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An all cycle algorithm by computational algebra

Giancarlo RINALDO

Department of Mathematics, University of Messina,
Messina, 98166, Italy
**E-mail: rinaldo@dipmat.unime.it*

Abstract.

We describe an algorithm to calculate all the cycles of a given undirected graph G by the algebraic technique of Gröbner basis specialized for toric ideals of semigroup algebras.

Introduction

In this work we describe an original algorithm for computing all the cycles of a given undirected graph $\mathcal{G}$.

In the first section we show the main result (see Theorem 1.1), where we describe a bijective correspondence between a set of generators of a toric ideal P and the cycles of the given graph $\mathcal{G}$. Each generator of P is a binomial, b_c, that describes completely a cycle C of $\mathcal{G}$: its vertices, its edges and its length given by the degree of b_c (see Remark 1.1).

The main tool to calculate a set of generators of the toric ideal P is the Buchberger algorithm (see [1], Chapter 3) that gives a method for eliminating variables from systems of polynomial equations. In these last years some improvements were given when we specialize the algorithm for special purpose. One of them is related to toric ideals and was given by B. Sturmfels (see [3], Algorithm 12.3).

The main idea of this algorithm is to construct the basis of a generic toric ideal P starting from an associated lattice basis related to P, and then construct via "Gröbner basis" of quotient ideals the generators of P itself.

In the second section we describe how we specialize and optimize the algorithm of [3] in the specific case of graphs.

The first observation is that in our case the lattice is related to a matrix that is the incidence matrix of a bipartite graph $\mathcal{B}$ associated to $\mathcal{G}$ (see Remark 2.1).

Therefore one can easily calculate the lattice kernel either by Gaussian reduction of the incidence matrix of $\mathcal{B}$ or considering the spanning tree $\mathcal{T}$ of $\mathcal{B}$ and then calculating the fundamental cycles of $\mathcal{B}$ related to $\mathcal{T}$ (see [2], Chapter 4).

The second step is to lift the lattice kernel to the kernel of semigroup algebra that is the toric ideal P. To reach this goal we need to calculate n ideal quotients, with n that is the number of edges of $\mathcal{B}$. Even in this case we optimize the algorithm of B. Sturmfels by Lemma 2.3 where we show that $n/2$ calculations are sufficient in this case.

In the last section we summarize the full algorithm.

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1. Toric ideals and Graphs

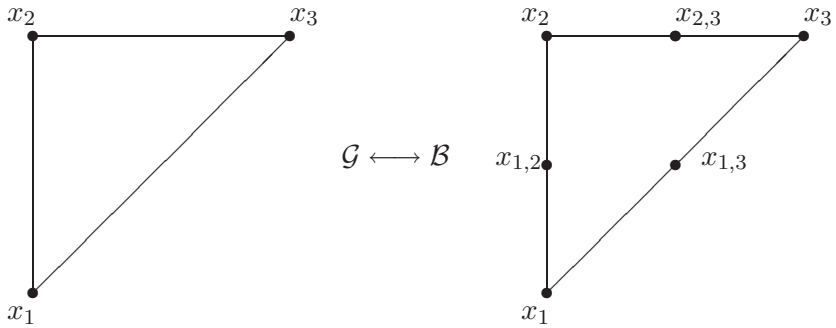
Let $\mathcal{G}$ be a simple undirected graph with n vertices, $V(\mathcal{G}) = \{x_1, \ldots, x_n\}$, and q edges, $E(\mathcal{G}) = \{\{x_i, x_j\} | x_i \text{ adjacent to } x_j\}$.

Definition 1.1. Let $\mathcal{B}$ a graph related to $\mathcal{G}$ such that

1. $V(\mathcal{B}) = \{x_1, \ldots, x_n\} \cup \{x_{ij} | \{x_i, x_j\} \in E(\mathcal{G})\}$;
2. $E(\mathcal{B}) = \{x_i x_{ij}, x_j x_{ij} | \forall \{x_i, x_j\} \in E(\mathcal{G})\}$.

It is easy to observe that $\mathcal{B}$ is bipartite with $n + q$ vertices and $2q$ edges (see fig.1).

