

The three-state toric homogeneous Markov chain model has Markov degree two

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Abstract

We prove that the three-state toric homogeneous Markov chain model has Markov degree two. In algebraic terminology this means, that a certain class of toric ideals are generated by quadratic binomials. This was conjectured by Haws, Martin del Campo, Takemura and Yoshida, who proved that they are generated by degree six binomials.

1. Introduction

This paper concerns the algebraic statistics of time homogeneous Markov chains. Markov chains are simple yet important random processes but the algebra surrounding them is relatively unexplored. A Markov chain give a distribution on the set of words of a given length on the alphabet consisting of the states of the Markov chain. We are interested in the toric ideals generated by the binomial equations satisfied by all such distributions. The Markov chains considered are time homogeneous, meaning that the transition probabilities do not depend on time.

One motivation to study these ideals is that the generating sets of these ideals can be used to do hypothesis testing, this idea was proposed by Diaconis and Sturmfels [6]. When the Markov chain only have two states Hara and Takemura [7] found generating sets consisting of binomials of degree at most two. In this paper we are interested in Markov chains with more states but with the restriction that the initial distribution is uniform and that the transition probabilities from a state to itself are zero. In this setting Haws, Martin del Campo, Takemura and Yoshida [9] conjectured that there are generating sets consisting of binomials of degree at most $S - 1$, where S is the number of states. The main contribution of this paper is to prove the conjecture for the three state case. The conjecture is false in general, a counterexample for the four state case is provided. We also investigate Gröbner bases for these ideals.

The results of this paper are about algebraic statistics, an area further surveyed in the book by Drton, Sturmfels, and Sullivan [2].

The rest of the introduction is a more formal setup of the problem and the description of the results, in Section 2 the main tools used in the proofs are introduced and in Section 3 the main theorem is proved.

Let S and T be positive integers, set

$$R_{S,T} = \mathbb{K}[x_w \mid w \text{ is a } T\text{-letter word } i_1 \dots i_T \text{ on the alphabet } [S] \text{ with } i_j \neq i_{j+1}],$$

and define the S -state toric homogeneous Markov T -chain ideal, $I_{S,T}$, as the kernel of the ring homomorphism

$$\Phi_{S,T} : R_{S,T} \rightarrow R_{S,2}$$

given by $\Phi(x_{i_1 \dots i_T}) = x_{i_1 i_2} x_{i_2 i_3} \cdots x_{i_{T-1} i_T}$. When the T is clear from context this is sometimes abbreviated to S -state model ideal. The *Markov degree* of an ideal is the smallest upper bound of the degree of the generators of the ideal, and the *Gröbner degree* is the smallest upper bound for the degrees of the elements in a Gröbner basis.

Theorem (Haws, Martin del Campo, Takemura and Yoshida, [8], [9]). *The Markov degree of the three-state model ideal is at most six.*

Conjecture ([8], [9]). *For $S > 2$, the S -state model ideal has Markov degree $S - 1$ and Gröbner degree S .*

We prove the Markov part of the conjecture for the three-state model ideal by combinatorial arguments.

Theorem 3.7. *The Markov degree of the three-state model ideal is two.*

Before this paper only the two state case was settled. For more states only conjectures were known.

Example 1.1. When T is less than or equal to two then the ideal is trivial. The ideal $I_{3,3}$ is

$$\langle x_{123}x_{321} - x_{121}x_{232}, x_{231}x_{132} - x_{131}x_{232}, x_{312}x_{213} - x_{121}x_{131}, x_{121} - x_{212}, x_{131} - x_{313}, x_{232} - x_{323} \rangle.$$

The S -state toric homogeneous Markov T -chain ideal is similar to the ideal of graph homomorphisms from the path of length T to the complete graph on S vertices. The following result motivates the belief that the structure of $I_{S,T}$ should be possible to understand.

Theorem (Engström and Norén [5]). *The ideal of graph homomorphisms from any forest to any graph has a square-free quadratic Gröbner basis.*

This theorem was proved using the toric fiber product. In this paper, we will use an adaption of that object, similar to those in [3], [4] and [10], for ideals that are not always toric fiber products right off.

