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:
  \[ \begin{align*}
  \min & \quad f(x) \\
  Ax = b & \quad l \leq x \leq u
  \end{align*} \]

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 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

min \( f(x) \)

\[ Ax = b \]
\[ x \text{ integer, non-negative} \]

\[ Ax = 0 \]
\[ x \text{ integer} \]

\[ Ax = b \]
\[ x \text{ integer, non-negative} \]

QUBO_1 to get kernel elements
Embed into D-Wave

D-Wave outputs stuff_1

Post-process to get some Graver basis elements.

(If stop with single quantum call, we get partial Graver basis.)

QUBO_2 to get some feasible solutions
Embed into D-Wave

D-Wave outputs stuff_2

Post-process to get some feasible solutions.

Start with any/many feasible solutions
Augment via (partial) Graver basis using \( f(x) \) computation
Stop when no improvement found

Report result(s)
Background Material

Test Sets in Optimization
Graver Basis
Test Sets in Optimization

- Nonlinear integer program:

\[
\begin{align*}
\min \left\{ f(x) : \quad & Ax = b, \quad x \in \mathbb{Z}^n , \quad l \leq x \leq u \right\} \\
(IP)_{A,b,l,u,f} : \\
& A \in \mathbb{Z}^{m \times n} , \quad b \in \mathbb{Z}^m , \quad l,u \in \mathbb{Z}^n , \quad f: \mathbb{R}^n \rightarrow \mathbb{R}
\end{align*}
\]

- 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 \( A \):
  \[
  \mathcal{L}^*(A) = \left\{ x \mid Ax = 0, \ x \in \mathbb{Z}^n, \ A \in \mathbb{Z}^{m \times n} \right\} \setminus \{0\}
  \]
- 2. Partial Order
  \[
  \forall x, y \in \mathbb{R}^n \quad x \sqsubseteq y \quad \text{s.t.} \quad x_i y_i \geq 0 \quad \& \quad |x_i| \leq |y_i| \quad \forall \quad i = 1, ..., n
  \]
  - \( x \) 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:

- \( \min cx, \text{ Linear} \)
- \( \max f(Wx), W \in \mathbb{Z}^{d \times n}, f \text{ convex on } \mathbb{Z}^d \)
- \( \min \sum f_i(x_i), f_i \text{ convex (separable convex)} \)
- \( \min \|x - x_0\|_p \)
- Some other nonlinear costs \( x^T V x \quad P(x) \)
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 $\subseteq$ (minimal) elements by comparisons, using classical computer

3. Repeating (1) and (2) while adjusting the “QUBO” variables in each run adaptively
QUBO for Kernel

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

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

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

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

\[ \mathbf{X}_i^T = \begin{bmatrix} \mathbf{X}_{i,1} & \mathbf{X}_{i,2} & \ldots & \mathbf{X}_{i,k_i} \end{bmatrix} \in \{0,1\}^{k_i} \]

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

- Unary encoding: \[ \mathbf{e}_i^T = \underbrace{\begin{bmatrix} 1 & 1 & \ldots & 1 \end{bmatrix}}_{k_i} \]
QUBO for Kernel....

\[
x = L + EX = \begin{bmatrix}
Lx_1 \\
Lx_2 \\
\vdots \\
Lx_n
\end{bmatrix} + \begin{bmatrix}
e_1^T & 0^T & \cdots & 0^T \\
0^T & e_2^T & \cdots & 0^T \\
\vdots & \vdots & \ddots & \vdots \\
0^T & 0^T & \cdots & e_n^T
\end{bmatrix} \begin{bmatrix}
X_1 \\
X_2 \\
\vdots \\
X_n
\end{bmatrix}
\]

(L is the lower bound vector)

- **QUBO:**

\[
\min \quad X^T Q_B X , \quad Q_B = E^T Q_1 E + \text{diag}(2L^T Q_1 E)
\]

\[
X \in \{0,1\}^{nk} , \quad Q_1 = A^T A
\]

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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
QUBO for Feasible Solutions

\[ \begin{align*}
Ax &= b \\
l &\leq x &\leq u
\end{align*} \]

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

\[ X \in \{0,1\}^{nk}, \quad Q_I = A^T A \]

- Using adaptive centering and encoding width for feasibility bound

- Results in many feasible solutions!
Capital Budgeting

- Important canonical Finance problem
  - $\mu_i$ expected return
  - $\sigma_i$ variance
  - $\varepsilon$ risk

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

$$\min \quad -\sum_{i=1}^{n} \mu_i x_i + \sqrt{\frac{1-\varepsilon}{\varepsilon} \sum_{i=1}^{n} \sigma_i^2 x_i^2}$$

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

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

when $t = 1$ we have: $G(A) \in M_{50 \times 304}(\{-1, 0, +1\})$
~ 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
- \( G(A) \in M_{25 \times 616} (\{-4, \ldots, +4\}) \) 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
  
  \[ g^P(A) \in M_{25 \times 418} (\{-4, \ldots, +4\}) \]

- 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

$$
\begin{align*}
t = 1 & \Rightarrow \left\{ \begin{array}{ll}
0.2 \text{ sec} & t = 10 \Rightarrow \left\{ \begin{array}{ll}
16 \text{ sec} & t = 20 \Rightarrow \left\{ \begin{array}{ll}
3 \text{ min} \\
6 \text{ terms} & 230 \text{ terms}
\end{array} \right. \\
21 \text{ min} & t = 100 \Rightarrow \left\{ \begin{array}{ll}
> 8 \text{ hours} & 1070 \text{ terms}
\end{array} \right. \\
1030 \text{ terms} & t = 100 \Rightarrow \left\{ \begin{array}{ll}
1190 \text{ terms}
\end{array} \right. \\
\end{array} \right. \\
\end{align*}
$$

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

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

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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


Thank You

Contact
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