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

Graver Augmented Multiseed Algorithm (GAMA)

Lecture 07

09.26.2022







Agenda

- Hybrid Quantum-Classical Algorithms
- Graver Basis via Quantum Annealing
- Toy Example: Quantum Graver in 10 Steps
- Non-linear Integer Optimization on an Ising Solvers
- How to surpass Classical Best-in Class?
- Quantum-inspired Classical algorithm (special structured A)







A New Approach is Needed

Naive method of solving *IP*:
$$\begin{cases} & \text{min } f(x) \\ & Ax = b \quad l \le x \le u \end{cases}$$

by a Ising Solver is to:

- 1) Convert non quadratic f(x) into quadratic
- 2) Add constraint to quadratic and solve:

$$x^T Q x + \lambda (Ax - b)^T (Ax - b)$$

which has a balancing problem, and other issues.

We want to do something very different!







[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing

Solution methods for Combinatorial Optimization

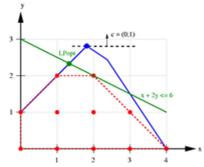
Current status and perspectives

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



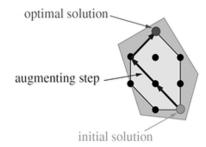


Not very popular classical methods

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**





^[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

GAMA: Hybrid Quantum-Classical Optimization

Calculate Graver Basis (Quantum-Classical)

Find Many Initial Feasible Solutions (Quantum)

Augmentation: Improve feasible solutions using Graver Basis (Classical)

Graver Augmented Multi-Seed Algorithm



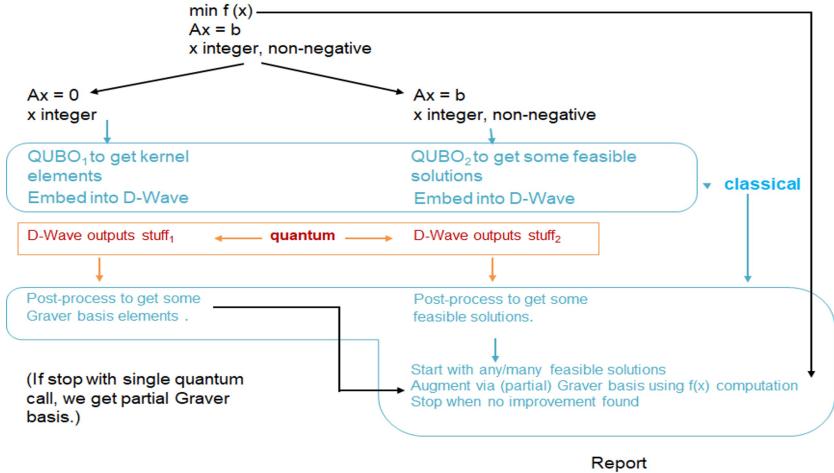




[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing

Carnegie Mellon University

GAMA



Report result(s)

[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing with application to non-linear integer programs." arXiv preprint arXiv:1902.04215 (2019).







Test Sets in Optimization

• Nonlinear integer program:

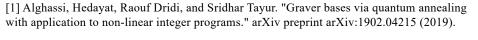
$$(IP)_{A,b,l,u,f}: \min \left\{ f(x) : Ax = b, x \in \mathbb{Z}^n, l \le x \le u \right\}$$

$$A \in \mathbb{Z}^{m \times n}, b \in \mathbb{Z}^m, l,u \in \mathbb{Z}^n, f : \mathbb{R}^n \to \mathbb{R}$$

- Can be solved via *augmentation procedure*:
- 1. Start from a feasible solution
- 2. Search for augmentation direction to improve
- 3. If none exists, we are at an optimal solution.







