A Novel Algebraic Geometry Compiling Framework for Adiabatic Quantum Computation

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Plan

What is algebraic geometry ?

Algebraic geometry is the study of geometric objects defined by polynomial equations, using algebraic means. Its roots go back to Descartes' introduction of coordinates to describe points in Euclidean space and his idea of describing curves and surfaces by algebraic equations.

The basic correspondence in algebraic geometry

$$\textbf{Algebraic varieties} \simeq \textbf{Polynomial rings} \tag{1}$$

(Equivalence of categories !)

Example : Circle

The variety : $\mathcal{V} := \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 - 1 = 0\}$.
The ring : $\mathbb{Q}[x, y]/ < x^2 + y^2 - 1 >$ = polynomials mod $x^2 + y^2 - 1$

What is algebraic geometry ?

Introducing some terminology :

- Let $\mathcal{S}$ be a set of polynomials $f \in \mathbb{Q}[x_0, \ldots, x_{n-1}]$.
- $\mathcal{V}(S)$ is the affine variety defined by the polynomials $f \in S$, that is, the set of common zeros of the equations $f = 0,\ f \in \mathcal{S}$.
- The system $\mathcal{S}$ generates an ideal $\mathcal{I}$ by taking all linear combinations over $\mathbb{Q}[x_0, \ldots, x_{n-1}]$ of all polynomials in $\mathcal{S}$; we have $\mathcal{V}(\mathcal{S}) = \mathcal{V}(\mathcal{I})$. The ideal $\mathcal{I}$ reveals the hidden polynomials that are the consequence of the generating polynomials in $\mathcal{S}$. For instance, if one of the hidden polynomials is the constant polynomial 1 (i.e., $1 \in \mathcal{I}$), then the system $\mathcal{S}$ is inconsistent (because $1 \neq 0$).

- Strictly speaking, the set of all hidden polynomials is given by the so-called radical ideal $\sqrt{\mathcal{I}}$, which is defined by $\sqrt{\mathcal{I}} = \{g \in \mathbb{Q}[x_0, \ldots, x_{n-1}] | \exists r \in \mathbb{N} : g^r \in \mathcal{I}\}$.
- In practice, the ideal $\sqrt{\mathcal{I}}$ is infinite, so we represent such an ideal using a Groebner basis $\mathcal{B}$, which one might take to be a triangularization of the ideal $\sqrt{\mathcal{I}}$.
- In fact, the computation of Groebner bases generalizes Gaussian elimination in linear systems.
- We also have

$$\mathcal{V}(\mathcal{S}) = \mathcal{V}(\mathcal{I}) = \mathcal{V}(\sqrt{\mathcal{I}}) = \mathcal{V}(\mathcal{B}).$$

What is algebraic geometry ? Solving system of polynomial equations

Example

Consider the system

$$\mathcal{S} = \{x^2 + y^2 + z^2 - 4, x^2 + 2y^2 - 5, xz - 1\}.$$

We want to solve $\mathcal{S}$. We need to compute a Groebner basis for $\mathcal{S}$!

Notebook 1.

Algebraic geometry in optimization

Given a binary optimization problem

$$(\mathcal{P}) : \ argmin_{(y_0,\cdots,y_{m-1})\in\mathbb{B}^m} f(y_0,\cdots,y_{m-1}), \qquad (2)$$

where $\mathbb{B} = \{0,1\}$ and $f \in \mathbb{Q}[y_0,\cdots,y_{m-1}]$.

Algebraic geometry appears naturally !

First appearance :

The objective function f defines an ideal

$$\mathcal{I} = \{z - f(y_0,\cdots,y_{m-1}), y_i^2 - y_i\},$$

subset of the larger ring

$$\mathbb{Q}[z, y_0,\cdots,y_{m-1}].$$

The variety $\mathcal{V}(\mathcal{I})$ is the graph of the objective function f (we will solve $(\mathcal{P})$ later with Groebner bases).

Algebraic geometry in optimization

Given the binary optimization problem

$$(\mathcal{P}) : \; argmin_{(y_0,\cdots,y_{m-1})\in\mathbb{B}^m} f(y_0,\cdots,y_{m-1}), \tag{3}$$

where $\mathbb{B} = \{0,1\}$.

Second appearance : The variety of local minima

Define

$$\tilde{f} := f + \sum_{i=1}^{n} \alpha_i^2 y_i(y_i - 1).$$

The gradient ideal of $(\mathcal{P})$ is

$$\tilde{I} :=< \partial_{y_i}\tilde{f},\cdots,\partial_{\alpha_i^2}\tilde{f} > .$$

Its variety is the set of local minima of $(\mathcal{P})$.

Algebraic geometry in optimization

Given a binary optimization problem

$$(\mathcal{P}) : \; argmin_{(y_0,\cdots,y_{m-1})\in\mathbb{B}^m} f(y_0,\cdots,y_{m-1}), \tag{4}$$

where $\mathbb{B} = \{0,1\}$.

Third connection : Solving $(\mathcal{P})$ as an eigenvalue problem !