Fig.1



Let $R = K[x_i, x_{ij} \in V(\mathcal{B})]$ be the polynomial ring where K is a field with the standard grading. A monomial $f_{ij} = x_i x_{ij}$ is said a generator of $\mathcal{B}$. Let f_{ij}, f_{ji}, $\forall \{x_i, x_j\} \in E(\mathcal{G})$ be the generators of $\mathcal{B}$, the monomial subring $K[\mathcal{B}] \subset R$ related to the graph $\mathcal{B}$ is

$$K[\mathcal{B}] = K[f_{ij}, f_{ji} | \{x_i, x_j\} \in E(\mathcal{G})].$$

There exists a graded epimorphism of K-algebras

$$\Phi : S = K[T_{ij}, T_{ji} | \{x_i, x_j\} \in E(\mathcal{G})] \longrightarrow K[\mathcal{B}]$$

with $\Phi(T_{ij}) = f_{ij}$, with kernel $P(\mathcal{B})$ that is a graded prime ideal, called toric ideal, and is generated by a finite set of binomials (see Proposition 7.1.2, [4]).

Remark 1.1. If C is a cycle of $\mathcal{G}$, $C = \{x_{i_1}, x_{i_2}, \ldots, x_{i_r}\}$ then there exists a binomial b_c in $P(\mathcal{B})$ such that $b_c = T_{i_1 i_2} T_{i_2 i_3} \cdots T_{i_r i_1} - T_{i_2 i_1} T_{i_3 i_2} \cdots T_{i_1 i_r}$. In fact

$$\begin{aligned} \Phi(b_c) &= f_{i_1 i_2} f_{i_2 i_3} \cdots f_{i_r i_1} - f_{i_2 i_1} f_{i_3 i_2} \cdots f_{i_1 i_r} \\ &= x_{i_1 i_2} x_{i_2 i_3} \cdots x_{i_{r-1} i_r} x_{i_r i_1} (x_{i_1} \cdots x_{i_r} - x_{i_r} \ldots x_{i_1}). \end{aligned}$$

It is easy to observe that the sequence of vertices $\{i_1, i_2, \ldots, i_r\}$ describe the cycle C in one direction say the directed cycle C^+, while the sequence of vertices $\{i_r, i_{r-1}, \ldots, i_1\}$ describe the cycle C in the other direction say the directed cycle C^-, therefore we write each binomial b_c as $T_{c^+} - T_{c^-}$.

Remark 1.2. We set on the ring $S = K[T_{ij}, T_{ji} | \{x_i, x_j\} \in E(\mathcal{G})]$ an $\mathbb{N}^q$ graduation assigning to each pair of variable T_{ij}, T_{ji}, the following multidegree

$$\deg(T_{ij}) = \deg(T_{ji}) = (0, \ldots, 0, 1, 0, \ldots, 0) \in \mathbb{N}^q$$

where 1 is at kth position and k is the position of the edge $\{x_i, x_j\} \in E(\mathcal{G})$, such that $k = 1, \ldots, q$.

With this assumption the binomial b_c of Remark 1.1 is $\mathbb{N}^q$ homogeneous.

Definition 1.2. Let $<$ a term order on the ring S. For every pure binomial $b \in P$ we call $\mathrm{in}(b)$ the initial term in b with respect to $<$, and $\mathrm{tr}(b) = b - \mathrm{in}(b)$ the trailing term of b.

Theorem 1.1. *Let G_P the set of binomial*

$$G_P = \{b_c | C \text{ is a cycle of } \mathcal{G}\}.$$

Then G_P is a minimal set of generators of the toric ideal $P(\mathcal{B})$.

Proof. Since the graph $\mathcal{B}$ is bipartite the set G_P generates the toric ideal $P(\mathcal{B})$ (see [4], Proposition 8.1.2).

