hadfield,[2,3] Jeffrey Marshall,[2,3] Zhihui Wang,[2,3] and Eleanor Rieffel[2]
[1] *Department of Physics and Astronomy, and Center for Quantum Information Science & Technology, University of Southern California, Los Angeles, California 90089, USA*
[2] *QuAIL, NASA Ames Research Center, Moffett Field, California 94035, USA*
[3] *USRA Research Institute for Advanced Computer Science, Mountain View, California 94043, USA*
(Dated: June 16, 2020)

Leveraging Quantum Annealing for Large MIMO Processing in Centralized Radio Access Networks

Minsung Kim, Princeton University, minsungk@cs.princeton.edu
Davide Venturelli, USRA Research Institute for Advanced Computer Science, DVenturelli@usra.edu
Kyle Jamieson, Princeton University, kylej@cs.princeton.edu

NOTE: ≈30 papers on applied use of quantum annealers in 2021 as of August (**61** papers in 2020)

Quantumness:

REPORT

Phase transitions in a programmable quantum spin glass simulator

R. Harris[1,*], Y. Sato[1], A. J. Berkley[1], M. Reis[1], F. Altomare[1], M. H. Amin[1,2], K. Boothby[1], P. Bunyk[1], C. Deng[1], ...
+ See all authors and affiliations

Science 13 Jul 2018:
Vol. 361, Issue 6398, pp. 162-165
DOI: 10.1126/science.aat2025

Letter | Published: 22 August 2018

Observation of topological phenomena in a programmable lattice of 1,800 qubits

Andrew D. King, Juan Carrasquilla, [...] Mohammad H. Amin

Nature **560**, 456–460(2018) | Cite this article

Benchmarking:

REPORT

Defining and detecting quantum speedup

Troels F. Rønnow[1], Zhihui Wang[2,3], Joshua Job[3,4], Sergio Boixo[5,6], Sergei V. Isakov[7], David Wecker[8], John M. Martinis[9], Dan...
+ See all authors and affiliations

Science 25 Jul 2014:
Vol. 345, Issue 6195, pp. 420-424
DOI: 10.1126/science.1252319

What is the Computational Value of Finite-Range Tunneling?

Vasil S. Denchev, Sergio Boixo, Sergei V. Isakov, Nan Ding, Ryan Babbush, Vadim Smelyanskiy, John Martinis, and Hartmut Neven

Phys. Rev. X **6**, 031015 – Published 1 August 2016

Recent Results: QAOA

Optimizing Variational Quantum Algorithms Using Pontryagin's Minimum Principle

Zhi-Cheng Yang,[1] Armin Rahmani,[2,3] Alireza Shabani,[4] Hartmut Neven,[4] and Claudio Chamon[1]

Low depth mechanisms for quantum optimization

Jarrod R. McClean,[1,*] Matthew P. Harrigan,[1] Masoud Mohseni,[1] Nicholas C. Rubin,[1] Zhang Jiang,[1] Sergio Boixo,[1] Vadim N. Smelyanskiy,[1] Ryan Babbush,[1] and Hartmut Neven[1]
[1] *Google Research, 340 Main Street, Venice, CA 90291, USA*
(Dated: August 21, 2020)

Behavior of Analog Quantum Algorithms

Lucas T. Brady,[1,2,*] Lucas Kocia,[3] Przemyslaw Bienias,[1,2] Aniruddha Bapat,[1,2] Yaroslav Kharkov,[1,2] and Alexey V. Gorshkov[1,2]
[1] *Joint Center for Quantum Information and Computer Science, NIST/University of Maryland, College Park, Maryland 20742, USA*
[2] *Joint Quantum Institute, NIST/University of Maryland, College Park, Maryland 20742, USA*
[3] *Sandia National Laboratories, Livermore, California 94550, USA*
(Dated: July 6, 2021)

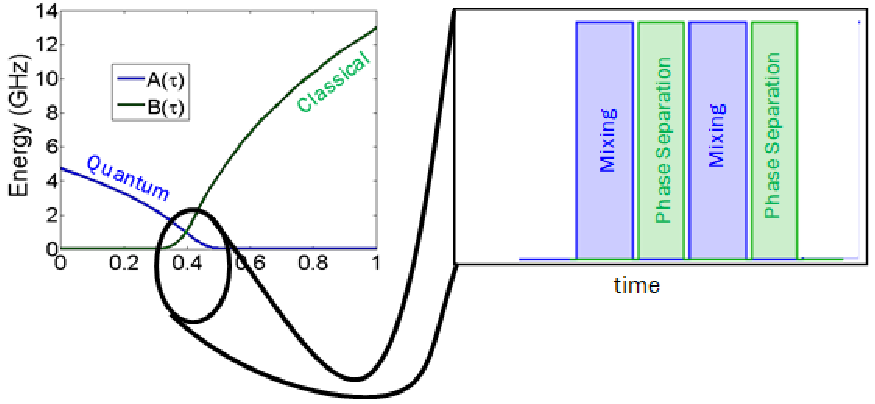
NOTE: ≈35 papers on quantum optimization algorithms in 2021 as of August (**77** in 2020)