Definitions

Ax = 0; Linear Frobenius problem

1. The lattice integer kernel of: A

$$\mathcal{L}^*(A) = \left\{ x \middle| Ax = \mathbf{0}, x \in \mathbb{Z}^n , A \in \mathbb{Z}^{m \times n} \right\} \setminus \left\{ \mathbf{0} \right\}$$

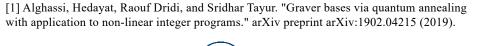
1. Partial Order

$$\forall x, y \in \mathbb{R}^n \quad x \sqsubseteq y \quad st. \quad x_i y_i \ge 0 \quad \& \quad |x_i| \le |y_i| \quad \forall \quad i = 1, ..., n$$

x is conformal (minimal) to y, $x \sqsubseteq y$







Partial order **⊑**

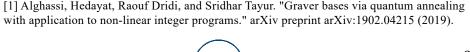
•
$$x = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \sqsubseteq y = \begin{bmatrix} 3 \\ 0 \\ -2 \end{bmatrix}$$
, x is conformal to y

•
$$x = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$
, $y = \begin{bmatrix} 3 \\ 0 \\ 2 \end{bmatrix}$, x and y are incomparable

•
$$x = \begin{bmatrix} 1 \\ 0 \\ -3 \end{bmatrix} \not\sqsubseteq y = \begin{bmatrix} 3 \\ 0 \\ -2 \end{bmatrix}$$
, x and y are not conformal







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Graver Basis

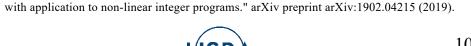
$$\mathcal{G}(A)
i g_i\subset \mathbb{Z}^n$$

Finite set of conformal (\sqsubseteq -minimal) elements in

$$\mathcal{L}(\mathbf{A}) = \{\mathbf{x}: \mathbf{A}\mathbf{x} = \mathbf{0}, \mathbf{x} \in \mathbb{Z}^n\} \setminus \{\mathbf{0}\}$$







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[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing

Test-sets and valid objectives

Test-set

Given an integer linear program $\min_{\mathbf{x}} f(\mathbf{x})$ s.t. $\mathbf{A}\mathbf{x} = \mathbf{b}, \mathbf{l} \leq \mathbf{x} \leq \mathbf{u}, \mathbf{x} \in \mathbb{Z}^n$ there exists a finite set denotes test-set $\mathcal{T} = \{\mathbf{t}^1, \dots, \mathbf{t}^N\}$ that only depends on \mathbf{A} , that assures that a feasible solution nonoptimal point \mathbf{x}_0 satisfies for some $\alpha \in \mathbb{Z}_+$

- $ullet f(\mathbf{x}_0 + lpha \mathbf{t}^i) < f(\mathbf{x}_0)$
- $\mathbf{x}_0 + \alpha \mathbf{t}^i$ is feasible

For which objective functions $f(\mathbf{x})$?

- Separable convex minimization: $\sum_i f_i(\mathbf{c}_i^{\top}\mathbf{x})$ with f_i convex
- Convex integer maximization: $-f(\mathbf{W}\mathbf{x})$ where $\mathbf{W} \in \mathbb{Z}^{d \times n}$ and f convex
- Norm p minimization: $f(\mathbf{x}) = ||\mathbf{x} \hat{\mathbf{x}}||_p$
- Quadratic minimization: $f(\mathbf{x}) = \mathbf{x}^{\top} \mathbf{Q} \mathbf{x}$ where \mathbf{Q} lies on the dual of the quadratic Graver cone of \mathbf{A}
 - \circ this includes certain nonconvex $\mathbf{Q} \not\succeq 0$
- Polynomial minimization: $f(\mathbf{x}) = P(\mathbf{x})$ where P is a polynomial of degree d, that lies on cone $\mathcal{K}_d(\mathbf{A})$, dual of d^{th} degree Graver cone of \mathbf{A}





Test-set methods - Example

Primal method for Integer Programs

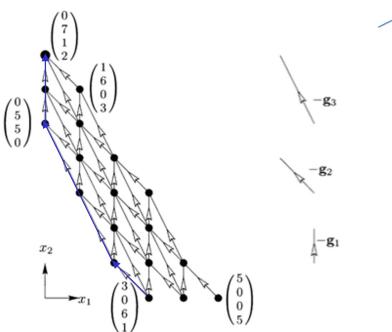
We require:

