

Quantum Integer Programming

47-779

**Graver Augmented
Multiseed Algorithm (GAMA)**



Agenda

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



A New Approach is Needed

Naive method of solving IP:

$$\left\{ \begin{array}{l} \min f(x) \\ Ax = b \quad l \leq x \leq u \end{array} \right.$$

by a Quantum Annealer is to:

- 1) Convert non quadratic $f(x)$ into $x^T Q x$
- 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!



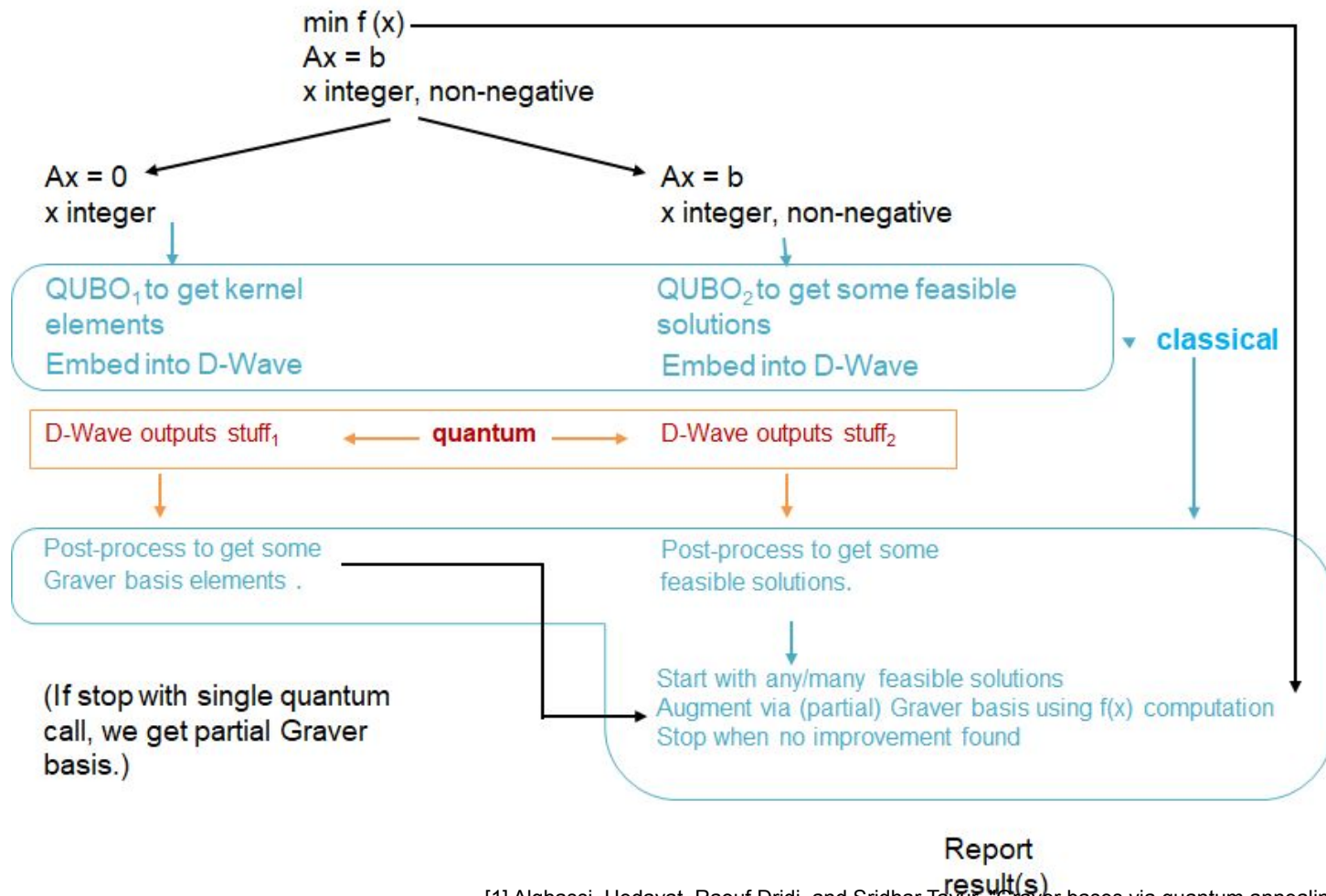
GAMA: Hybrid Quantum-Classical Optimization