Consider again the gradient ideal ($\tilde{f} := f + \sum_{i=1}^{n} \alpha_i^2 y_i(y_i - 1)$)

$$\tilde{\mathcal{I}} :=< \partial_{y_i}\tilde{f}, \cdots, \partial_{\alpha_i^2} f > .$$

Its coordinate ring is the residue algebra $A := \mathbb{Q}[y_0,\ldots,y_{m-1},\alpha_1,\ldots,\alpha_n]/\tilde{I}$. Define the linear map

$$\begin{aligned} m_{\tilde{f}} : \quad A &\to A \\ g &\mapsto \tilde{f}g \end{aligned} \tag{5}$$

Solving $(\mathcal{P})$ as ev problem : Continued

Since the number of local minima is finite, the algebra A is always finite-dimensional. Additionally, we have :

- **The values of $\tilde{f}$, on the set of critical points $\mathcal{V}(\tilde{\mathcal{I}})$, are given by the eigenvalues of the matrix $m_{\tilde{f}}$.**
- Eigenvalues of m_{y_i} and m_{α_i} give the coordinates of the points of $\mathcal{V}(\tilde{\mathcal{I}})$.
- If v is an eigenvector for $m_{\tilde{f}}$, then it is also an eigenvector for m_{y_i} and m_{α_i} for $1 \leq i \leq m$.

Refs :

- D. Cox's Using algebraic geometry.
- RD and H. Alghassi, Prime factorization using QA and algebraic geometry, nature srep 2017.

Solving optimization pbs with Groebner bases : S. Tayur's method

Consider the ideal

$$\mathcal{I} = \{z - f(y_0, \cdots, y_{m-1}), y_i^2 - y_i\} \subset Q[z, y_0, \cdots, y_{m-1}].$$

associated to the binary optimization :

$$(\mathcal{P}) : \; argmin_{(y_0, \cdots, y_{m-1}) \in \mathbb{B}^m} f(y_0, \cdots, y_{m-1}), \tag{6}$$

We would like to solve $(\mathcal{P})$ using the ideal $\mathcal{I}$.

Example

Solve the IP

$$\begin{cases} argmin_{y_i \in \{0,1\}} & y_1 + 2y_2 + 3y_3 + 3y_4, \\ & y_1 + y_2 + 2y_3 + y_4 = 3 \end{cases} \tag{7}$$

Notebook 2.

Reduction to QUBOs without slack variables

Consider the quadratic polynomial

$$H_{ij} := Q_i P_j + S_{i,j} + Z_{i,j} - S_{i+1,j-1} - 2\,Z_{i,j+1},$$

with the binary variables $P_j, Q_i, S_{i,j}, S_{i+1,j-1}, Z_{i,j}, Z_{i,j+1}$.

- The goal is solve H_{ij} (obtain its zeros) as a QUBO (eg., using DWave)
- We can square H_{ij} and reduce using slack variables !
- Or, instead, we compute a Groebner basis $\mathcal{B}$ of the system

  $$\mathcal{S} = \{H_{ij}\} \cup \{x^2 - x,\ x \in \{P_j, Q_i, S_{i,j}, S_{i+1,j-1}, Z_{i,j}, Z_{i,j+1}\}\},$$

  and look for a positive quadratic polynomial $H_{ij}{}^{+} = \sum_{t \in \mathcal{B} |\, deg(t) \leq 2} a_t t$. Note that global minima of $H_{ij}{}^{+}$ are the zeros of H_{ij}.

The Groebner basis $\mathcal{B}$ is

$$t_1 := Q_i P_j + S_{i,j} + Z_{i,j} - S_{i+1,j-1} - 2\,Z_{i,j+1}, \tag{8}$$

$$t_2 := \left(-Z_{i,j+1} + Z_{i,j}\right) S_{i+1,j-1} + \left(Z_{i,j+1} - 1\right) Z_{i,j}, \tag{9}$$

$$t_3 := \left(-Z_{i,j+1} + Z_{i,j}\right) S_{i,j} + Z_{i,j+1} - Z_{i,j+1} Z_{i,j}, \tag{10}$$

$$t_4 := \left(S_{i+1,j-1} + Z_{i,j+1} - 1\right) S_{i,j} - S_{i+1,j-1} Z_{i,j+1}, \tag{11}$$

$$t_5 := \left(-S_{i+1,j-1} - 2\,Z_{i,j+1} + Z_{i,j} + S_{i,j}\right) Q_i - S_{i,j} - Z_{i,j} + S_{i+1,j-1} + 2\,Z_{i,j+1}, \tag{12}$$

$$t_6 := \left(-S_{i+1,j-1} - 2\,Z_{i,j+1} + Z_{i,j} + S_{i,j}\right) P_j - S_{i,j} - Z_{i,j} + S_{i+1,j-1} + 2\,Z_{i,j+1}, \tag{13}$$

$$\text{in addition to 3 more cubic polynomials,} \tag{14}$$

We take ${H_{ij}}^{+} = \sum_{t \in \mathcal{B} | \, deg(t) \leq 2} a_t t$, and solve for the a_t. We can require that the coefficients a_t are subject to the dynamic range allowed by the quantum processor (eg., the absolute values of the coefficients of H_{ij}^{+}, with respect to the variables $P_j, Q_i, S_{i,j}, S_{i+1,j-1}, Z_{i,j}$, and $Z_{i,j+1}$, be within $[1-\epsilon, 1+\epsilon]$).

Ref : RD and HA srep 2017.

Solving IPs using Groebner bases of toric ideals

These are ideals generated by differences of monomials. Their Groebner bases enjoy a clear structure given by kernels of integer matrices. Specifically, let $A = (a_1, \cdots, a_n)$ be any integer $m \times n$-matrix. Each column $\mathbf{a}_i = (a_{1i}, \cdots, a_{ni})^T$ is identified with a Laurent monomial $y^{\mathbf{a}_i} = y_1^{a_{1i}} \cdots y_m^{a_{ni}}$. The toric ideal $\mathcal{J}_A$ is the kernel of the algebra homomorphism

$$\mathbb{Q}[x] \to \mathbb{Q}[y] \tag{15}$$

$$x_i \mapsto y^{\mathbf{a}_i}. \tag{16}$$

Proposition

The toric ideal $\mathcal{J}_A$ is generated by the binomials $x^{\mathbf{u}_+} - x^{\mathbf{u}_-}$, where the vector $\mathbf{u} = \mathbf{u}_+ - \mathbf{u}_- \in {\mathbb{Z}^+}^n \oplus {\mathbb{Z}^+}^n$ runs over all integer vectors in $\mathrm{Ker}_{\mathbb{Z}} A$, the kernel of the matrix A.

