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

Fall 2021

Room: Tepper Quad 4219	**Time:** Tuesday and Thursday 4:40pm-6:30pm

Instructors:

Sridhar Tayur	**Email:** stayur@cmu.edu	**Office:** 4216 Tepper Quad
Elias Towe	**Email:** towe@ece.cmu.edu	**Office:** 147 Roberts Engineering Hall
Davide Venturelli	**Email:** DVenturelli@usra.edu	**Office:** Online
David E. Bernal	**Email:** bernalde@cmu.edu	**Office:** 3116 Doherty Hall

Teaching Assistant:

Maximiliano Stock	**Email:** maximils@andrew.cmu.edu	**Office:** 4218A Tepper Quad

Course Description: This course is primarily designed for graduate and advanced undergraduate students. It covers recent developments in Quantum Computing for the solution of combinatorial optimization problems and machine learning. The course will cover integer programming and machine learning (ML), 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 is currently implemented in various hardware incarnations will be explained. The course explores how these machines will potentially be used for hardware-tailored machine learning algorithms to solve problems that classical computers struggle with. The course contains a series of lectures exposing students to 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 Bracket. The demand for this new workforce is extremely high with more than $22 Billion dollars invested worldwide in Quantum Information Sciences. Analysts forecast that in the next 5 years the demand for trained Ph.D. or master level Technicians, Engineers, Scientists and application researchers will outpace the offer in the U.S. by far, as evidenced by recent reports by the NSF, the White House Office of Science and Technology Policy, and the Quantum Economic Development Consortium (QED-C) and by the fact that as of March 2021 more than 250 companies are advertising over 750 open positions through recruiting websites. 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.

Objectives: This course is primarily designed for graduate students (and advanced undergraduates) interested in integer programming (with non-linear objective functions) and the potential of near-term quantum and quantum-inspired computing for solving combinatorial optimization problems. By the end of the semester, someone enrolled in this course should be able to:

- Describe the current status of quantum computing and its potential use for integer programming
- Access and use quantum computing resources (such as Quantum Annealers and Gate-based computers) as well as specialized hardware
- Set up a given integer program to be solved with quantum computing
- Work in groups collaboratively on a state-of-the-art project involving applications of quantum computing and integer programming

This course is not going to focus on the following topics:

- Computational complexity theory
- Quantum Information Theory
- Analysis of speedup using differential geometry, algebraic topology, etc.

Prerequisite classes and capabilities: Although this class has no explicit prerequisites we consider a list of recommended topics and skills that the student should feel comfortable with. 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 for this course. Programming skills are strongly recommended. 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.

Students with backgrounds in operations research, industrial engineering, chemical engineering, electrical engineering, physics, computer science, or applied mathematics are strongly encouraged to consider taking this course.

Tentative Course Outline:

Part 0 - Introduction to Linear Algebra for Quantum Mechanics and Machine Learning .... 1 week
- Complex numbers, vectors and vector spaces, functions as vectors, inner product, norms, projections.
- Hilbert spaces, basis vectors, matrices, Hermitian operators, and special matrices.

Part 1 - Mathematical Programming basics (classical methods) . 1 week
- Linear, nonlinear, continuous and discrete optimization.
- Integer Programming basics.
- Cutting plane theory and relaxations.

Part 2 - Basic classical machine learning .... 1 week
- 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.

Part 3 - Ising, QUBO .... 1 week
- Ising model basics.
- Simulated Annealing.
- Markov-chain Monte Carlo methods.
- Benchmarking classical methods.
- Formulating combinatorial problems as QUBOs.

Part 4 - GAMA: Graver Augmented Multiseed algorithm .... 1 week
- GAMA.
  - Applications: Portfolio Optimization.
  - Quantum Inspired: Quadratic (Semi-)Assignment Problem.
  - Test sets.

Part 5 - Hardware for solving Ising/QUBO .... 1 week
- Graphical Processing Units.
- Tensor Processing Units.
- Complementary metal-oxide-semiconductors (CMOS).
- Digital Annealers.
- Oscillator Based Computing.
- Coherent Ising Machines.

Part 6 - Axioms of Quantum Mechanics .... 1 week
- Postulates of Quantum of quantum mechanics.
- Quantum measurements, quantum operations.
- Multiple quantum states, observables.

Part 7 - Qubit Gate model of quantum computing .... 1 week
- 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.

Part 8 - Quantum methods for solving Ising/QUBO .... 1 week
- AQC, Quantum Annealing and D-Wave.
- QAOA: Quantum Approximate Optimization Algorithm.

Part 9 - Intermediate Project presentations .... 1 weeks

Part 10 - Recent advances and other topics .... 1 week
- Compiling
  - Quantum Annealing.
  - Gate-based Noisy Intermediate Scale Quantum (NISQ) devices.
- Adiabatic Quantum Computing and Algebraic Geometry.
  - Minimizing Polynomial Functions.
  - Prime Factorization.

Break .... 1 week

Part 11 - Quantum Algorithms for future quantum processors .. 1 week
- HHL Algorithms for solving a system of linear eqations ($Ax = b$).
- Factorizing large numbers.
- Quantum Fourier Transform.
- Quantum Shell game.
- Grover's search algorithm.