Quantum Approximate Optimization of Non-Planar Graph Problems on a Planar Superconducting Processor

Google AI Quantum and Collaborators*
(Dated: April 10, 2020)

Reference	Date	Problem topology	$\Delta(G)$	n	p	Optimization
Otterbach *et al.* [22]	2017-12	Hardware	3	19	1	Yes
Qiang *et al.* [27]	2018-08	Hardware	1	2	1	No
Pagano *et al.* [26]	2019-06	Hardware[1] (system 1)	n	12, 20	1	Yes
		Hardware[1] (system 2)	n	20–40	1–2[(2)]	No
Willsch *et al.* [23]	2019-07	Hardware	3	8	1	No
Abrams *et al.* [24]	2019-12	Ring	2	4	1	No
		Fully-connected	n			No
Bengtsson *et al.* [25]	2019-12	Hardware	1	2	1, 2	Yes
This work		Hardware	4	2–23	1–5	Yes
		3-regular	3	4–22	1–3	Yes
		Fully-connected	n	3–17	1–3	Yes

Relationship between QA and QAOA:



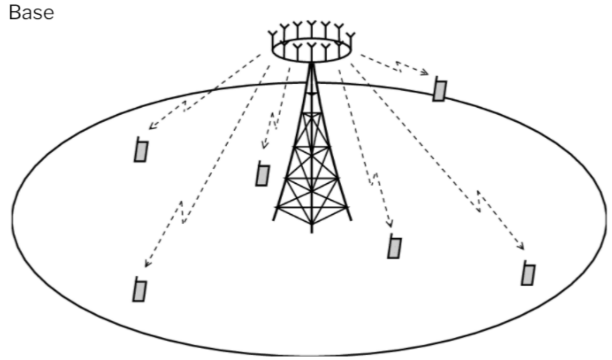
Grading Policy

- The final project accounts for 70% of the grade and weekly short quizzes account for 30% of the grade

- Bi-weekly homework or quizzes (50%)
  - Each week will have a short quiz to evaluate concepts covered in previous lectures
  - Worst quizzes won't be counted
- Final Project (70%)
  - Group project (2-4 people).
  - Formulate a relevant practical problem as an IP or ML in multiple ways (formulations)
  - Generate a family of instances of the problem to test solution methods
  - Review current state-of-the-art classical solution methods. Replicate it if possible.
  - Identify opportunities for unconventional computing solution methods
  - Map the problem into a formalism fit for physics-based or -inspired methods
  - Perform resource estimation and solve a proof-of-concept instance(s) on a real device or simulator
- Deliverables:
  - Ungraded project proposal at the 3rd week to evaluate validity of idea (or for us to provide a problem)
  - Provide a mid-term report with initial results and plan (15 points /70) with a short presentation (10/70)
  - Code to implement project
  - Write a report outlining strengths-limitations-functional requirements-opportunities of the different approaches used, highlighting the knowledge obtained while developing the project supported by computational results (25/70)
  - Make a presentation to the class reporting the findings of the project (20/70)

Project proposal ideas

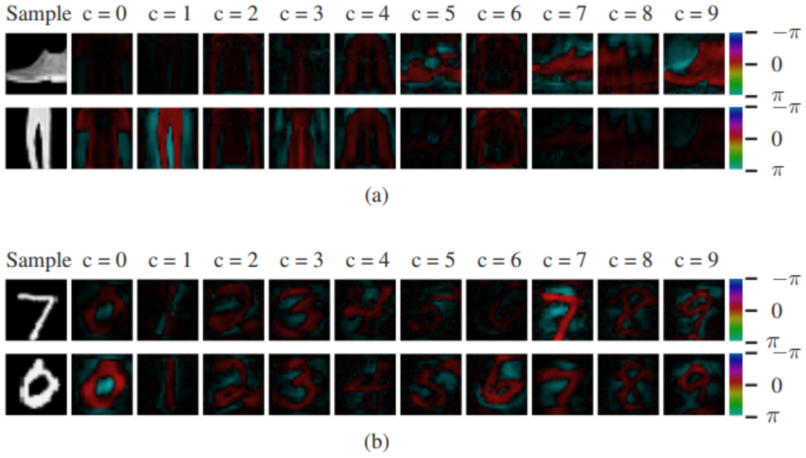
Multi-Input Multi-Output (MIMO) Maximum Likelihood Decoding problem