Notebook 3

Part 2 : Algebraic geometry for Graph Minor Theory

Toric ideals again ! Reduction to QUBO

Consider the binary optimization problem :

$$(\mathcal{P}) : \ argmin_{(y_0, \cdots, y_{m-1}) \in \mathbb{B}^m} f(y_0, \cdots, y_{m-1}). \tag{17}$$

Define the ideal

$$\begin{aligned} \mathcal{K}_A \ = \ \langle & x_1 - y_1, \, x_2 - y_2, \, x_3 - y_3, \, \cdots, \, x_m - y_m, \\ & x_k - y_{i_1} y_{i_2}, \ \text{for each pair } (y_{i_1}, y_{i_2}) \text{ contained in } f \rangle, \end{aligned} \tag{18}$$

where k runs from 1 to $m + n'$, where n' is the total number of such pairs (with $n' + m \leq n$).

Proposition

The minimal reduction of the polynomial function f into a quadratic function is given by the toric ideal $\mathcal{J}_A = \mathcal{K}_A \cap \mathbb{Q}[x]$.

From embeddings to fiber-bundles

Consider the QUBO

$$argmin_{(y_0,\cdots,y_{m-1})\in\mathbb{B}^m} \sum_{(y_{i_1},y_{i_2})\in\textbf{Edges}(Y)} J_{i_1 i_2} y_{i_1} y_{i_2} + \sum_{j=0}^{m-1} h_j y_j. \quad (19)$$

We recall the following definition

Definition (Embedding)

Let X be a fixed hardware graph. A *minor-embedding* (embedding for short) of the graph Y is a map

$$\phi : \textbf{Vertices}(Y) \to \textbf{Subtrees}(X) \quad (20)$$

that satisfies the following condition for each : $(y_1, y_2) \in \textbf{Edges}(Y)$, there exists at least one edge in $\textbf{Edges}(X)$ connecting the two subtrees $\phi(y_1)$ and $\phi(y_2)$.

An embedding is a mapping

$$\phi : \textbf{Logical graph} \rightarrow \textbf{Hardware graph}.$$

We flip the direction and define the surjection

$$\pi : \textbf{Hardware graph} \rightarrow \textbf{Logical graph}$$

such that for each logical qubit y

$$\pi^{-1}(y) = \phi(y).$$

The chain $\phi(y)$ is projected into the logical qubit y.
The triplet : (X, Y, π) is a fiber bundle.

A direct corollary of this representation, is that the map π has the form :

$$\pi(x_i) = \sum_{ij} \alpha_{ij} y_j \tag{21}$$

$$\text{with} \quad \sum_{ij} \alpha_{ij} = \beta_i, \quad \alpha_{ij_1}\alpha_{ij_2} = 0, \quad \alpha_{ij}(\alpha_{ij} - 1) = 0,$$

where the binary number β_i is 1 if the physical qubits x_i is used and 0 otherwise. We write $domain(\pi) = \textbf{Vertices}(X)$ and $support(\pi) = \textbf{Vertices}(X^\beta)$ with $X^\beta \subset_{subgraph} X$.

The fiber of the map π at $y_j \in \textbf{Vertices}(Y)$ is given by

$$\pi^{-1}(y_j) = \phi(y_j) = \{x_i \in \textbf{Vertices}(X) | \quad \alpha_{ij} = 1\}. \tag{22}$$

The conditions on the parameters α_{ij} guarantee that fibers don't intersect (i.e., π is well defined map).

Example :

Let X and Y be the two graphs depicted in Figure 1. An example of the map π is defined by $\pi(x_1) = \pi(x_4) = y_1$ and $\pi(x_2) = y_2$ and $\pi(x_3) = y_3$.

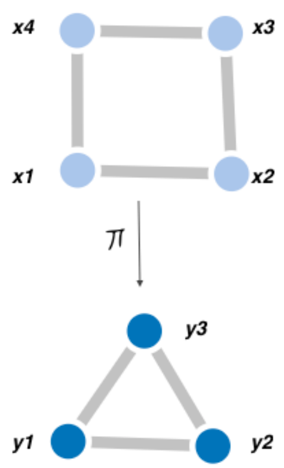


FIGURE – An example of a fiber bundle.

We this new definition, we systematically answer the following questions :

- Existence (or non existence) of embeddings.
- Calculating all embeddings in a *compact form* given by a Groebner basis.
- Counting all embeddings without solving any equations.

We do so for any fixed size of the chains.

Consider the surjection $\pi : X \to Y$

$$\begin{aligned}\pi(x_i) &= \sum_{ij} \alpha_{ij} y_j \qquad (23)\\ \text{with} \quad & \sum_{ij} \alpha_{ij} = \beta_i, \quad \alpha_{ij_1}\alpha_{ij_2} = 0,\\ \text{and} \quad & \alpha_{ij}(\alpha_{ij} - 1) = 0,\ \beta_j(\beta_j - 1) = 0,\end{aligned}$$

The fiber at y is

$$\pi^{-1}(y_j) = \phi(y_j) = \{x_i \in \textbf{Vertices}(X) | \quad \alpha_{ij} = 1\}. \qquad (24)$$

Task : Translate the definition of embedding into a system of algebraic constraints on the parameters αij and β_j.