It remains to show that the set G_P is a minimal set of generators. Suppose that $b_c = T_{c^+} - T_{c^-}$ is a binomial in G_P and is generated by $G_P - \{b_c\}$. We have

$$b_c = \sum_i f_i(\mathbf{T}) b_{c_i} = \sum_i f_i(\mathbf{T}) T_{c_i^+} - \sum_i f_i(\mathbf{T}) T_{c_i^-}$$

such that $b_{c_i} \in G_P - \{b_c\}$, $f_i(\mathbf{T})$ are polynomials in $B = K[\mathbf{T}]$. In particular b_c and $\sum_i f_i(\mathbf{T}) T_{c_i^+} - \sum_i f_i(\mathbf{T}) T_{c_i^-}$ have the same multidegree.

Therefore it exists either $T_{c_i^+}$ or $T_{c_i^-}$ that divides T_{c^+}. This implies that exists a cycle C_i subgraph of the cycle C but this is absurd. □

Therefore we have an algebraic tool to describe all the cycles of $\mathcal{G}$.

The classic algorithm to compute the generators of $P(\mathcal{B})$ is elimination "via" Grö bner basis. That is we consider a bigger ring $R[T_{ij}, T_{ji} | \{x_i, x_j\} \in E(\mathcal{G})]$ and eliminate all the "x" in the relations $T_{ij} - f_{ij}$ induced by the epimorphism Φ (see [1], Chapter 3).

Unfortunately this method is slow since Buchberger algorithm is sensitive to the number of variables involved.

Example 1.1. Let $\mathcal{G}$ be a triangle with vertices $V(\mathcal{G}) = \{x_1, x_2, x_3\}$ and edges $E(\mathcal{G}) = \{\{x_1, x_2\}, \{x_1, x_3\}, \{x_2, x_3\}\}$ (see fig.1). If we consider the ideal

$$(T_{12} - x_1x_{12}, T_{21} - x_2x_{12}, T_{13} - x_1x_{13}, T_{31} - x_3x_{13}, T_{23} - x_2x_{23}, T_{32} - x_3x_{23})$$

and consider a lexicographic term ordering to eliminate the x's we obtain a Gröbner basis of 16 elements. Using the algorithm that we describe at the end we obtain only one element (the generator related to the cycle).

2. Lattices and graphs

We recall that a (point) lattice $\mathcal{L}$ is a discrete subgroup of the euclidean space generated by linear combinations of the vectors $\mathbf{a_1}, \ldots \mathbf{a_r} \in \mathbb{Z}^d$ with integral coefficients, that is

$$\mathcal{L} = \{\sum_{i=1}^{r} \lambda_i \mathbf{a_i} | \lambda_i \in \mathbb{Z}\}.$$

We consider the semigroup homomorphism φ

$$\varphi : \mathbb{N}^r \longrightarrow \mathbb{Z}^d$$

such that $\varphi(\mathbf{u}) = \varphi((u_1, \ldots, u_r)) = \sum_{i=1}^{r} u_i \mathbf{a_i}$. We call $\mathcal{L} = \ker \varphi \subset \mathbb{Z}^r$ the lattice kernel of φ and M the matrix related to φ.

We observe that in the case of a graph $\mathcal{B}$, defined as in the previous section, we have $r = 2q$, $d = n + q$ and $\{\mathbf{a_1}, \ldots, \mathbf{a_{2q}}\} \subset \mathbb{N}^{n+q}$ where each vector $\mathbf{a_i}$ is the exponent vector of the monomial f_i related to the ith edge of the graph $\mathcal{B}$.

Remark 2.1. In general the computation of $\ker \varphi$ is not easy. One of the best algorithm is LLL-algorithm (Lenstra-Lenstra-Lovasz algorithm, see [3], Chapter 12), but in our case it is sufficient the Gaussian reduction to reach a reduced echelon form for M. In fact every column in the matrix M related to φ has only two 1 entries and by a correct subtraction in $q+n-1$ steps we obtain our matrix M reduced. We also observe that M is the incidence matrix of the bipartite graph $\mathcal{B}$.

Remark 2.2. A different, and more combinatorial, way to calculate the lattice kernel of φ is the following (see [2], Chapter 4).