Many devices communicate with a base station. How to recover original message from noisy measurement?

https://arxiv.org/pdf/2001.04014.pdf

Image processing and classification



Given an image and a group of categories. How to use quantum computing to help with image classification?

https://arxiv.org/pdf/2008.05859.pdf

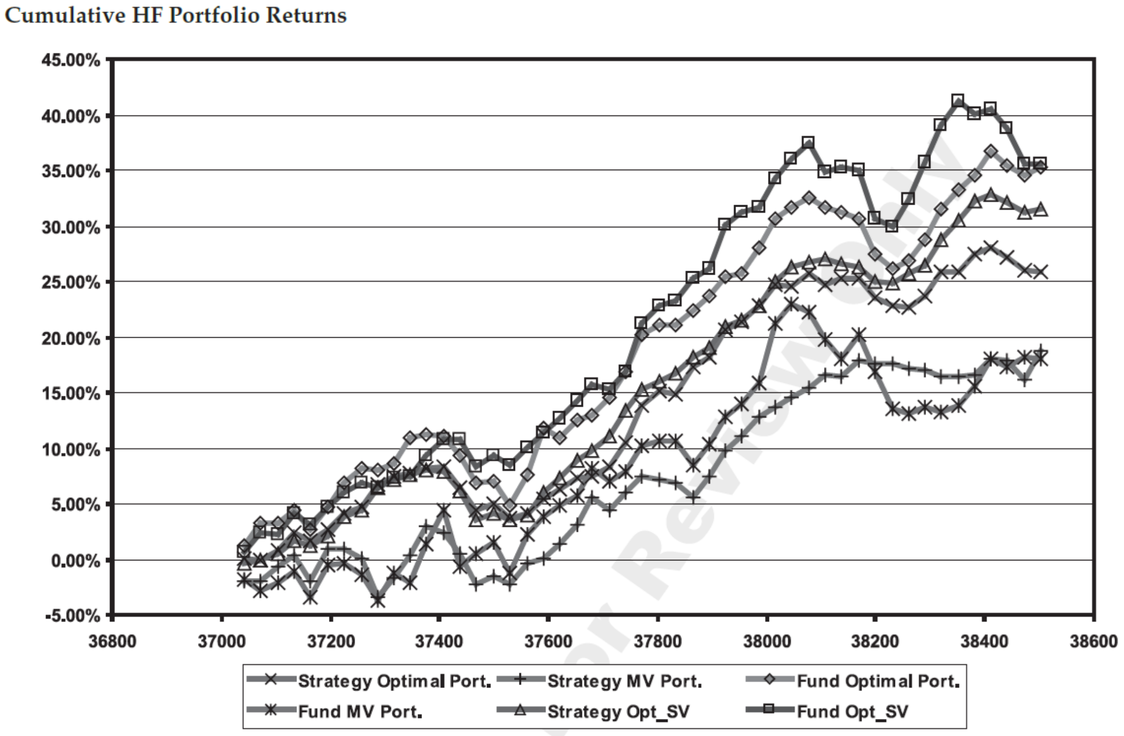
- Other projects:

  Bring your own application!

  It must be a machine learning / combinatorial optimization problem of interest suited for quantum computing

Project proposal from Industry

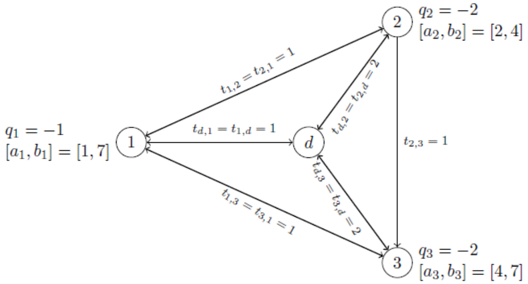
Principal Financial Group: Hedge Fund portfolio optimization with Kurtosis and Skewness