Size constraint

The number of usable physical qubits can be constrained : fix the maximum size of the fibers $\pi^{-1}(y_j)$ to a certain size $k \leq \mathrm{card}(\mathbf{Edges}(X))$. This can be enforced using :

$$\forall j : \quad \sum_{x_i \in \mathbf{Vertices}(X)} \alpha_{ij} \leq k \quad \text{or equivalently} \tag{25}$$

$$\Pi_{\kappa=1}^{k} \left(\sum_{x_i \in \mathbf{Vertices}(X)} \alpha_{ij} - \kappa \right) = 0. \tag{26}$$

Additionally, we have

$$\forall j : \quad \alpha_{i_1 j} \alpha_{i_2 j} = 0, \tag{27}$$

for all pairs (x_{i_1}, x_{i_2}) with $d(x_{i_1}, x_{i_2}) > k$, where $d(x_{i_1}, x_{i_2})$ is the size of the shortest chain connecting x_{i_1} and x_{i_2}.

Fiber condition

Fiber Condition

Each fiber $\pi^{-1}(y)$ of π is a connected subtree.

We need the following notations :

- $c_k(x_{i_1}, x_{i_2})$ is a chain of size $\leq k$ connecting x_{i_1} and x_{i_2}. Our convention here is to define a chain as an ordered list of vertices that includes the end points x_{i_1} and x_{i_2}, thus, $\mathrm{card}(C_k(x_{i_1}, x_{i_2})) \leq k + 1$.
- $\mathcal{C}_k(x_{i_1}, x_{i_2})$ is the set of all chains of size $\leq k$ connecting x_{i_1} and x_{i_2}.

Fiber condition

We impose :

$$\alpha_{i_1 j}\alpha_{i_2 j} \times \left(\sum_{c_k(x_{i_1},x_{i_2}) \in \mathcal{C}_k(x_{i_1},x_{i_2})} \Pi_{x_\ell \in c_k(x_{i_1},x_{i_2}) \setminus \{x_{i_1},x_{i_2}\}} \alpha_{\ell j} - 1 \right) = 0. \tag{28}$$

For each pair of vertices in $\pi^{-1}(y_j)$, condition (28) implies the existence of a unique chain connecting the pair and that is completely contained in the fiber $\pi^{-1}(y_j)$. Note that, the existence of chains implies that $\pi^{-1}(y_j)$ is connected.

Fiber condition

In case we wish the fiber $\pi^{-1}(y_j)$ to be a chain, a preferred minimal structure for the logical qubits, we constrain the degree of each vertex x_{i_1} to be in $\{1, 2\}$, which translates into

$$-1 + \sum_{i_2 \colon (x_{i_1}, x_{i_2}) \in \mathbf{Edges}(X)} \alpha_{i_1 j} \alpha_{i_2 j} \tag{29}$$

is binary for all $x_{i_1} \in \pi^{-1}(y_j)$.

Pullback condition

Each edge (y_{j_1}, y_{i_2}) in Y there exists at least one edge connecting the fibers $\pi^{-1}(y_{j_1})$ and $\pi^{-1}(y_{i_2})$.

We need a few more constructions. The map π given by the equations (23) extends to a *linear and multiplicative* map

$$\pi : \mathbb{Q}[\textbf{Vertices}(X)] \to \mathbb{Q}[\textbf{Vertices}(Y)] \tag{30}$$

by

$$\pi(x_{i_1} x_{i_2}) = \pi(x_{i_1})\pi(x_{i_2}) \text{ and } \pi(a_{i_1} x_{i_1} + a_{i_2} x_{i_2}) = a_{i_1}\pi(x_{i_1}) + a_{i_2}\pi(x_{i_2}), \tag{31}$$

for all $a_i \in \mathbb{Q}$. Additionally, the *pullback* of the polynomial $P(x)$ by π is the polynomial

$$\pi^*(P)(y) = P(\pi(x)) \quad \in \mathbb{Q}[\textbf{Vertices}(Y)]. \tag{32}$$

Pullback condition

In particular, the pullback of the quadratic form

$$Q_X(x) = \sum_{(x_{i_1}, x_{i_2}) \in \mathbf{Edges}(X)} x_{i_1} x_{i_2}$$

by π is the quadratic form

$$\begin{aligned}
\pi^*(Q_X)(y) &= \sum_{(x_{i_1}, x_{i_2}) \in \mathbf{Edges}(X)} \pi(x_{i_1})\pi(x_{i_2}) \\
&= \sum_{(x_{i_1}, x_{i_2}) \in \mathbf{Edges}(X)} \left(\sum_{0 \le j_1 < j_2 \le m-1} \left(\alpha_{i_1 j_1} \alpha_{i_2 j_2} + \alpha_{i_1 j_2} \alpha_{i_2 j_1} \right) y_{j_1} y_{j_2} + \sum_{j=0}^{m-1} \alpha_{i_1, j} \alpha_{i_2, j} {y_j}^2 \right) \\
&= \sum_{0 \le j_1 < j_2 \le m-1} \left(\sum_{(x_{i_1}, x_{i_2}) \in \mathbf{Edges}(X)} \left(\alpha_{i_1 j_1} \alpha_{i_2 j_2} + \alpha_{i_1 j_2} \alpha_{i_2 j_1} \right) \right) y_{j_1} y_{j_2} \\
&\quad + \sum_{j=0}^{m-1} \left(\sum_{(x_{i_1}, x_{i_2}) \in \mathbf{Edges}(X)} \alpha_{i_1 j} \alpha_{i_2 j} \right) {y_j}^2 . \qquad (33)
\end{aligned}$$

Fiber condition

The sum

$$\sum_{(x_{i_1}, x_{i_2}) \in \mathbf{Edges}(X)} \left(\alpha_{i_1 j_1} \alpha_{i_2 j_2} + \alpha_{i_1 j_2} \alpha_{i_2 j_1} \right)$$

gives the number of edges in **Edges**(X) that connect $\pi^{-1}(y_{j_1})$ and $\pi^{-1}(y_{j_2})$. The Pullback Condition is equivalent to the fact that this number is strictly non zero if the pair $\{y_{j_1}, y_{j_2}\}$ is an edges of Y.