Calculate Graver Basis (Quantum-Classical)

Find Many Initial Feasible Solutions (Quantum)

Augmentation: Improve feasible solutions using Graver Basis (Classical)

Graver Augmented Multi-Seed Algorithm



Test Sets in Optimization

- Nonlinear integer program:

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

- 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

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

2. Partial Order

$$\forall x, y \in \mathbb{R}^n \quad x \sqsubseteq y \quad \text{s.t.} \quad x_i y_i \geq 0 \quad \& \quad |x_i| \leq |y_i| \quad \forall \quad i = 1, \dots, n$$

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

Partial order $\sqsubseteq$

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

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

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

Graver Basis

$$\mathcal{G}(A) \ni g_i \in \mathbb{Z}^n$$

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

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

Test-sets and valid objectives

Test-set

Given an integer linear program $\min_{\mathbf{x}} f(\mathbf{x})$ s.t. $\mathbf{Ax} = \mathbf{b}, \mathbf{l} \leq \mathbf{x} \leq \mathbf{u}, \mathbf{x} \in \mathbb{Z}^n$ 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 $\alpha \in \mathbb{Z}_+$

- $f(\mathbf{x}_0 + \alpha \mathbf{t}^i) < f(\mathbf{x}_0)$
- $\mathbf{x}_0 + \alpha \mathbf{t}^i$ 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 $\mathbf{A}$
 - this includes certain nonconvex $\mathbf{Q} \not\geq 0$
- 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 $\mathbf{A}$

Hybrid Quantum- Classical Graver

1. Finding the lattice kernel $\mathcal{L}^*(A)$ using many reads of quantum annealer : need a QUBO
2. Filtering conformal $\sqsubseteq$ minimal elements by comparisons, using classical methods
3. If QUBO solver has limitations: Repeating (1) and (2) while *adjusting* the “QUBO” variables in each run *adaptively*



QUBO for Kernel

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

$$\min \quad \mathbf{x}^T \mathbf{Q}_1 \mathbf{x}, \quad \mathbf{Q}_1 = \mathbf{A}^T \mathbf{A}, \quad \mathbf{x} \in \mathbb{Z}^n$$

$$\mathbf{x}^T = \begin{bmatrix} x_1 & x_2 & \dots & x_i & \dots & x_n \end{bmatrix}, \quad x_i \in \mathbb{Z}$$

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

$$\mathbf{X}_i^T = \begin{bmatrix} X_{i,1} & X_{i,2} & \dots & X_{i,k_i} \end{bmatrix} \in \{0,1\}^{k_i}$$

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

- Unary encoding $\mathbf{e}_i^T = \underbrace{\begin{bmatrix} 1 & 1 & \dots & 1 \end{bmatrix}}_{k_i}$

QUBO for Kernel

$$\mathbf{x} = \mathbf{L} + \mathbf{E}\mathbf{X} = \begin{bmatrix} Lx_1 \\ Lx_2 \\ \vdots \\ Lx_n \end{bmatrix} + \begin{bmatrix} \mathbf{e}_1^T & \mathbf{0}^T & \cdots & \mathbf{0}^T \\ \mathbf{0}^T & \mathbf{e}_2^T & \cdots & \mathbf{0}^T \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}^T & \mathbf{0}^T & \cdots & \mathbf{e}_n^T \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{bmatrix}$$

(L is the lower bound vector)

- QUBO

$$\min \quad \mathbf{X}^T \mathbf{Q}_B \mathbf{X} \quad , \quad \mathbf{Q}_B = \mathbf{E}^T \mathbf{Q}_I \mathbf{E} + \text{diag}\left(2\mathbf{L}^T \mathbf{Q}_I \mathbf{E}\right)$$

$$\mathbf{X} \in \{0,1\}^{nk} \quad , \quad \mathbf{Q}_I = \mathbf{A}^T \mathbf{A}$$