Purpose ***(What is the project motivation?)***	• The purpose of this project is to adopt Ising's model to solve a complex Optimization problem incorporating higher moments i.e. Skewness and Kurtosis into the objective function. • The goal is to establish a framework through which a reformulation of the problem is possible. • Its purpose is also to push the boundaries of optimization problem by incorporating other practical constraints such as mixed-integer formulation.
Objectives ***(What are we going to do?)***	• Perform a literature review of Ising's model with particular focus on its relevance to Portfolio Optimization • Reformulate the Optimization problem incorporating higher order moments so that it is amenable to be solved using the Ising's model. • Develop a working prototype of the proposed methodology • Define metrics and validation procedures for evaluating model performance – both accuracy as well speed. • Define and prototype benchmarks for comparison. Consider baseline Mean Variance Optimization for this purpose. • Demonstrate a prototype of the developed methodology on a large dataset
Output ***(What are the project deliverables?)***	• A thorough report of literature review identifying literature relevant to adopting Ising's model to Portfolio Optimization. • Establish a framework for reformulating the optimization problem using Ising's model. • A working prototype implementing Ising's model for addressing complex Portfolio Optimization problem. • Documentation for the proposed mathematical formulation.
Outcome ***(Expected impact on which sub-system(s)?)***	• A richer formulation incorporating higher order moments of returns namely, Skewness and Kurtosis in addition to Mean and Variance leads to renewed focus on traditionally neglected aspects of return distribution. • This reformulation would play a pivotal role in transforming the portfolio manager mindset and development of this framework would allow us to rapidly prototype and readily implement it. • Incorporating higher order moments of return is beset with mathematical complexities and obstacles arising from practical computational limitations. This novel approach to solve this problem circumvents these traditional limitations.

Project examples

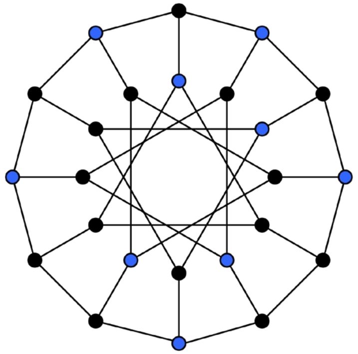
Maritime Routing Problem



Real-life application problem

https://ieeexplore.ieee.org/iel7/8924785/9347847/09314905.pdf

Max-k-coloring and stable-set of a graph



Graph theoretical

https://arxiv.org/pdf/2101.09462.pdf

- Other applications in Finance, Engineering, and Sciences

Other applications

Applied:

- Air Traffic Management
- Portfolio Optimization
- Airport Gate Scheduling
- Autoencoders
- Anomaly detection in networks
- Vehicle Routing
- Robot Operations Planning

Paradigmatic:

- SAT
- Traveling Salesman Problem
- Job Shop Scheduling
- Spin Glasses

Course Policy

- Auditing students are encouraged to participate actively in the lectures
  - Consider doing the project, one learns by doing
- Regular attendance is essential and expected
- CMU students: use canvas
  - The quizzes are being posted there
  - Questions should be asked there to make it available to everyone

- Academic honesty is expected. Refer to the CMU’s policies on academic integrity when in doubt.

Videos and extra resources

- This year's website
  - https://bernalde.github.io/QuIPML/
- Last year's Course Website
  - https://bernalde.github.io/QuIP/
- Teaser video
  - https://www.linkedin.com/posts/carnegie-mellon-tepper-school-of-business_quantum-computing-activity-6698655542186913792-001_
- CMU Quantum Computing Group Website
  - https://lnkd.in/d6m5ECV
- Pittsburgh Quantum Institute
  - https://www.pqi.org/
- Prof. Tayur's seminar at Cornell on GAMA
  - https://cornell.hosted.panopto.com/Panopto/Pages/Viewer.aspx?id=3d46643f-03ea-4e3f-ad7a-ab9901290472

USRA collaboration and NASA/USRA resources

- USRA Research Institute for Advanced Computer Science (RIACS) Quantum Group Website
  - https://riacs.usra.edu/quantum (includes a full login-protected QC course and last year's QIP Lectures)

- NASA Quantum and Artificial Intelligence Laboratory (QuAIL)
  - https://quantum.nasa.gov

- Students of this course are encouraged to apply to the Feynman Academy Internship program https://riacs.usra.edu/quantum/qacademy that sponsors research projects at NASA Ames Research Center.

Why Universities Exist

"The justification for a university is that it preserves the connection between knowledge and zest of life, by uniting the young and old in the imaginative consideration of learning…The task of the university is to weld together imagination and experience…..The task of the university is the creation of the future…."