- An initial feasible solution
- An oracle to compare objective function
- The test-set (set of directions)
- Given the objective, the test set will point us a direction where to improve it, and if no improvement, we have the optimal solution.
- The Graver basis test-set only depends on the constraints and objective and can be computed for equality constraints with integer variables

Example

$$A\mathbf{x} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix} \mathbf{x} = \begin{bmatrix} 10 \\ 15 \end{bmatrix}$$







^[2] Integer Programming (1st ed. 2014) by Michele Conforti, Gérard Cornuéjols, and Giacomo Zambelli







Test-set methods - Example

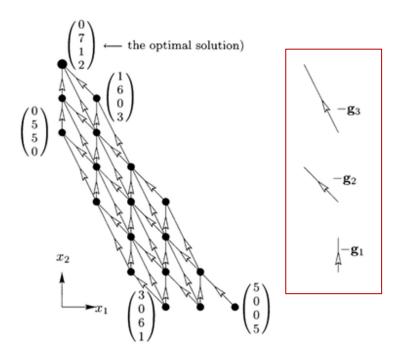
Combinatorial problems are usually NP Unless P=NP, they don't accept polynomial algorithms.

Where is the NP?

Obtaining the test-set!

Example

$$A\mathbf{x} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \end{bmatrix} \mathbf{x} = \begin{bmatrix} 10 \\ 15 \end{bmatrix}$$



[1] Gröbner Bases and Integer Programming, G. Ziegler. 1997







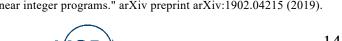
Definitions

- Finding the lattice kernel $\mathcal{L}^*(A)$ using many reads of an Ising solver: need a QUBO
- Filtering conformal

 minimal elements by comparisons, using classical methods
- If QUBO solver has limitations: Repeating (1) and (2) while *adjusting* the "QUBO" variables in each run adaptively







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QUBO for Kernel

$$\mathbf{A}\mathbf{x} = \mathbf{0}, \quad \mathbf{x} \in \mathbb{Z}^{n} \quad , \quad \mathbf{A} \in \mathbb{Z}^{m \times n}$$

$$\min \quad \mathbf{x}^{T}\mathbf{Q}_{\mathbf{I}}\mathbf{x} \quad , \quad \mathbf{Q}_{\mathbf{I}} = \mathbf{A}^{T}\mathbf{A} \quad , \quad \mathbf{x} \in \mathbb{Z}^{n}$$

$$\mathbf{x}^{T} = \left[\begin{array}{cccc} x_{1} & x_{2} & \dots & x_{i} & \dots & x_{n} \end{array} \right] \quad , \quad x_{i} \in \mathbb{Z}$$

• Integer to binary transformation: $x_i = \mathbf{e}_i^T X_i$

$$X_i^T = \begin{bmatrix} X_{i,1} & X_{i,2} & \cdots & X_{i,k_i} \end{bmatrix} \in \{0,1\}^{k_i}$$

- Binary encoding $\mathbf{e}_i^T = \begin{bmatrix} 2^0 & 2^1 & \cdots & 2^{k_i} \end{bmatrix}$
- Unary encoding $\mathbf{e}_i^T = \begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix}$

[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing with application to non-linear integer programs." arXiv preprint arXiv:1902.04215 (2019).





QUBO for Kernel

$$\mathbf{x} = \mathbf{L} + \mathbf{E} \mathbf{X} = \begin{bmatrix} L x_1 \\ L x_2 \\ \vdots \\ L x_n \end{bmatrix} + \begin{bmatrix} \mathbf{e}_1^T & \mathbf{0}^T & \cdots & \mathbf{0}^T \\ \mathbf{0}^T & \mathbf{e}_2^T & \cdots & \mathbf{0}^T \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}^T & \mathbf{0}^T & \cdots & \mathbf{e}_n^T \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{bmatrix}$$

