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

Graver Augmented Multiseed Algorithm (GAMA)

Lecture 08 2021.09.28







## Quiz 2

This quiz is intended to familiarize you with the use of Google Collab for the creation and training of a deep neural network (DNN) and a convolutional neural network (CNN), through the Keras library. For this they can use the google colab present in the following link: <u>https://colab.research.google.com/github/bernalde/QuIPML/blob/master/notebooks/Notebook%206%20-%20CNN.ipynb</u>

We ask you to answer the following:

For the DNN we asked you to run the next models and examine the accuracy and run time for each of them. Also, when comparing models b) and a), which scenario is more efficient.

- a) 2 hidden layers with 256 nodes each.
- b) 4 hidden layers, with the same number of nodes each (256).
- c) 2 hidden layers with 512 nodes each.

For the CNN we asked you to run the next models and examine the accuracy and run time for each of them. Also, comment on impact of number of convolutions on accuracy.

- a) 3 convolutions only.
- b) 4 convolutions.
- c) 5 convolutions.

Finally, compare and comment on accuracy and run time of each approach (DNN and CNN) on the same classification problem







#### 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*:

$$\min f(x)$$
$$Ax = b \quad l \le x \le u$$

by a Ising Solver is to:

1) Convert non quadratic f(x) into quadratic

2) Add constraint to quadratic and solve:

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

which has a balancing problem, and other issues.

We want to do something very different!







## **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

test-set



[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







#### GAMA



Report result(s)







## **Test Sets in Optimization**

• Nonlinear integer program:

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

- 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** ⊑

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

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

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







#### **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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#### **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  $\alpha \in \mathbb{Z}_+$ 

- $\bullet \ \ f(\mathbf{x}_0 + \alpha \mathbf{t}^i) < f(\mathbf{x}_0)$
- $\mathbf{x}_0 + \alpha \mathbf{t}^i$  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  $\mathbf{W} \in \mathbb{Z}^{d imes n}$  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  $\mathbf{Q} \nsucceq \mathbf{0}$
- 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  $\mathbf{A}$





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#### **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



Gröbner Bases and Integer Programming, G. Ziegler. 1997
 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





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







#### Definitions

- 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**

$$\mathbf{A}\mathbf{x} = \mathbf{0}, \quad \mathbf{x} \in \mathbb{Z}^n \quad , \quad \mathbf{A} \in \mathbb{Z}^{m \times n}$$
  
min  $\mathbf{x}^T \mathbf{Q}_{\mathbf{I}} \mathbf{x} \quad , \quad \mathbf{Q}_{\mathbf{I}} = \mathbf{A}^T \mathbf{A} \quad , \quad \mathbf{x} \in \mathbb{Z}^n$   
 $\mathbf{x}^T = \begin{bmatrix} x_1 & x_2 & \dots & x_i & \dots & x_n \end{bmatrix}, \quad x_i \in \mathbb{Z}$ 

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

$$X_{i}^{T} = \begin{bmatrix} X_{i,1} & X_{i,2} & \cdots & X_{i,k_{i}} \end{bmatrix} \in \{0,1\}^{k_{i}}$$
  
Binary encoding  $\mathbf{e}_{i}^{T} = \begin{bmatrix} 2^{0} & 2^{1} & \cdots & 2^{k_{i}} \end{bmatrix}$ 

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 $k_i$ 

• Unary encoding 
$$\mathbf{e}_i^T = \begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix}$$

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







## **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

$$A = \left[ \begin{array}{ccc} 1 & 2 & 1 \end{array} \right]$$

Quadratic Unconstrained Integer Optimization QUIO:

$$Ax = 0 \quad \rightarrow \quad \min \quad x^{T} \underbrace{\left(A^{T} A\right)}_{\mathcal{Q}_{I}} x$$
$$Q_{I} = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$$







## **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**









#### **Step 5: Quadratic Unconstrained Binary Optimization** (QUBO)

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

• QUBO







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#### **Step 6: Mapping to Ising variables**

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

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

[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).

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#### **Step 7: Reframing in Ising Model**

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

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

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

• Note:

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







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

• Note that there are 4 unique elements of *J* 

• Ising Solver (such as D-Wave) gives S

$$S_i = +1 \rightarrow X_i = 1$$
$$S_i = -1 \rightarrow X_i = 0$$

• Get *X* back from *S* (see Step 6)

• Optimal *X*'s:

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





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

 $x = L + EX \rightarrow$ 

[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).

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#### **Step 10: Convert Kernel to Graver Basis**

$$\begin{bmatrix} x \end{bmatrix} \rightarrow \sqsubseteq -\text{minimal classical filteration} \rightarrow \mathcal{G}(A)$$

• Negative basis elements are also part of Graver Basis:

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

**EPPER** 

[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).

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#### **QUBO for Feasible Solutions**

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

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

• 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

•  $\mu_i$  expected return •  $\sigma_i$  variance •  $\varepsilon$  risk  $\begin{array}{l} \min -\sum_{i=1}^n \mu_i x_i + \sqrt{\frac{1-\varepsilon}{\varepsilon}} \sum_{i=1}^n \sigma_i^2 x_i^2 \\ Ax = b , x \in \{0,1\}^n \end{array}$ 

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

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

when t = 1 we have:

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







#### **GAMA** in Action

Let's go to the Colab

https://colab.research.google.com/github/bernalde/QuIPML/blob/master/notebooks/Notebo ok%205%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









## Augmenting...

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

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

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



[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).

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#### **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



[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).

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## **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 Nonlinear 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.