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:

$$Ax = 0 \rightarrow \min x^T \underbrace{(A^T A)}_{Q_I} x$$

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



Step 2: Encoding

Two bit encoding:

$$e_i = \begin{bmatrix} 2^0 & 2^1 \end{bmatrix}$$

- 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

$$E = \begin{bmatrix} 1 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 \end{bmatrix}$$

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)

$$\min (L + EX)^T Q_l (L + EX) \rightarrow \min X^T \underbrace{(E^T Q_l E + 2 \text{diag}(L^T Q_l E))}_{Q_B} X$$

o QUBO

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



Step 6: Mapping to Ising variables

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

$$S = 2X - 1$$

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



Step 7: Reframing in Ising Model

$$\min S^T JS + h^T S$$

$$X^T QX = \frac{(S+1)^T}{2} Q \frac{(S+1)}{2} \rightarrow \frac{1}{4} S^T QS + \frac{1}{2} \mathbf{1}^T QS + \underbrace{\frac{1}{4} \mathbf{1}^T Q \mathbf{1}}_{cte} \rightarrow J = \frac{1}{4} Q \quad h = \frac{1}{2} \mathbf{1}^T Q$$

$$J = \begin{bmatrix} 0 & 0.5 & 0.5 & 1 & 0.25 & 0.5 \\ 0.5 & 0 & 1 & 2 & 0.5 & 1 \\ 0.5 & 1 & 0 & 2 & 0.5 & 1 \\ 1 & 2 & 2 & 0 & 1 & 2 \\ 0.25 & 0.5 & 0.5 & 1 & 0 & 0.5 \\ 0.5 & 1 & 1 & 2 & 0.5 & 0 \end{bmatrix}$$

$$h = \begin{bmatrix} 2 \\ 4 \\ 4 \\ 8 \\ 2 \\ 4 \end{bmatrix}$$

o Note:

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

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

- Note that there are 4 unique elements of J

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

- Quantum Annealer (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:

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

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

$$x = L + EX \rightarrow$$

$$[x] = \begin{pmatrix} -1 & -1 & 0 & 0 & 1 & 1 & 2 \\ 0 & 1 & -1 & 0 & -1 & 0 & -1 \\ 1 & -1 & 2 & 0 & 1 & -1 & 0 \end{pmatrix}$$



Step 10: Convert Kernel to Graver Basis

$$[x] \rightarrow \sqsubseteq\text{-minimal classical filtration} \rightarrow \mathcal{G}(A)$$

$$\mathcal{G}(A) = \begin{pmatrix} 0 & 1 & 1 & 2 \\ -1 & -1 & 0 & -1 \\ 2 & 1 & -1 & 0 \end{pmatrix}$$

- Negative basis elements are also part of Graver Basis:

$$-\mathcal{G}(A) = \begin{pmatrix} 0 & -1 & -1 & -2 \\ 1 & 1 & 0 & 1 \\ -2 & -1 & 1 & 0 \end{pmatrix}$$



Sampling for Kernel

- Each anneal starts with an independent uniform superposition (10000 per D-Wave call):

$$|\hat{0}\rangle = \frac{1}{2^n} \sum_{i \in \mathbb{Z}_2^n} |i\rangle$$

- Symmetry in QUBO (for arbitrary A) implies similar spread in valleys
- Techniques:
 - Random column permutation
 - Adaptive resource allocation chases the non-extracted solutions



Post Processing

Experimental observation:

- Majority ($\sim 90\%$) of sub-optimal solutions have small overall sum-errors: most **near-optimal!**
- **Post-processing**: Systematic pairwise error vector addition and subtraction to yield zero columns of these near-optimal solutions
- Overall numerical complexity low (and polynomial) by limiting range of errors post-processed



Post Processing: Analysis

Optimal and suboptimal percentages for various sizes

	(2x5)	(3x5)	(3x6)	(3x7)	(4x8)	(5x8)	Overall
0	15	12	10	13	12	9	11.8
1	24	28	26	31	30	33	28.7
2	31	28	27	24	21	25	26.0
3	20	21	25	19	20	17	20.3
4	7	8	10	9	9	8	8.5
5	2	1	0	3	4	5	2.5
6	1	2	2	1	4	3	2.2



Computational Experience

For all matrices that have a small span of integral values (± 4) the Graver basis acquired with less than 7 calls.