The Pullback Condition is equivalent to the following statement : for each $\{y_{j_1}, y_{j_2}\}$ in **Edges**(Y) we have

$$\sum_{(x_{i_1}, x_{i_2}) \in \mathbf{Edges}(X)} \left(\alpha_{i_1 j_1} \alpha_{i_2 j_2} + \alpha_{i_1 j_2} \alpha_{i_2 j_1} \right) = 1 + \delta_{j_1 j_2}^2, \tag{34}$$

for some integer $\delta_{j_1 j_2} \in \mathbb{Z}$.

Equations (23), in addition to the conditions in the previous Fiber and Pullback conditions define an algebraic ideal $\mathcal{I} \subset \mathbb{Q}[\alpha, \beta, \delta]$. The variety $\mathcal{V}(\mathcal{I})$ gives all embeddings of Y (of size $\leq k$) inside the hardware graph X. In fact, one has :

Proposition

Let $\mathcal{B}$ be a reduced Groebner basis for the ideal $\mathcal{I}$. The following statements are true :

- A Y minor exists if and only if $1 \notin \mathcal{B}$.
- If $\mathcal{B}$ is computed using the elimination order $\alpha \succ \beta \succ \delta$ and $1 \notin \mathcal{B}$, then the intersection $\mathcal{B} \cap \mathbb{Q}[\beta, \delta]$ gives all subgraphs X^{β} of X that are minors for Y. The remainder of the reduced Groebner basis gives the corresponding embedding $\pi_{\beta} : X^{\beta} \to Y$.

Example

Consider the two graphs in Figure 2.

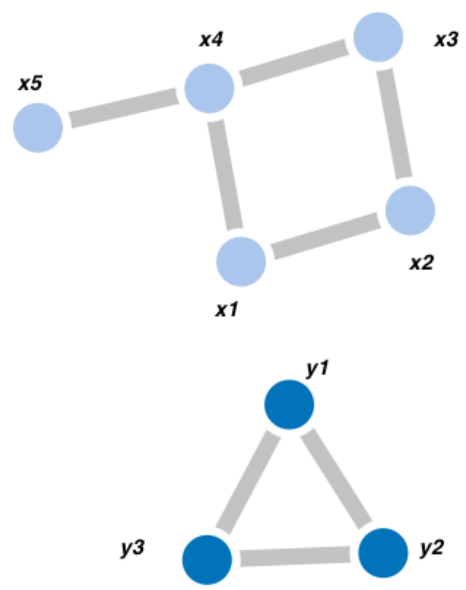


FIGURE – The set of *all* fiber bundles $\pi : X \to Y$ defines an algebraic variety. This variety is given by the Groebner basis (40).

In this case, equations (23) are given by

$$\alpha_{1,1}\alpha_{1,2},\ \alpha_{1,1}\alpha_{1,3},\ \alpha_{1,2}\alpha_{1,3}, \tag{35}$$

$$\alpha_{2,1}\alpha_{2,2},\ \alpha_{2,1}\alpha_{2,3},\ \alpha_{2,2}\alpha_{2,3}, \tag{36}$$

$$\alpha_{3,1}\alpha_{3,2},\ \alpha_{3,1}\alpha_{3,3},\ \alpha_{3,2}\alpha_{3,3}, \tag{37}$$

$$\alpha_{4,1}\alpha_{4,2},\ \alpha_{4,1}\alpha_{4,3},\ \alpha_{4,2}\alpha_{4,3}, \tag{38}$$

$$\alpha_{5,1}\alpha_{5,2},\ \alpha_{5,1}\alpha_{5,3},\ \alpha_{5,2}\alpha_{5,3}, \tag{39}$$

and

$$\alpha_{1,1}+\alpha_{1,2}+\alpha_{1,3}-\beta_1,\quad \alpha_{2,1}+\alpha_{2,2}+\alpha_{2,3}-\beta_2,\quad \alpha_{3,1}+\alpha_{3,2}+\alpha_{3,3}-\beta_3,$$
$$\alpha_{4,1}+\alpha_{4,2}+\alpha_{4,3}-\beta_4,\quad \alpha_{5,1}+\alpha_{5,2}+\alpha_{5,3}-\beta_5.$$