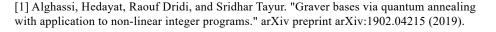
(L is the lower bound vector)

QUBO

min
$$\mathbf{X}^T$$
 $\mathbf{Q_B}\mathbf{X}$, $\mathbf{Q_B} = \mathbf{E}^T\mathbf{Q_I}\mathbf{E} + diag(2\mathbf{L}^T\mathbf{Q_I}\mathbf{E})$
 $\mathbf{X} \in \{0,1\}^{nk}$, $\mathbf{Q_I} = \mathbf{A}^T\mathbf{A}$







Ten Steps to obtain Graver basis of A

- 1. Matrix A into QUIO
- 2. Encoding to have only binary variables
- 3. Encoding Matrix
- 4. Encoded Equation
- 5. QUBO
- 6. Mapping binary to Ising variables
- 7. Ising Model
- 8. Solution of Ising Model
- 9. Kernel of A
- 10. Graver basis from Kernel







Step 1: Matrix to Quadratic Unconstrained Integer Optimization (QUIO)

Consider

$$A = \begin{bmatrix} 1 & 2 & 1 \end{bmatrix}$$

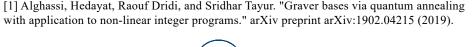
Quadratic Unconstrained Integer Optimization QUIO:

$$Ax = 0 \rightarrow \min_{Q_I} x^T (A^T A) x$$

$$Q_{I} = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$$







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Step 2: Encoding

Two bit encoding:

$$e_i = \left[\begin{array}{cc} 2^0 & 2^1 \end{array} \right]$$

• Two bit normally (L=0), covers:

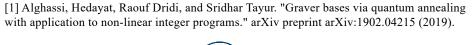
$$\{0,1,2,3\}$$

• —If shifted one step left (L=-1), covers:

$$\{-1,0,1,2\}$$



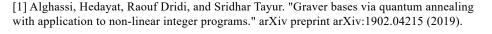




Step 3: Encoding Matrix







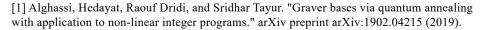
Step 4: Encoded Equation

$$x = L + EX$$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix} + \begin{bmatrix} 1 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{bmatrix}$$







Step 5: Quadratic Unconstrained Binary Optimization (QUBO)

$$\min \quad (L + EX)^T \quad Q_I(L + EX) \to \quad \min \quad X^T \underbrace{\left(E^T Q_I E + 2 diag(L^T Q_I E)\right)}_{Q_B} X$$

QUBO

$$\min \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{bmatrix}^T \begin{bmatrix} -7 & 2 & 2 & 4 & 1 & 2 \\ 2 & -12 & 4 & 8 & 2 & 4 \\ 2 & 4 & -12 & 8 & 2 & 4 \\ 4 & 8 & 8 & -16 & 4 & 8 \\ 1 & 2 & 2 & 4 & -7 & 2 \\ 2 & 4 & 4 & 8 & 2 & -12 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{bmatrix}$$

[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing with application to non-linear integer programs." arXiv preprint arXiv:1902.04215 (2019).





Step 6: Mapping to Ising variables

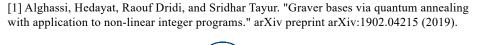
• We need to take X which are $\{0,1\}$ to S which are $\{-1,+1\}$

$$S = 2X - 1$$

$$X = \frac{1}{2} \left(S + \mathbf{1} \right)$$







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Step 7: Reframing in Ising Model

min
$$S^T J S + h^T S$$

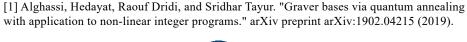
$$X^{T}QX = \frac{\left(S+\mathbf{1}\right)^{T}}{2}Q\frac{\left(S+\mathbf{1}\right)}{2} \to \frac{1}{4}S^{T}QS + \frac{1}{2}\mathbf{1}^{T}QS + \frac{1}{4}\mathbf{1}^{T}Q\mathbf{1} \to J = \frac{1}{4}Q \quad h = \frac{1}{2}\mathbf{1}^{T}Q$$