All embeddable ($m \times 16$) *binary matrices* Graver basis acquired in less than 5 calls.

The quantum approach performs very well for narrow truncated band, i.e. $\{-1, 0, 1\}$, attractive as test set for nonlinear combinatorial or low span integer programming.

QUBO for Feasible Solutions

$$\mathbf{Ax} = \mathbf{b} \quad l \leq \mathbf{x} \leq u$$

$$\min \quad \mathbf{X}^T \mathbf{Q}_B \mathbf{X}, \quad \mathbf{Q}_B = \mathbf{E}^T \mathbf{Q}_I \mathbf{E} + 2 \text{diag} \left[\left(\mathbf{L}^T \mathbf{Q}_I - \mathbf{b}^T \mathbf{A} \right) \mathbf{E} \right]$$

$$\mathbf{X} \in \{0, 1\}^{nk}, \quad \mathbf{Q}_I = \mathbf{A}^T \mathbf{A}$$

- Using adaptive centering and encoding width for feasibility bound
- Results in **many feasible solutions!**



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

$$\left\{ \begin{array}{l} \circ \mu_i \text{ expected return} \\ \circ \sigma_i \text{ variance} \\ \circ \varepsilon \text{ risk} \end{array} \right. \quad \min -\sum_{i=1}^n \mu_i x_i + \sqrt{\frac{1-\varepsilon}{\varepsilon} \sum_{i=1}^n \sigma_i^2 x_i^2}$$

$$Ax = b \quad , \quad x \in \{0,1\}^n$$

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

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

when $t = 1$ we have:

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



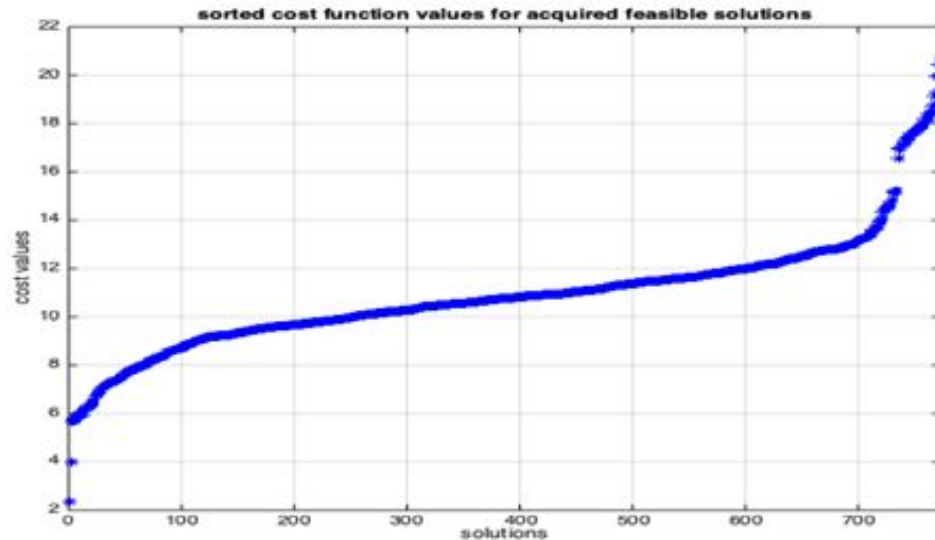
GAMA in Action

Let's go to the Colab

<https://colab.research.google.com/github/bernalde/QuIP/blob/master/notebooks/Notebook%206%20-%20GAMA.ipynb>

Non-binary Integer Variables

- Low span integer $x \in \{-2, -1, 0, 1, 2\}^n$
 $A \in M_{5 \times 50}(\{0, 1\}) \quad \mu \in [0, 1]^{25 \times 1} \quad \sigma \in [0, \mu_i]^{25 \times 1}$
- 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



