Minimizing Polynomial Functions

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Agenda

- Overview of Research Program
- GAMA: A Novel Approach for Optimization
- Background: Test Sets, Graver Basis
- Graver Basis via Quantum Annealing
- Multiple Feasible Solutions via QA
- Non-linear Integer Optimization on D-Wave
- How to surpass Classical Best-in Class?
- Concluding Remarks

Overview of Research Program

- Non-Linear Integer Optimization
  - GAMA: A Brand New Approach
- Compiling
  - AQC and Gate (circuit) models
- Analysis of Speedup
- Real Applications
  - Finance, Chemical Engineering, Cancer Genomics

A New Approach is Needed

- Naive method of solving IP:

$$\begin{cases} \min \quad f(x) \\ Ax = b \quad l \le x \le u \end{cases}$$

by a Quantum Annealer is to:

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

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

- which has balancing problem, and more.
  - We want to do something very different!

GAMA: Hybrid Quantum- Classical Optimization

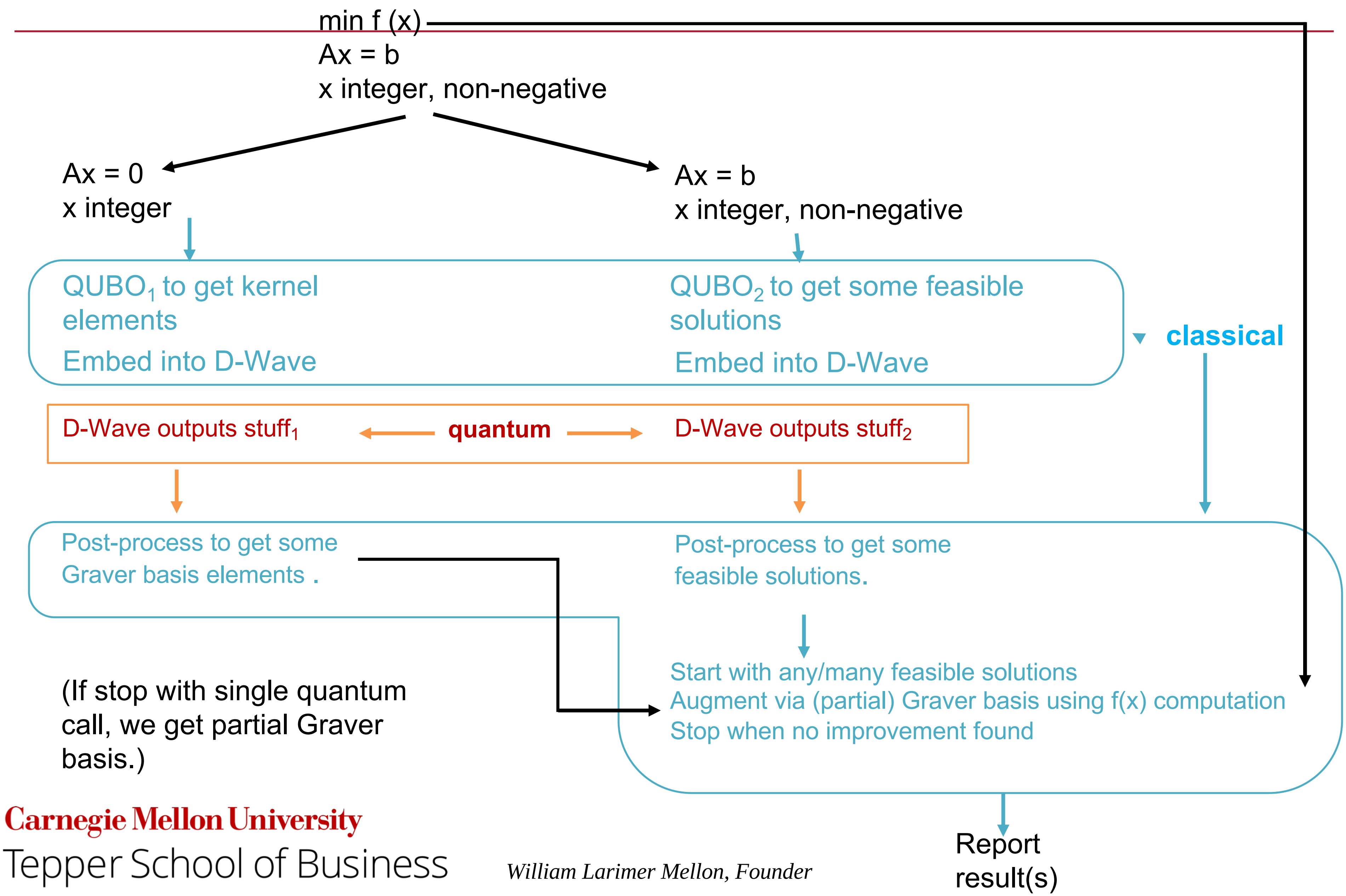
Calculate Graver Basis (Quantum-Classical)