Part 12 - Noise and quantum error correction .... 1 week
- Review of classical error correction methods.
- Quantum error correction.

Part 13 - Guest speakers .... 1 weeks

Part 14 - Project completion .... 2 weeks

Part 15 - Project presentations .... 1 weeks

Grading Algorithm: The final course grade will be based on a term project accounting for 70% of the grade and periodic quizzes accounting for 30% of the grade. There will be 4 quizzes, each worth 10 points. Only the best 3 quizzes will count toward the 30%.
Note: While lower cut-offs may be used, the following cut-offs are guaranteed
Final Grade (% of Points): A (89 - 100%), B (79 - 88%), C (69 - 78%).

- Each lecture will have a short quiz (10 minutes at most) to evaluate the concepts covered in the previous lecture(s). Each quiz will be counted equally towards the final grade and the two worst quizzes won't be counted in that average.
- There will be ungraded exercises during the lectures on which the quizzes will be based on, whose solutions will be given at the end of each lecture for allowing the students to practice.
- Although the quizzes are designed to be completed in fewer than 10 minutes, in order to accommodate for students being unable to submit them during the lecture time, we will allow the quizzes to be submitted until midnight (11:59 p.m. EST) of the lecture day. Quizzes submitted after that deadline will not be graded. In case of emergency, see the details below.
- Given the long time-frame for the project completion, the presentation and report must be submitted **at least** two days before the last day of classes. Reports and presentations submitted in the 24 hours after the due date will only be eligible for 80% of the maximum number of point allotted. Assignments submitted more than 24 hours after the due date will not be accepted.
- If you experience extenuating circumstances (e.g., you are hospitalized) that prohibit you from submitting your assignments on time, please let us know via email. We will evaluate these instances on a case-by-case basis.

Office Hours: Post your questions in the forum provided for this purpose on Canvas. This course will be conducted online.

Project description: This project will be completed in groups of 2-4 students and will reflect the understanding of the students of the material covered in the lecture. The components of this project are the following

- Identify a problem that can be posed as an Integer Optimization Problem or a Machine Learning Problem. Discuss the importance of this problem.
- Summarize the literature surrounding the problem. How is it solved at this point? Which computational methods are employed to tackle these problems?
- Find or generate a family of instances or input data of the problem to test solution algorithms on it (consistent with literature or industrial application).
- Attempt to reproduce the state-of-the-art approach to address the problem using classical computing. Identify the sources of complexity while solving this problem that might benefit from quantum/quantum-inspired/unconventional (physics-inspired) methods.
- Map the problem and solve it using physics-inspired methods:

  If you choose an Integer Optimization Problem:

  Model the problem as a Quadratic Unconstrained Binary Optimization (QUBO). Verify that the reformulation of the problem is valid, in the sense that it represents the original problem.

  Solve it using simulated annealing as a benchmark.

  If you choose a Machine Learning Problem:

  Formulate a machine learning problem that is amenable to solution by a noisy intermediate-scale quantum (NISQ) device such as those available in computing cloud (e.g., Amazon Could Services).

  Solve it using neural networks and classical computing methods (consider solving it without using GPUs as a baseline for the comparison) as a benchmark.
- Perform simulations of NISQ devices and/or analytical resource estimates for this problem (so that we know what would be needed at scale when more mature NISQ devices become available in the future).

  If you choose an Integer Optimization Problem:

  Tackle the resulting QUBO using non-conventional methods, e.g. Quantum Annealing, QAOA, simulated annealing in GPUs/TPUs, etc. Compare at least two different methods.

  If you choose a Machine Learning Problem:

  Solve the learning task using hardware accelerators, e.g., GPUs or TPUs. Perform simulations or runs in limited-sized instances in NISQ devices.
- Provide a mid-term report with initial results and plan (15/70) with a short presentation (10/70).
- 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).

There will be an ungraded submission at the beginning of week 3 with the proposed problem to be solved (we can guide you in case you are out of ideas). There is a presentation at the middle of the semester (when the mid-term report is submitted) allowing students to present in front of the class their partial progress and receive feedback.

Much of the second half of the course is devoted to the final project completion, with the office hours aimed at each final project group.

The groups are self-created although we will support you in finding a group in case that you want to join one. Individual projects are only allowed under exceptional cases. One of the important learning objectives of this course is completing the project in a group (with a considerable amount of work distributed among several individuals).

Important Dates:

No Final Exam.
Project Proposal: Tuesday, September 21.
Intermediate Project Presentations in week 6-7.
Presentations in weeks 14.

Course Policy:

- Auditing students are encouraged to participate actively in the lectures.

- Regular attendance is essential and expected. Given that each lecture will build on top of the previous ones, we strongly suggest you to attend to each one of them. In order to accommodate for each situation, each lecture will be recorded and made available in the course's Canvas and attendance won't be counted towards the final grade. Keep in mind that attending to the lectures live will give you the chance to interact with the lecturers; therefore, we encourage it.
- Please sign up using Canvas.