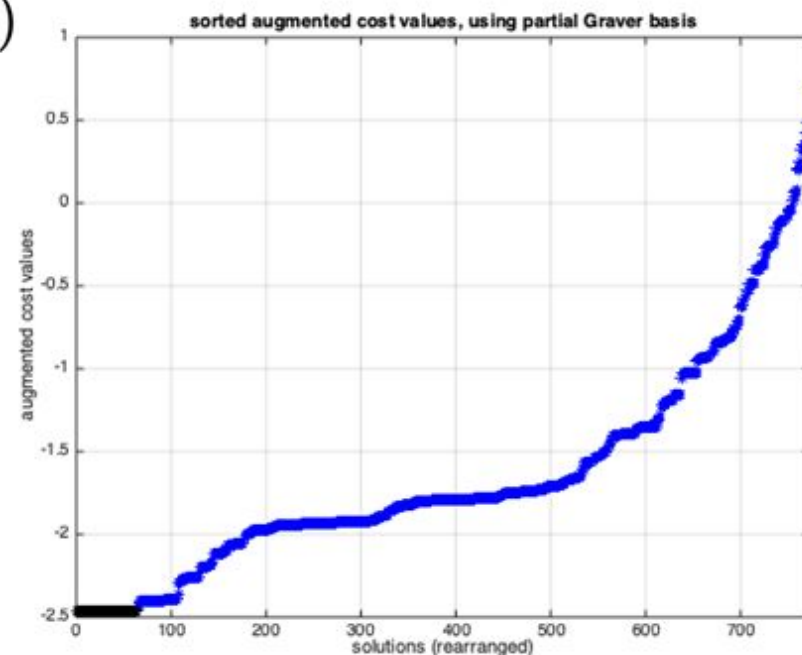
[1] Alghassi, Hedayat, Raouf Dridi, and Sridhar Tayur. "Graver bases via quantum annealing with application to non-linear integer programs." arXiv preprint arXiv:1902.04215 (2019).

Augmenting...

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

$$\mathcal{G}^P(A) \in M_{25 \times 418} (\{-4, \dots, +4\})$$

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



How to Surpass Best-in-Class Classical Methods?

Gurobi 8.0

- Random $A \in M_{5 \times 50} (\{0, \dots, t\})$
- “terms” designates cardinality of set of J values

$$\begin{array}{lll} t=1 \Rightarrow \begin{cases} 0.2 \text{ sec} \\ 6 \text{ terms} \end{cases} & t=10 \Rightarrow \begin{cases} 16 \text{ sec} \\ 230 \text{ terms} \end{cases} & t=20 \Rightarrow \begin{cases} 3 \text{ min} \\ 620 \text{ terms} \end{cases} \\ t=40 \Rightarrow \begin{cases} 21 \text{ min} \\ 1030 \text{ terms} \end{cases} & t=50 \Rightarrow \begin{cases} 75 \text{ min} \\ 1070 \text{ terms} \end{cases} & t=100 \Rightarrow \begin{cases} > 8 \text{ hours} \\ 1190 \text{ terms} \end{cases} \end{array}$$

D-Wave

- Chimera but improved coupler precision to handle more unique **J** elements for 0-1 matrices.

$$\begin{array}{lll} \left\{ \begin{array}{l} t=1 \\ A^{20 \times 80} \end{array} \right\} \Rightarrow \begin{cases} 135 \text{ sec} \\ 13 \text{ terms} \end{cases} & \left\{ \begin{array}{l} t=1 \\ A^{25 \times 100} \end{array} \right\} \Rightarrow \begin{cases} \sim 2 \text{ hours} \\ 15 \text{ terms} \end{cases} & \left\{ \begin{array}{l} t=1 \\ A^{30 \times 120} \end{array} \right\} \Rightarrow \begin{cases} > 3 \text{ hours} \\ 16 \text{ terms} \end{cases} \end{array}$$

How and Where to Surpass?