Find Many Initial Feasible Solutions (Quantum)

Augmentation: Improve feasible solutions using Graver Basis (Classical)

Graver Augmented Multi-Seed Algorithm

Hybrid Quantum-Classical Approach



Background Material

Test Sets in Optimization
Graver Basis

Test Sets in Optimization

- Nonlinear integer program:

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

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

- 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:

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

- 2. Partial Order

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

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

Partial order $\sqsubseteq$

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

Definition: Graver Basis

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

- Finite set of conformal (minimal) elements in

$$\mathcal{L}^*(A)$$

Graver Basis is Test Set for:

- $\min cx$, Linear
- $\max f(Wx), W \in \mathbb{Z}^{d \times n}$, f *convex on* $\mathbb{Z}^d$
- $\min \sum f_i(x_i)$, f_i convex (separable convex)
- $min\ |x - x_0|_p$
- Some other nonlinear costs $x^T V x$ $P(x)$

Graver Basis via Quantum Annealing

QUBO for Kernel
Sampling the Kernel
Post-processing Near-Optimal Solutions
Adaptive Centering and Encoding
Computational Results

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 computer

3. Repeating (1) and (2) while *adjusting* the "QUBO" variables in each run *adaptively*

QUBO for Kernel

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

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

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

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

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

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

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

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:

$$\min \quad \mathbf{X}^T \quad \mathbf{Q_B X} \quad , \quad \mathbf{Q_B} = \mathbf{E}^T \mathbf{Q_I E} + diag\left(2\mathbf{L}^T \mathbf{Q_I E}\right)$$

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

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 via control of center(lower) and width

Post Processing

Experimental observation:

- Majority (~ 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

Non-Linear Integer Optimization on D-Wave

QUBO for Feasible Solution(s)
Hybrid Quantum- Classical Algorithm
Computational Results

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William Larimer Mellon, Founder

QUBO for Feasible Solutions

- $\mathbf{Ax} = \mathbf{b} \qquad l \le \mathbf{x} \le u$

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

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

- Using adaptive centering and encoding width for feasibility bound

- Results in many feasible solutions!