The Pullback Condition reads

$$-1+\alpha_{4,1}\alpha_{5,2}+\alpha_{3,1}\alpha_{4,2}+\alpha_{1,1}\alpha_{2,2}+\alpha_{3,2}\alpha_{4,1}+\alpha_{1,2}\alpha_{2,1}+\alpha_{1,2}\alpha_{4,1}+\alpha_{2,2}\alpha_{3,1}$$
$$+\alpha_{1,1}\alpha_{4,2}+\alpha_{2,1}\alpha_{3,2}+\alpha_{4,2}\alpha_{5,1},$$
$$-1+\alpha_{3,3}\alpha_{4,1}+\alpha_{1,3}\alpha_{2,1}+\alpha_{2,3}\alpha_{3,1}+\alpha_{4,1}\alpha_{5,3}+\alpha_{1,3}\alpha_{4,1}+\alpha_{1,1}\alpha_{2,3}+\alpha_{4,3}\alpha_{5,1}$$
$$+\alpha_{2,1}\alpha_{3,3}+\alpha_{3,1}\alpha_{4,3}+\alpha_{1,1}\alpha_{4,3},$$
$$-1+\alpha_{3,3}\alpha_{4,2}+\alpha_{1,2}\alpha_{2,3}+\alpha_{1,2}\alpha_{4,3}+\alpha_{1,3}\alpha_{2,2}+\alpha_{1,3}\alpha_{4,2}+\alpha_{2,3}\alpha_{3,2}+\alpha_{2,2}\alpha_{3,3}$$
$$+\alpha_{4,2}\alpha_{5,3}+\alpha_{3,2}\alpha_{4,3}+\alpha_{4,3}\alpha_{5,2}.$$

The Fiber Condition is given by

$$-\alpha_{1,1}\alpha_{2,1}\alpha_{5,1},\ -\alpha_{1,1}\alpha_{3,1}\alpha_{5,1},\ -\alpha_{1,2}\alpha_{2,2}\alpha_{5,2},\ -\alpha_{1,2}\alpha_{3,2}\alpha_{5,2},\ -\alpha_{1,3}\alpha_{2,3}\alpha_{5,3},\ -\alpha_{1,3}\alpha_{3,3}\alpha_{5,3}$$
$$-\alpha_{2,1}\alpha_{3,1}\alpha_{5,1},\ -\alpha_{2,1}\alpha_{4,1}\alpha_{5,1},\ -\alpha_{2,2}\alpha_{3,2}\alpha_{5,2},\ -\alpha_{2,2}\alpha_{4,2}\alpha_{5,2},\ -\alpha_{2,3}\alpha_{3,3}\alpha_{5,3},\ -\alpha_{2,3}\alpha_{4,3}\alpha_{5,3},$$
$$\alpha_{2,1}\alpha_{5,1},\ \alpha_{2,2}\alpha_{5,2},\ \alpha_{2,3}\alpha_{5,3}.$$

A part of the reduced Groebner basis of the resulted system is given by

$$\mathcal{B} = \Big\{\beta_1 - 1, \beta_2 - 1, \beta_3 - 1, \beta_4 - 1, \beta_i^2 - \beta_i, \alpha_{ij}^2 - \alpha_{ij},$$

$$\alpha_{1,2}\alpha_{1,3}, \alpha_{1,2}\alpha_{3,2}, \alpha_{1,3}\alpha_{3,3}, \alpha_{2,2}\alpha_{2,3}, \alpha_{2,2}\alpha_{4,2}, \alpha_{2,2}\alpha_{5,2},$$

$$\alpha_{4,2}\alpha_{5,3}, \alpha_{4,3}\alpha_{5,2}, \alpha_{5,2}\alpha_{5,3}, \alpha_{4,2}\alpha_{5,2} - \alpha_{5,2}, \alpha_{4,2}\beta_5 - \alpha_{5,2},$$

$$\vdots$$

$$-\alpha_{2,2}\alpha_{5,3} - \alpha_{3,2}\alpha_{5,3} + \alpha_{1,2}\beta_5 + \alpha_{2,2}\beta_5 + \alpha_{3,2}\beta_5 + \alpha_{3,3}\beta_5 + \alpha_{5,2}$$

In particular, the intersection $\mathcal{B} \cap \mathbb{Q}[\beta] = (\beta_1 - 1, \beta_2 - 1, \beta_3 - 1, \beta_4 - 1, {\beta_5}^2 - \beta_5)$ gives the two Y minors (i.e., subgraphs X^β) inside X. The remainder of $\mathcal{B}$ gives the explicit expressions of the corresponding mappings.

Counting embeddings without solving equations

The number of zeros of an ideal $\mathcal{I} \subset \mathbb{Q}[x_0, \cdots, x_{n-1}]$ can be determined without solving any equation in $\mathcal{I}$. This is done using *staircase diagrams*, as follows. To each polynomial in $\mathcal{I}$ we assign a point in the Euclidean space $\mathbb{E}^n$ given by the exponents of its leading term (with respect to the given monomial order). Figure 3 depicts three staircase diagrams.

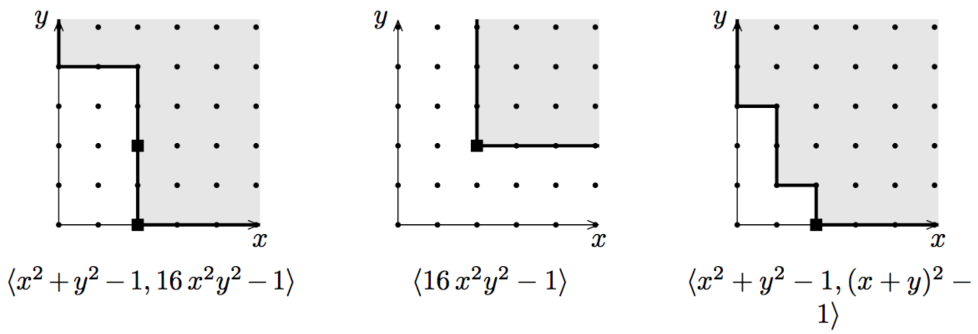


FIGURE – Staircase diagrams of three ideals in $\mathbb{Q}[x, y]$. The number of zeros of the three ideals (left to right) are 8, ∞ and 4 respectively.