$$J = \begin{bmatrix} 0 & 0.5 & 0.5 & 1 & 0.25 & 0.5 \\ 0.5 & 0 & 1 & 2 & 0.5 & 1 \\ 0.5 & 1 & 0 & 2 & 0.5 & 1 \\ 1 & 2 & 2 & 0 & 1 & 2 \\ 0.25 & 0.5 & 0.5 & 1 & 0 & 0.5 \\ 0.5 & 1 & 1 & 2 & 0.5 & 0 \end{bmatrix} \qquad h = \begin{bmatrix} 2 \\ 4 \\ 4 \\ 8 \\ 2 \\ 4 \end{bmatrix}$$

$$h = \left[\begin{array}{c} 2\\4\\4\\8\\2\\4 \end{array} \right]$$

Note:

$$S_i^2 = 1 \rightarrow diag(J) = \mathbf{0}$$







Step 8: Solve Ising Model to get S and convert to X

Note that there are 4 unique elements of *J*

$$\{0,0.25,0.5,1,2\}$$

Ising Solver (such as D-Wave) gives S

$$\begin{cases} S_i = +1 \rightarrow X_i = 1 \\ S_i = -1 \rightarrow X_i = 0 \end{cases}$$

Get X back from S (see Step 6)

Optimal *X's*:

$$\begin{bmatrix} X \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 \end{bmatrix}$$







[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing with application to non-linear integer programs." arXiv preprint arXiv:1902.04215 (2019).

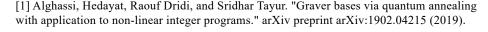
Step 9: Recover Kernel of A (in original integer variables)

$$x = L + EX \rightarrow$$

$$[x] = \left(\begin{array}{ccccccccc} -1 & -1 & 0 & 0 & 1 & 1 & 2 \\ 0 & 1 & -1 & 0 & -1 & 0 & -1 \\ 1 & -1 & 2 & 0 & 1 & -1 & 0 \end{array} \right)$$







Step 10: Convert Kernel to Graver Basis

$$\lceil x \rceil \rightarrow \sqsubseteq -\text{minimal classical filteration} \rightarrow \mathcal{G}(A)$$

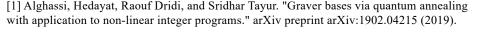
$$\mathcal{G}(A) = \left(\begin{array}{cccc} 0 & 1 & 1 & 2 \\ -1 & -1 & 0 & -1 \\ 2 & 1 & -1 & 0 \end{array} \right)$$

• Negative basis elements are also part of Graver Basis:

$$-\mathcal{G}(A) = \left(\begin{array}{cccc} 0 & -1 & -1 & -2 \\ 1 & 1 & 0 & 1 \\ -2 & -1 & 1 & 0 \end{array}\right)$$







QUBO for Feasible Solutions

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$
 $l \le \mathbf{x} \le u$

min
$$\mathbf{X}^{T} \mathbf{Q}_{\mathbf{B}} \mathbf{X}$$
, $\mathbf{Q}_{\mathbf{B}} = \mathbf{E}^{T} \mathbf{Q}_{\mathbf{I}} \mathbf{E} + 2 diag \left[\left(\mathbf{L}^{T} \mathbf{Q}_{\mathbf{I}} - \mathbf{b}^{T} \mathbf{A} \right) \mathbf{E} \right]$
 $\mathbf{X} \in \left\{ 0, 1 \right\}^{nk}$, $\mathbf{Q}_{\mathbf{I}} = \mathbf{A}^{T} \mathbf{A}$

Results in many feasible solutions!