Capital Budgeting

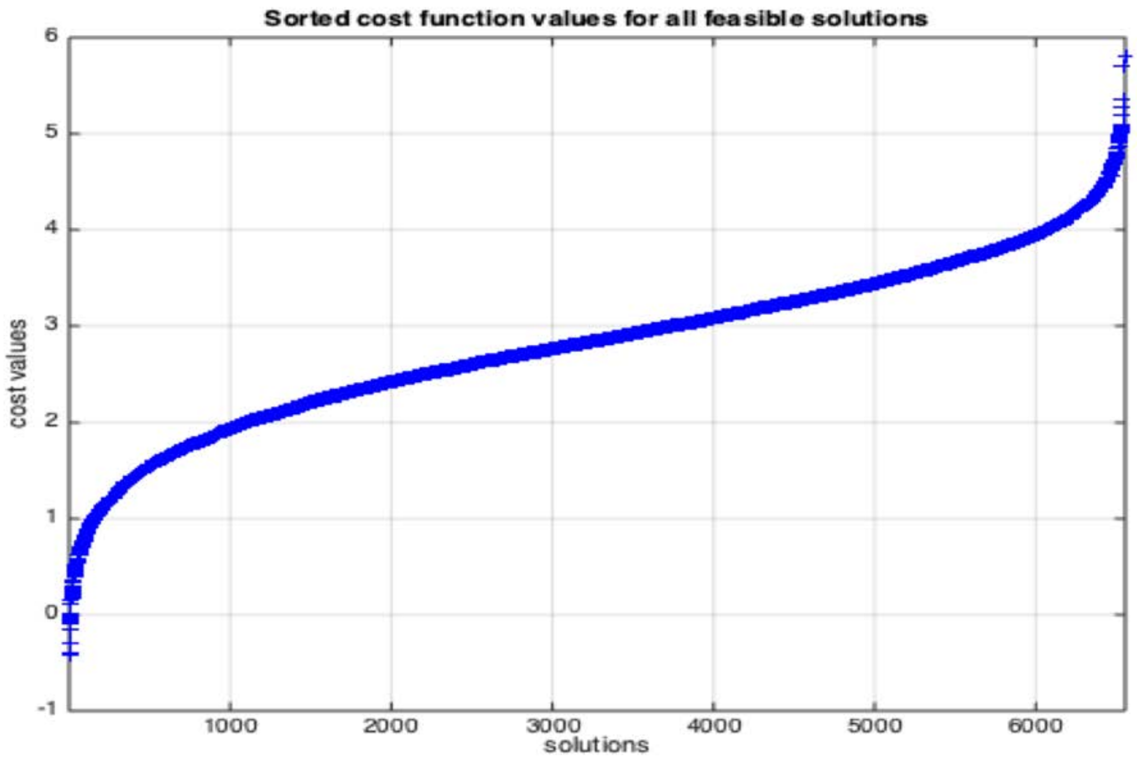
- Important canonical Finance problem
- μ_i expected return
- σ_i variance
- ε risk
- Graver Basis in 1 D-Wave call (1 bit encoding)

$$\begin{cases} \min \quad -\sum_{i=1}^{n} \mu_i x_i + \sqrt{\frac{1-\varepsilon}{\varepsilon} \sum_{i=1}^{n} \sigma_i^2 x_i^2} \\ Ax = b \quad , \quad x \in \{0,1\}^n \end{cases}$$

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

when t = 1 we have: $\mathcal{G}(A) \in M_{50\times 304}(\{-1,0,+1\})$

~ 6500 Solutions in One Call!



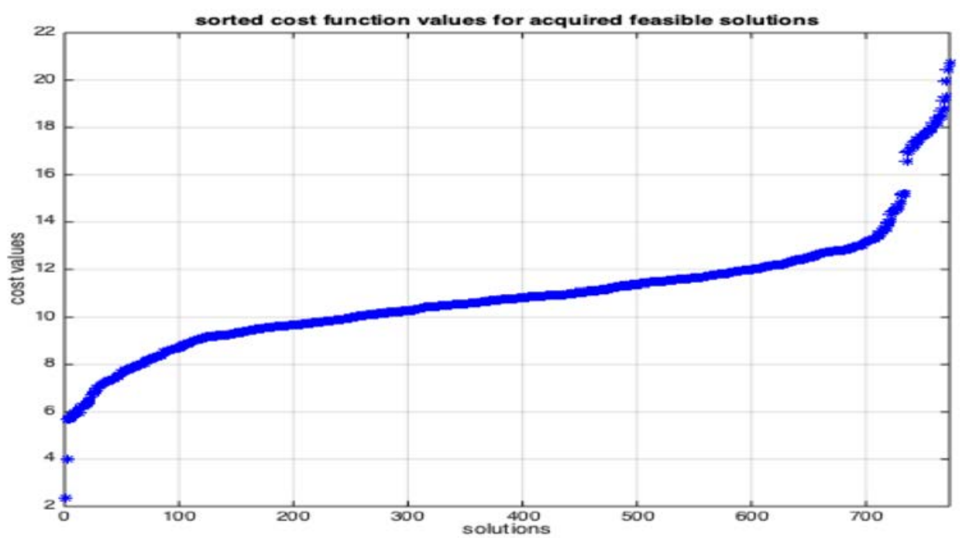
- From any feasible point in ~24-30 augmenting steps reach optimal cost = -3.69