Learning Objectives and gained skills: By the end of the semester, those enrolled in the course should be able to:

1. Describe the current status of quantum computing and its potential use for discrete optimization and machine learning.
2. Access and use quantum computing resources (such as Quantum Annealears, gate-based Quantum Computers and other photonics emergent hardware).
3. Set up a given integer program to be solved with quantum computing.
4. Acquire an expanded perspective on quantum-inspired algorithms and physics-based approaches for machine learning.
5. Work in groups collaboratively on a state-of-the-art project involving applications of quantum computing, integer programming, and machine learning.

USRA Collaboration

1. 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 QuIP Lectures)
2. NASA Quantum and Artificial Intelligence Laboratory (QuAIL)
   `https://quantum.nasa.gov`
3. Students of this course are encouraged to apply to the USRA Feynman Academy Internship program `https://riacs.usra.edu/quantum/qacademy` that sponsors research projects at NASA Ames Research Center.

Amazon Braket Collaboration

1. Access to D-Wave, Rigetti and ionQ have been made available by Amazon Braket.
2. Students will be provided individual sub-accounts for use with pre-funded amounts to access the quantum machines.

Academic Honesty: Lack of knowledge of the academic honesty policy is not a reasonable explanation for a violation. Any form of plagiarism can earn you a failing grade for the entire course. For more information you can refer to CMU's policies on academic integrity. When in doubt, add a citation. The quizzes are to be taken individually and with all the resources that a student might consider useful, except for another student. The project on the other hand is to be completed collaboratively within the given groups and shared with the rest of the class through the presentations.

Casual References: There is no single text book for the course. On the other hand, the lecture notes for the Quantum Integer Programming Lecture can be found at David E Bernal, Sridhar Tayur, and Davide Venturelli. "Quantum Integer Programming (QuIP) 47-779: Lecture Notes". In: *arXiv preprint arXiv:2012.11382* (2020). This is a short list of various interesting and useful books that will be mentioned during the course. You need to consult them occasionally.

- Richard J Lipton and Kenneth W Regan. *Quantum algorithms via linear algebra: a primer.* MIT Press, 2014
- Eleanor G Rieffel and Wolfgang H Polak. *Quantum computing: A gentle introduction.* MIT Press, 2011
- N David Mermin. *Quantum computer science: an introduction.* Cambridge University Press, 2007
- Georges Ifrah. *The universal history of computing: From the abacus to the quantum computer.* John Wiley & Sons, Inc., 2001
- Michael A Nielsen and Isaac Chuang. *Quantum computation and quantum information.* 2002

- Arnab Das and Bikas K Chakrabarti. *Quantum annealing and related optimization methods.* Vol. 679. Springer Science & Business Media, 2005

Accommodations for Students with Disabilities: If you have a disability and require accommodations, please contact Catherine Getchell, Director of Disability Resources, 412-268-6121, getchell@cmu.edu. If you have an accommodations letter from the Disability Resources office, we encourage you to discuss your accommodations and needs with us as early in the semester as possible. We will work with you to ensure that accommodations are provided as appropriate.

Well-being policy: As a student, you may experience a range of challenges that can interfere with learning, such as strained relationships, increased anxiety, substance use, feeling down, difficulty concentrating and/or lack of motivation. These mental health concerns or stressful events may diminish your academic performance and/or reduce your ability to participate in daily activities. CMU services are available, and treatment does work. You can learn more about confidential mental health services available on campus at: `http://www.cmu.edu/counseling/`. Support is always available (24/7) from Counseling and Psychological Services: 412-268-2922.

Diversity statement: We must treat every individual with respect. We are diverse in many ways, and this diversity is fundamental to building and maintaining an equitable and inclusive campus community. Diversity can refer to multiple ways that we identify ourselves, including but not limited to race, color, national origin, language, sex, disability, age, sexual orientation, gender identity, religion, creed, ancestry, belief, veteran status, or genetic information. Each of these diverse identities, along with many others not mentioned here, shape the perspectives our students, faculty, and staff bring to our campus. We, at CMU, will work to promote diversity, equity and inclusion not only because diversity fuels excellence and innovation, but because we want to pursue justice. We acknowledge our imperfections while we also fully commit to the work, inside and outside of our classrooms, of building and sustaining a campus community that increasingly embraces these core values.

Each of us is responsible for creating a safer, more inclusive environment.

Unfortunately, incidents of bias or discrimination do occur, whether intentional or unintentional. They contribute to creating an unwelcoming environment for individuals and groups at the university. Therefore, the university encourages anyone who experiences or observes unfair or hostile treatment on the basis of identity to speak out for justice and support, within the moment of the incident or after the incident has passed. Anyone can share these experiences using the following resources:

- Center for Student Diversity and Inclusion: csdi@andrew.cmu.edu, (412) 268-2150
- Report-It online anonymous reporting platform: `reportit.net` username: *tartans* password: *plaid*

All reports will be documented and deliberated to determine if there should be any following actions. Regardless of incident type, the university will use all shared experiences to transform our campus climate to be more equitable and just.