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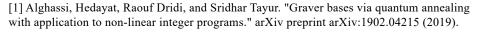
[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing

Hybrid Quantum-Classical Optimization

- 1. Calculate Graver Basis
- 2. Find Initial Feasible Solution(s) (Quantum)
- 3. Augmentation: Improve feasible solutions (Classical)









Example: Capital Budgeting

Important canonical Finance problem

- μ_i expected return
- σ_i variance
- **E** risk

$$\begin{cases}
\min & -\sum_{i=1}^{n} \mu_{i} x_{i} + \sqrt{\frac{1-\varepsilon}{\varepsilon}} \sum_{i=1}^{n} \sigma_{i}^{2} x_{i}^{2} \\
Ax = b , x \in \{0,1\}^{n}
\end{cases}$$

Graver Basis in 1 D-Wave call (1 bit encoding)

$$A \in M_{5 \times 50}(\{0, \dots, t\})$$
 $\mu \in [0,1]^{50 \times 1}$ $\sigma \in [0, \mu_i]^{50 \times 1}$

when t = 1 we have:

$$\mathcal{G}(A) \in M_{50 imes 304}(\{-1,0,+1\})$$

[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing with application to non-linear integer programs." arXiv preprint arXiv:1902.04215 (2019).





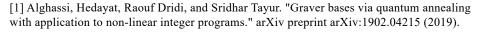
GAMA in Action

Let's go to the Colab

https://colab.research.google.com/github/bernalde/QuIPML22/blob/master/notebook s/Notebook%203%20-%20GAMA.ipynb





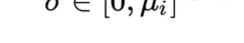


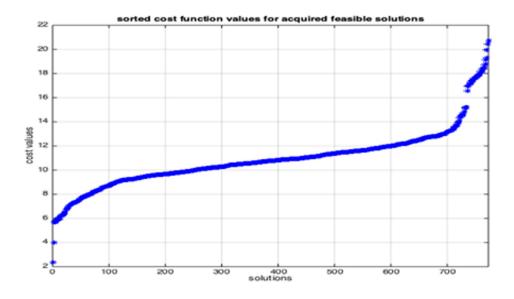
Non-binary Integer Variables

• Low span integer $x \in \{-2, -1, 0, 1, 2\}^n$

$$A \in M_{5 imes 50} \left(\{0,1\}
ight) \hspace{0.5cm} \mu \in [0,1]^{25 imes 1} \hspace{0.5cm} \sigma \in [0,\mu_i]^{25 imes 1}$$

- 2 Bit Encoding
- $\mathcal{G}(A) \in M_{25 \times 616} (\{-4, \dots, +4\})$ in 2 D-Wave calls
- 773 feasible solutions in one D-Wave call





[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing with application to non-linear integer programs." arXiv preprint arXiv:1902.04215 (2019).



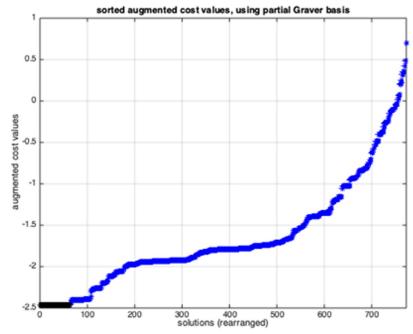


Augmenting...

- From any feasible points in \sim 20-34 augmenting steps, reach global optimal cost = -2.46
- Partial Graver Basis: One D-Wave call only

• 64 out of 773 feasible starting points end up at global solutions.

$$\mathcal{G}^P(A) \in M_{25 imes418}\left(\{-4,\ldots,+4\}
ight)$$



[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing with application to non-linear integer programs." arXiv preprint arXiv:1902.04215 (2019).





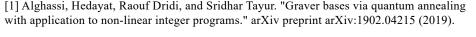


D-Wave: How and Where to Surpass Classical?

- If coupler precision doubles, with the same number of qubits and connectivity, we can be competitive on 0-1 problems and $\{0,...,t\}$ matrices of size 50.
- Pegasus can embed a size 180 problem with shorter chains, could surpass Gurobi on {0,1} matrices of sizes 120 to 180, but for limited fidelity.
- An order of magnitude increase in maximum number of anneals per call.
- Global optimization with difficult convex (and non-convex) objective functions.