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

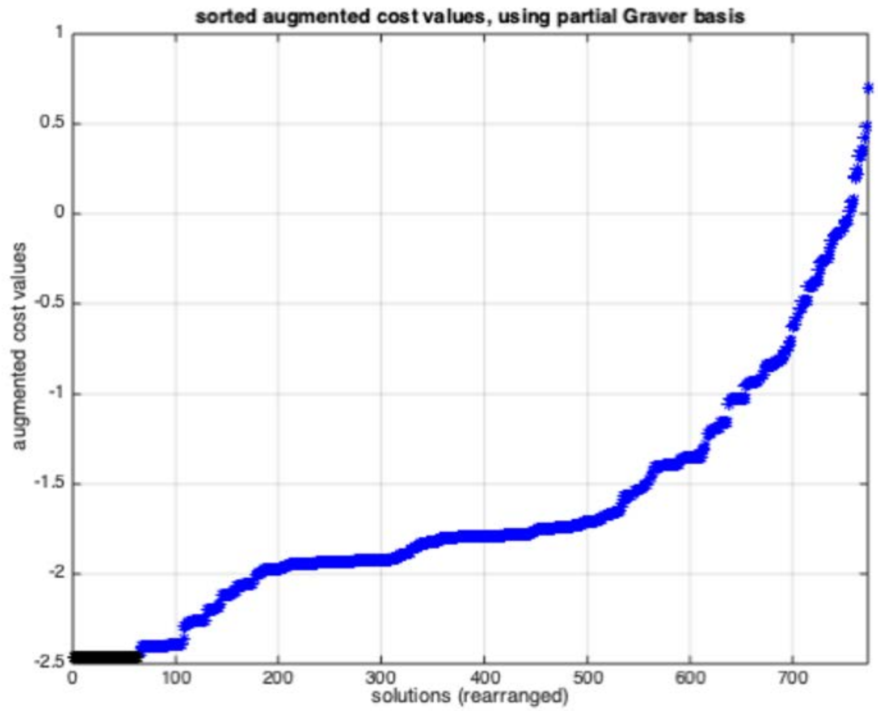


Augmenting…

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

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

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



How to Surpass Best-in-Class Classical Methods?

Gurobi Optimizer 8.0

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

$t=1 \Rightarrow \begin{cases} 0.2 & \text{sec} \\ 6 & \textit{terms} \end{cases}$ $t=10 \Rightarrow \begin{cases} 16 & \text{sec} \\ 230 & \textit{terms} \end{cases}$ $t=20 \Rightarrow \begin{cases} 3 & \text{min} \\ 620 & \textit{terms} \end{cases}$

$t=40 \Rightarrow \begin{cases} 21 & \text{min} \\ 1030 & \textit{terms} \end{cases}$ $t=50 \Rightarrow \begin{cases} 75 & \text{min} \\ 1070 & \textit{terms} \end{cases}$ $t=100 \Rightarrow \begin{cases} >8 & \textit{hours} \\ 1190 & \textit{terms} \end{cases}$

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

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

How and Where to Surpass?

- 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, should surpass Gurobi on {0,1} matrices of sizes 120 to 180, without an increase in precision.

- An order of magnitude increase in maximum number of anneals per call.

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

Thank You

<u>Contact</u>

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