We consider the graph $\mathcal{G}$ (or $\mathcal{B}$ is equivalent) and denote the edge set of $\mathcal{G}$

$$E(\mathcal{G}) = \{f_1, \ldots, f_q\}$$

and vertex set

$$V(\mathcal{G}) = \{x_1, \ldots, x_n\}.$$

We define two vector spaces over the field $\mathbb{Z}_2$, one generated by the 0-chains that are formal linear combination of points $\sum a_i x_i$, $a_i \in \mathbb{Z}_2$, and the other generated by the 1-chains that are formal linear combination of edges $\sum b_i f_i$, $b_i \in \mathbb{Z}_2$.

The boundary operator ∂ is a linear operator sending 1-chains to 0-chain according to the formula

$$\partial(f_i) = \partial(x_k x_l) = x_k + x_l.$$

The kernel of ∂ is called the cycle space of $\mathcal{G}$.

To calculate the generators of $\ker(\partial)$ we consider a spanning tree $\mathcal{T}$ (or a forest) of $\mathcal{G}$, and for each chord of $\mathcal{T}$ (edge of $\mathcal{G}$ that is not in $\mathcal{T}$) we calculate the corresponding cycle.

The set of the cycles calculated in this way is independent and generates $\ker(\partial)$. It is easy to see that exists a bijection between the generators of $\ker(\partial)$ and the generators of $\ker \varphi$.

The relation between $\ker \varphi$ and a generic toric ideal $P = \ker \Phi \subset K[T_1, \ldots, T_r]$ is given by the following Lemma (see [3], Chapter 4):

Lemma 2.1. *The toric ideal P is generated as a K-vector space by the set of binomials*

$$\{T^{\mathbf{u}} - T^{\mathbf{v}}, \mathbf{u}, \mathbf{v} \in \mathbb{N}^r, \varphi(\mathbf{u}) = \varphi(\mathbf{v})\}$$

We recall that the support of a vector $\mathbf{u} \in \mathbb{Z}^r$ is $\mathrm{supp}(u) = \{i : u_i \neq 0\}$. We observe also that any vector $\mathbf{u} \in \mathbb{Z}^r$ can be written as $\mathbf{u} = \mathbf{u}^+ - \mathbf{u}^-$ where $\mathbf{u}^+$ and $\mathbf{u}^-$ are non negative vector with disjoint support.

By this remark P is generated by

$$\{T^{\mathbf{u}^+} - T^{\mathbf{u}^-}, \mathbf{u} \in \ker \varphi\}.$$

We give the following definition of quotient ideal, necessary for our computation:

Definition 2.1. Let f be a polynomial of the ring $A = K[T_1, \ldots, T_r]$ and $J \subset A$ an ideal. We define the quotient ideals

$$(J : f) = \{g \in A : fg \in J\}$$

and

$$(J : f^\infty) = \{g \in A : f^s g \in J \text{ for some } s \in \mathbb{N}\}.$$

At this point we lift $\ker \varphi$ to $\ker \Phi$ by calculating the ideal quotients. That is we consider the ideal $P_0 = (T^{\mathbf{u}} - T^{\mathbf{v}} | \mathbf{u} - \mathbf{v})$, with $u - v$ is a generator of the lattice basis, and calculate the ideal quotients

$$P = P_0 : (T_1 T_2 \cdots T_r)^\infty = ((\cdots (P_0 : T_1^\infty) : T_2^\infty) \cdots) : T_r^\infty)$$

Therefore we have to calculate r ideal quotients, that in our case are $2q$.

By the following lemma (see [3], Lemma 12.1) we have the method to calculate ideal quotients using Gröbner basis:

Lemma 2.2. *Let $<$ the degree reverse lexicographic term order induced by*

$$T_1 > T_2 > \cdots > T_r,$$

and let G be the reduced Gröbner basis of a homogeneous ideal $J \subset K[T_1, \ldots, T_r]$. Then the set

$$G' = \{f \in G : T_r \nmid f\} \cup \{f/T_n : f \in G,\ T_r \mid f\}$$

is a Gröbner basis of $(J : T_r)$. A Gröbner basis of $(J : T_r^\infty)$ is obtained by dividing each element $f \in G$ by the highest power of T_r that divides f.