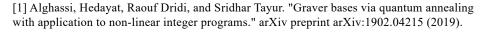


GAMA: Classical

- If A has special structure, we can construct Graver Basis from first principles and also randomly generate many feasible solutions.
- No need for quantum computer!
- Problem classes include QAP, QSAP and CBQP.
- Really, really fast! (100x compared to Gurobi!)





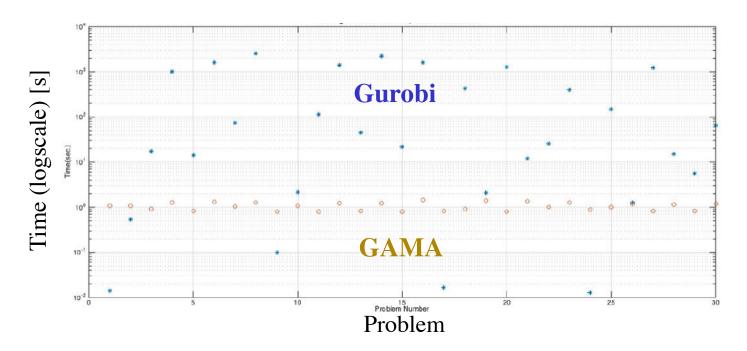


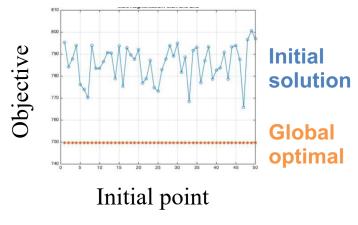


GAMA: Applications

Cardinality Constrained Quadratic Programs

$$\min \left\{ \mathbf{c}^T \mathbf{x} + \mathbf{x}^T Q \mathbf{x} : \mathbf{1}_n^T \mathbf{x} = b \right\}$$





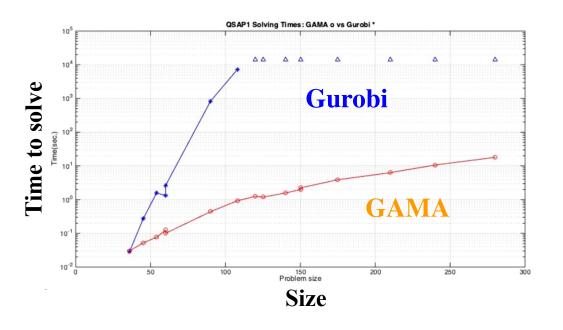
[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing with application to non-linear integer programs." arXiv preprint arXiv:1902.04215 (2019).



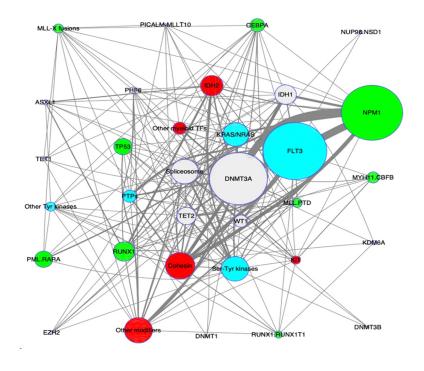


GAMA: Applications

Quadratic Semi-Assignment Problem



Cancer Genomics



- [1] Alghassi H., Dridi R., Tayur S. (2019) GAMA: A Novel Algorithm for Non-Convex Integer Programs. arXiv:1907.10930
- [2] Alghassi, Hedayat, et al. "Quantum and Quantum-inspired Methods for de novo Discovery of Altered Cancer Pathways." bioRxiv (2019): 845719.







References

[1] Alghassi H., Dridi R., Tayur S. (2018) Graver Bases via Quantum Annealing with Application to Non-linear Integer Programs. arXiv:1902.04215

[2] Alghassi H., Dridi R., Tayur S. (2019) GAMA: A Novel Algorithm for Non-Convex Integer Programs. arXiv:1907.10930

[3] Alghassi, Hedayat, et al. "Quantum and Quantum-inspired Methods for de novo Discovery of Altered Cancer Pathways." bioRxiv (2019): 845719.