The application of this construction to the problem of counting all embeddings $\pi : X \to Y$ is obvious. The ideal $\mathcal{I}$ is given by the different requirements on the coefficients α_{ij} of the map π as discussed previously. Note that the dimension of $Q[\alpha, \beta, \delta]/\mathcal{I}$ cannot be infinite because there is (if any) only finite number of possible embeddings. An example is depicted in Figure 4.

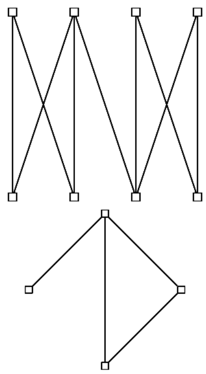


FIGURE – There are 360 embeddings, with chains of size at most 2, for the bottom graph into the upper graph.

Getting rid of redundancies

1. When determining the surjections π (or equivalently, the embeddings ϕ), many of the solutions are redundant : they are of the form $\pi \circ \sigma$ with $\sigma \in \mathbf{Aut}(X)$. This is not desirable because it affects the efficiency of the computations.

2. Instead of applying our method directly, we fold the hardware graph along it symmetries and proceed as before.

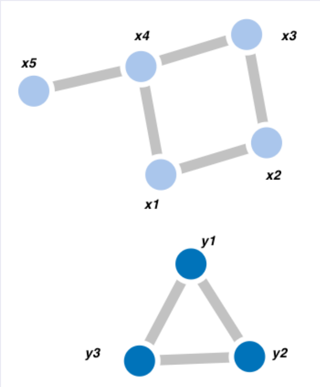
3. This amounts to re-expressing the quadratic form of the hardware graph in terms of the invariants !

Example

Consider the two graphs X and Y of the figure below. The quadratic form of X is :

$$Q_X(x) = x_1x_2 + x_2x_3 + x_3x_4 + x_1x_4 + x_4x_5. \tag{40}$$

Exchanging the two nodes x_1 and x_3 is a symmetry for X, and the quantities $K = x_1 + x_3$, x_2, x_4, and x_5 are invariants of this symmetry.



Example-Continued

In terms of these invariants, the quadratic function $Q_X(x)$, takes the simplified form :

$$Q_X(x, K) = Kx_2 + Kx_4 + x_4 x_5, \tag{41}$$

which shows (as expected) that graph X can be folded into a chain (given by $[x_2, K, x_4, x_5]$). The surjective homomorphism $\pi : X \to Y$ now takes the form

$$K = \alpha_{01} y_1 + \alpha_{02} y_2 + \alpha_{03} y_3. \tag{42}$$

$$x_i = \alpha_{i1} y_1 + \alpha_{i2} y_2 + \alpha_{i3} y_3 \text{ for } i = 2, 4, 5. \tag{43}$$

The coefficients are constrained as usual.

Example-Continued

The table below compares the computations of the surjections π with and without the use of invariants :

	original coords	invt coords
Time for computing a GB (in secs)	0.122	0.039
Number of defining equations	58	30
Maximum degree in the defining eqns	3	2
Number of variables in the defining eqns	20	12
Number of solutions	48	24

In particular, the number of solutions is down to 24, that is, four (non symmetric) minors times the six symmetries of the logical graph Y.

Part 3 : Applications

Flowchart of the Translator :

→ The user inputs the optimization problem $(\mathcal{P})$.

A Reduction to a quadratic form :

1. Generation of the toric ideal $\mathcal{J}_A$ from the monomials of the objective function of $(\mathcal{P})$.
2. Computation of a reduced Groebner basis for $\mathcal{J}_A$; return the quadratic function.

B Embedding inside the AQC processor graph :

3. Generation of the ideal $\mathcal{I}$ that gives the embeddings π.
4. Computation of a reduced Groebner basis $\mathcal{B}$ of the ideal $\mathcal{I}$.

C Solution using a selected embedding on the AQC processor.

← User gets the answer.

Notebook 4

Analytical dependance of the spectral gap on the points of the variety $\mathcal{V}(\mathcal{B})$

Consider a hardware graph X and a problem graph Y. Let $\mathcal{B}$ denote the reduced Groebner basis that gives the set of embeddings $\pi : X \to Y$. An important problem is to understand the dependence of the computational complexity of AQC on the points of the variety $\mathcal{V}(B)$. That is, the dependence of the spectrum of the adiabatic Hamiltonian

$$H(t) = \alpha(t) H_{initial} + \beta(t) H_{(\mathcal{P})} \quad (44)$$

on the different choices of embedding given by $\mathcal{B}$. One way to proceed is to obtain the most general expression of the (quadratic form of the) minor $\tilde{\phi}(Q_Y)(x)$ in terms of the parameters α_{ij}, and β_i determined by $\mathcal{B}$.

Ref : V. Choi, Minor-embedding in adiabatic quantum computation II, 2011.

Proposition

Given a hardware graph X and a problem graph Y. Let $\mathcal{B}$ denote the reduced Groebner basis that gives the set of embeddings $\pi : X \to Y$. The general form of the quadratic form of the Y minor is given by

$$\begin{aligned}\tilde{\phi}(Q_Y)(x) &= \sum_{x_{i_1} x_{i_2} \in \textbf{Edges}(X)} \text{NF}_{\mathcal{B}} \left\{ \left(\sum_j \alpha_{i_1 j} \right) \left(\sum_j \alpha_{i_2 j} \right) \right\} x_{i_1} x_{i_2} \\ &+ \quad M \times \text{NF}_{\mathcal{B}} \left\{ \sum_j \alpha_{i_1 j} \alpha_{i_2 j} \right\} (-2x_{i_1} + 1)(-2x_{i_2} + 1),\end{aligned}$$

with M being one (or more) strong ferromagnetic coupling that maintains the chain.