Remark 2.3. We may improve the speed of the calculation of P in the following manner: Let $P_i = P_{i-1} : T_i^\infty$, $i = 1, \ldots, r$, we have that

$$P_0 \subseteq P_1 \subseteq \cdots \subseteq P_r$$

is a filtration of the prime ideal $P = P_r$.

If $b = w(u - v) \in P_i$ where u, v and w are monomials in $K[T_1, \ldots, T_r]$, then $u - v$ is in P since it is a prime ideal generated by binomials.

Let $b_1, \ldots, b_s$ the minimal set of generators of P_i, we may calculate for each $b_i = u_i - v_i$ the binomial, $b_i' = u_i' - u_i'$, with u_i' and v_i' that have exponent vectors with disjoint support, that is

$$b_i' = \frac{u_i - v_i}{GCD(u_i, v_i)} = u_i' - v_i'$$

With this assumption we define $P_i' = (b_1', \ldots, b_s')$.

We observe that $P_i \subset P_i' \subset P$, $\forall i = 1, \ldots, r$ and $P_{i+1} = P_i : T_{i+1}^\infty \subset P_i' : T_{i+1}^\infty$.

Therefore we define a new filtration of P in this way $P_1' = (P_0 : T_1^\infty)'$, $P_2' = (P_1' : T_2^\infty)'$, $\ldots$, $P_r' = (P_{r-1}' : T_r^\infty)'$.

In this way for each computation of the Gröbner basis we construct a new ideal whose generators have a lower degree of the original generators, whose number of generators are less or equal than the number of the original ideal. We obtain a shorter filtration for P, too.

Even in this case we optimize this calculation by the following

Lemma 2.3. *The toric ideal $P(\mathcal{B})$ is generated by the quotients*

$$P_k'(\mathcal{B}) = (P_{k-1}'(\mathcal{B}) : T_{ij}^\infty)',$$

with $i < j$, $\{x_i, x_j\} \in E(\mathcal{G})$, $k = 1, \ldots, q$.

Proof. From now on for simplicity we set $P_k = P_k(\mathcal{B})$. We observe that is enough to prove that

$$((P'_k : T_{ij})' : T_{ji})' = (P'_k : T_{ij})'.$$

1) $((P'_k : T_{ij})' : T_{ji})' \supset (P'_k : T_{ij})'$. By definition of quotient ideal we have

$$(P'_k : T_{ij})' : T_{ji} \supset (P'_k : T_{ij})'$$

and since

$$((P'_k : T_{ij})' : T_{ji})' \supset (P'_k : T_{ij})' : T_{ji}$$

we have the first inclusion.

2) $((P'_k : T_{ij})' : T_{ji})' \subset (P'_k : T_{ij})'$. Let g be in the set of generators of $(P'_k : T_{ij})' : T_{ji}$, we want to show that g is in $(P'_k : T_{ij})'$.

Let G be the Gröbner basis of $(P'_k : T_{ij})'$ with respect to degree reverse lexicographic ordering with T_{ji} that is less than the other indeterminates, and let G' be the Gröbner basis of $(P'_k : T_{ij})' : T_{ji}$ with respect to the same term ordering.

By Lemma 2.2 we have

$$G' = \{f \in G : T_{ji} \nmid f\} \cup \{f/T_{ji} : f \in G, T_{ji} \mid f\}.$$

Without loss of generality we can take $g \in G'$ and prove that $g \in (G)$.

We observe that g is an $\mathbb{N}^q$ graded binomial in fact the s-polynomial of $\mathbb{N}^q$ graded binomials is an $\mathbb{N}^q$ graded binomial (see Lemma 2.2).

If we take $g \in \{f \in G : T_{ji} \nmid f\}$ the assertion is trivially true, so we take $g \in \{f/T_{ji} : f \in G, T_{ji} \mid f\}$.

That is $g = f/T_{ji}$, with $g \notin G$, $gT_{ji} \in G$. Since $gT_{ji} \in G$ it exists $b \in G$ such that $\mathrm{in}(b)$ divides $\mathrm{in}\, gT_{ji}$ with T_{ji} that divides $\mathrm{in}(b)$.