- o If **coupler precision** doubles, with the same number of qubits and connectivity, we can be competitive on 0-1 problems and $\{0, \dots, t\}$ matrices of size 50.
- o **Pegasus** can embed a size 180 problem with shorter chains, should surpass Gurobi on $\{0, 1\}$ matrices of sizes 120 to 180, without an increase in precision.
- o An order of magnitude increase in **maximum number of anneals per call**.
- o Global optimization with **difficult convex** (and non-convex) objective functions.

GAMA: Classical

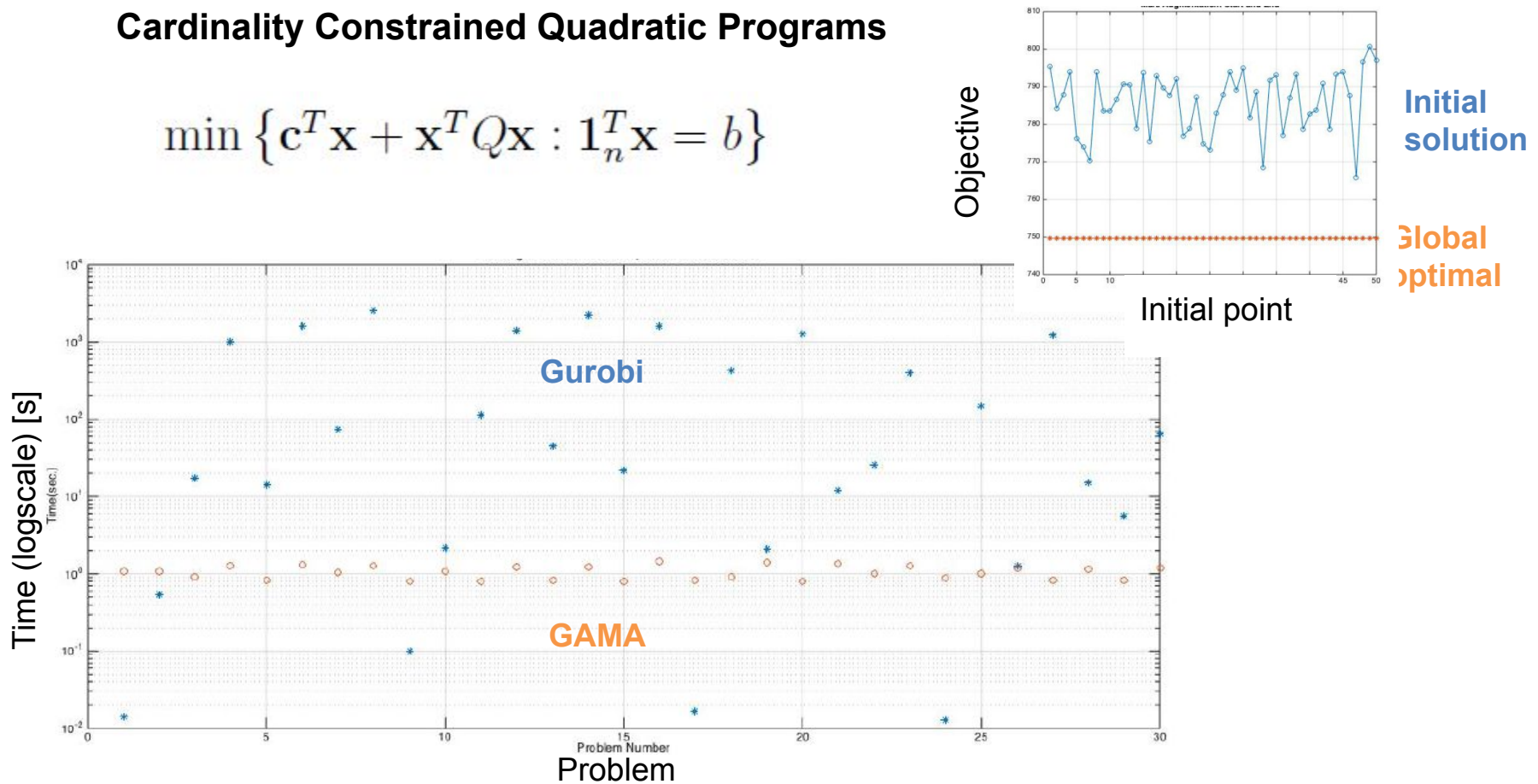
- If A has special structure, we can construct Graver Basis from first principles and also randomly generate many feasible solutions.
- No need for quantum computer!
- Problem classes include QAP, QSAP and CBQP.
- Really, really fast! (100x compared to Gurobi!)