Example

Consider the two graphs given by the quadratic functions $Q_X(x) = x_1x_2 + x_2x_3$ and $Q_Y(y) = y_1y_2$. In this case, the reduced Groebner basis is given by

$$\begin{gathered}
\beta_2 - 1, \quad (\beta_1 - 1)(\beta_3 - 1), \quad {\beta_3}^2 - \beta_3, \quad {\beta_1}^2 - \beta_1, \\
\alpha_{1,2}\alpha_{3,2}, \quad \alpha_{2,1} + \alpha_{2,2} - 1, \quad \alpha_{3,1} + \alpha_{3,2} - \beta_3, \quad \alpha_{1,1} + \alpha_{1,2} - \beta_1, \quad \alpha_{1,2}\beta_1 - \alpha_{1,2}, \quad \alpha_{3,2}\beta_3 - \alpha_{3,2}, \\
\alpha_{1,2}\beta_3 + 1 + \alpha_{2,2}\beta_3 - \alpha_{1,2} - \alpha_{2,2} - \beta_3, \quad \alpha_{3,2}\beta_1 - \alpha_{2,2}\beta_3 + \alpha_{1,2} + \alpha_{2,2} - \beta_1, \\
\alpha_{2,2}\beta_1 + 1 + \alpha_{2,2}\beta_3 - \alpha_{1,2} - 2\,\alpha_{2,2} - \alpha_{3,2}, \quad \alpha_{1,2}\alpha_{2,2} + 1 + \alpha_{2,2}\alpha_{3,2} - \alpha_{1,2} - \alpha_{2,2} - \alpha_{3,2}, \\
{\alpha_{1,2}}^2 - \alpha_{1,2}, \quad {\alpha_{3,2}}^2 - \alpha_{3,2}, \quad {\alpha_{2,2}}^2 - \alpha_{2,2}.
\end{gathered} \tag{45}$$

The first four polynomials give the reduced Groebner basis $\mathcal{B} \cap \mathbb{Q}[\beta_1, \beta_2, \beta_3]$, which gives the different domains for the projection π.

Example - Continued

The general form of Y minor is given by

$$\begin{aligned}\tilde{\phi}(Q_Y)(x) &= \beta_1 x_1 x_2 + \beta_3 x_2 x_3 - M\,(1-\beta_1-\gamma)\,(2x_1-1)(2x_2-1)\\ &+ M\,(\beta_3-\gamma)\,(2x_2-1)(2x_3-1),\end{aligned}$$

with $\gamma = \alpha_{3,2} + \alpha_{2,2}\beta_3 - 2\alpha_{2,2}\alpha_{3,2}$.

Ising architecture design

An important milestone in the development of AQC is the design of Ising architectures that satisfy the following :

- The degree of X cannot exceed a limited degree d (imposed by current manufacturing limitations).
- X contains a minor for each graph $Y \in \mathcal{Y}$, where $\mathcal{Y}$ represents a class of problems of interest.
- Each Y minor is explicitly computable.

This problem as described was posed in [V. Choi 2011], where the following nomenclature was introduced :

Definition (V. Choi 2011)

Let $\mathcal{Y}$ be a family of graphs. A graph X is called $\mathcal{Y}-$minor universal if for any graph $Y \in \mathcal{Y}$, there exists a minor embedding of Y in X.

Ref : V. Choi, Minor-embedding in AQC II, 2011.

The first requirement translates into the condition $\sum_j q_{ij} \leq d$, where $(q_{ij})_{1\leq i,j\leq n}$ is the unknown adjacency matrix of X. Additionally, if the family $\mathcal{Y}$ is given by a finite number of graphs Y_μ (where μ belongs to a finite range), then for each graph Y_μ, we define the transformation

$$\pi^\mu(x_i) = \sum_{y_i \in V(Y_i)} \alpha_{ij}^\mu y_j, \tag{46}$$

where the binary coefficients are subject to the conditions (23) for each index μ. These conditions, in addition to the pullback and chain conditions for all μ as well as the degree condition above, form a system of polynomials $\mathcal{L} \subset \mathbb{Q}[\alpha^\mu, q]$ that has all information needed to determine the coefficients q_{ij}.

More precisely, we have

Proposition

Let $\mathcal{B}$ be a reduced Groebner basis for the system $\mathcal{L}$ with respect to the elimination order $\{\alpha_{ij}^{\mu}\} \succ \{q_{ij}\}$. The following statements are true :

- the family of graphs $\mathcal{Y} = \{Y_\mu\}$ admits a $\mathcal{Y}-$minor universal graph of size n if and only if $1 \notin \mathcal{B}$ (the choice of the ordering used is not relevant for this statement).
- if $1 \notin \mathcal{B}$, the set of all $\mathcal{Y}-$minor universal graphs of size n is given by the intersection $\mathcal{B} \cap \mathbb{Q}[q]$.
- if $1 \notin \mathcal{B}$, the embeddings π^{μ} (i.e., the coefficients α_{ij}^{μ}) are also given by $\mathcal{B}$ (as functions of the q_{ij}).

This approach can be applied to forbidden minor characterizations. Consider for instance the following statement : A graph X is a forest if and only if it does not contain the triangle K_3 as a minor. This yields the following procedure :

(i) Generate the system of equations that gives all embeddings of K_3 inside X.

(ii) Compute a reduced Groebner basis $\mathcal{B}$: $1 \in \mathcal{B}$ if and only if X is a forest.

More generally, Robertson - Seymour theorem states that every family of graphs that is closed under minors can be defined by a finite set of forbidden minors. The membership to this class can be expressed as a Groebner basis computation using this finite set of forbidden minors.

Thank you !