Since b is $\mathbb{N}^q$ graded and T_{ji} is the least indeterminate with respect to the term ordering, we have that T_{ji} divides also the trailing term of b.

We observe that each generator of $(P'_k : T_{ij})'$ has monomials with disjoint support and to obtain the element $gT_{ji} \in G$, there exist f_1, f_2 in the minimal set of generators of $(P'_k : T_{ij})'$, such that $T_{ij} \mid \mathrm{in}(f_1)$ and $T_{ij} \mid \mathrm{in}(f_2)$, and since f_1 and f_2 are $\mathbb{N}^q$ graded $T_{ji} \mid \mathrm{tr}(f_1)$ and $T_{ji} \mid \mathrm{tr}(f_2)$. We have

$$S(f_1, f_2) \to T_{ji} g$$

where "$\to$" is the reduction step induced by multivariate division algorithm ([1], Chapter 2).

If we fix the degree reverse lexicographic ordering with T_{ij} as the least indeterminate, we obtain

$$S(f_1, f_2) \to T_{ij} g'$$

and $g' \in (P' : T_{ij})'$, that is g' has monomial with disjoint support, generates $T_{ji}g$ and since is $\mathbb{N}^q$ graded generates g itself.

With similar argument we prove the assertion for $P'_k : T_{ij}^{\infty}$. □

By this Lemma we succeed to calculate only q ideal quotients.

3. Conclusions: The algorithm

Now we are ready to describe the following

Algorithm 3.1. *(All cycles of a graph using Gröbner basis)*

1. *Define the graph* $\mathcal{B}$ *induced from* $\mathcal{G}$ *(see Definition 1.1);*
2. *Find the lattice basis of* $\ker\varphi$ *that is cycle space of* $\mathcal{B}$ *(see Remarks 2.1, 2.2);*
3. *Define the ring* $B = K[T_{i,j}, T_{j,i} | \{x_i, x_j\} \in E(\mathcal{G})]$*;*
4. *Let* $k = 0$*,* $P_k = (T^{\mathbf{u}} - T^{\mathbf{v}} | \mathbf{u} - \mathbf{v} \in \ker\varphi) \subset B$*;*
5. *For each* $i < j$ *,*$\{x_i, x_j\} \in E(\mathcal{G})$ *do* $P'_{k+1} = (P'_k : T_{i,j}^{\infty})'$*, increment* k *(see Lemmas 2.2, 2.3,);*
6. *Let* $P = P_k$*, for each generator of* P *find the corresponding cycle of* $\mathcal{G}$ *(see Theorem 1.1).*

Example 3.1. We consider the complete graph with 4 vertices K_4. By the second step of the algorithm we calculate a lattice basis of $\mathcal{B}$ that in our case is induced by the cycles $(1,2,3,4)$, $(1,2,3)$ and $(1,2,4)$, therefore

$$\begin{aligned} P_0 = (&T_{12}T_{23}T_{34}T_{41} - T_{21}T_{32}T_{43}T_{14}, \\ &T_{12}T_{23}T_{31} - T_{21}T_{32}T_{13}, T_{12}T_{24}T_{41} - T_{21}T_{42}T_{14}). \end{aligned}$$

By the computation of $P'_1 = (P_0 : T_{12})'$ and $P'_2 = (P'_1 : T_{13})'$ we obtain 3 binomials of degree 4 related to the 4-cycles:
$T_{12}T_{23}T_{34}T_{41} - T_{21}T_{32}T_{43}T_{14}, T_{12}T_{24}T_{43}T_{31} - T_{21}T_{42}T_{34}T_{13},$
$T_{13}T_{32}T_{24}T_{41} - T_{31}T_{23}T_{42}T_{14};$
and 4 binomials of degree 3 related to the 3-cycles:
$T_{12}T_{23}T_{31} - T_{21}T_{32}T_{13}, T_{12}T_{24}T_{41} - T_{21}T_{42}T_{14},$
$T_{13}T_{32}T_{21} - T_{31}T_{23}T_{12}, T_{23}T_{34}T_{42} - T_{32}T_{43}T_{24}.$

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