GAMA: Applications

Cardinality Constrained Quadratic Programs

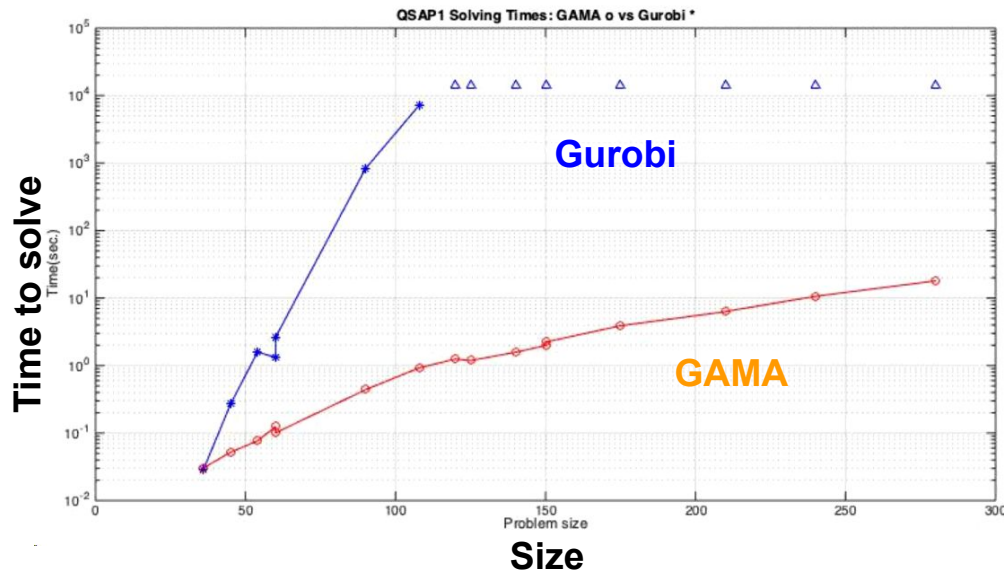
$$\min \{ \mathbf{c}^T \mathbf{x} + \mathbf{x}^T \mathbf{Q} \mathbf{x} : \mathbf{1}_n^T \mathbf{x} = b \}$$



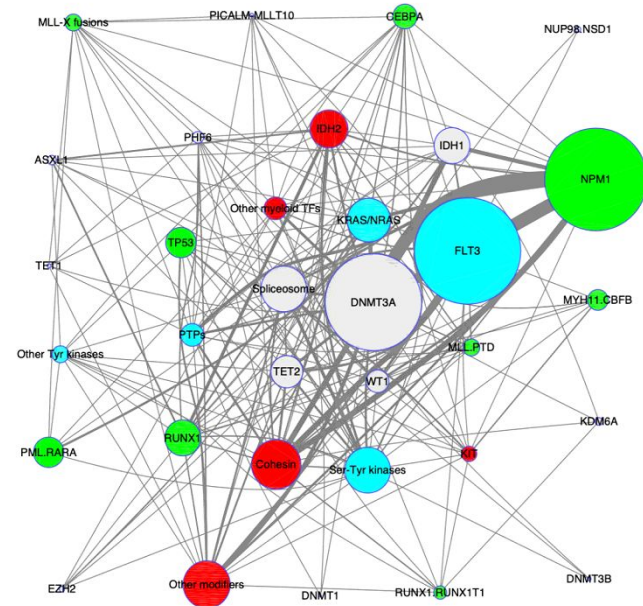


GAMA: Applications

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.](#)

Carnegie Mellon University

Tepper School of Business

William Larimer Mellon, Founder