The corresponding problem for general Markov chains where the transition probabilities are allowed to depend on time is easier, the ideals are then ideals of graph homomorphisms from a path to a complete graph with loops and these are always generated in degree at most two. This suggests that there should be an easier argument to settle the case with non-uniform initial distribution, as the ideals with non-uniform initial distribution is in some sense closer to be ideals of graph homomorphisms. The problem is still open when all transition probabilities are allowed to be nonzero, but it seems likely that similarly combinatorial methods can be used to settle this case too.

2. State graphs and normal monomials

Let P_T be the directed path on vertex set $[T]$ with edges $12, 23, \dots, (T-1)T$ and let K_3 be the directed complete graph on vertex set $[3]$. Each T -letter word $i_1 \dots i_T$ on the alphabet $[3]$ with $i_j \neq i_{j+1}$ encodes a graph homomorphism $P_T \rightarrow K_3$, by sending vertex j to i_j . A *state graph* is a directed graph on vertex set $[3]$ with multiple edges allowed but no loops.

The variables of $R_{3,T}$ are indexed by graph homomorphisms $P_T \rightarrow K_3$ each of which induces a state graph. If x and y are two variables with the same state graph, then $x - y \in I_{3,T}$. When describing the relations between higher degree monomials, it is enough to have one variable for each state graph.

The state graphs will be decomposed into paths and cycles. The notation for a path is ij or ijk depending on its length, the notation for a two-cycle is (ij) , and the notation for triangles is (ijk) (the cycle (ijk) have the edges ij, jk, ki .) We keep careful track of orientation: $12, 23, 31, 123, 231, 312$, and (123) are oriented one way and $13, 21, 32, 132, 213, 321$, and (132) are oriented the other way.

Proposition 2.1. *The state graph G of a variable can be uniquely decomposed into a collection of two-cycles, triangles with the same orientation, and potentially a leftover path oriented in the same way as the triangles.*

Proof. It is a basic fact in graph theory that a directed graph with the same in and out degree for each vertex can be decomposed into cycles.

The state graph comes from a graph homomorphism $P_T \rightarrow K_3$. If the homomorphism sends 1 and T to the same vertex, then the state graph can be decomposed into directed cycles. If there are triangles with different orientations, then any two oppositely oriented triangles can be replaced by a triple of two-cycles.

If the graph homomorphism sends 1 to i and T to j with $i \neq j$, then add an extra edge ji in G to get G' . Decompose G' as before into cycles, with triangles oriented the same way. Then remove ji from a triangle if possible, and otherwise from a two-cycle, to achieve compatible orientation.

That the decomposition is unique follows from the fact that all edges with one orientation are locked into two-cycles and the leftover edges are put into as many triangles as possible. \square

Proposition 2.2. *Any collection of two-cycles, triangles, and at most one path with the same orientation as the the triangles; with in total $T - 1$ edges, is a decomposition of the state graph of a variable.*

Proof. For each cycle α , let c_α be the number of copies of the cycle α in the collection. The goal is to construct a word realizing the decomposition as a state graph of a variable. There are four different cases depending on what kind of path and cycles that occur in the decomposition.

CASE 1. If the path 123 occurs in the collection, then the word

$$\underbrace{1212 \dots 12}_{c_{(12)}} \underbrace{1313 \dots 13}_{c_{(13)}} \underbrace{123123 \dots 123}_{c_{(123)}} \underbrace{132132 \dots 132}_{c_{(321)}} 1 \underbrace{2323 \dots 23}_{c_{(23)}}$$

realizes the collection as the state graph of a variable. The numbers under the brackets denote the number of times the small subword is repeated. For example,

$$\underbrace{132132 \dots 132}_{c_{(321)}}$$

represents $c_{(321)}$ copies of the word 132.

CASE 2. If the path 12 occurs, then the collection is realized by the word:

$$\underbrace{1212 \dots 12}_{c_{(12)}} \underbrace{1313 \dots 13}_{c_{(13)}} \underbrace{123123 \dots 123}_{c_{(123)}} \underbrace{132132 \dots 132}_{c_{(321)}} 1 \underbrace{2323 \dots 23}_{c_{(23)}} 2.$$

CASE 3. If the collection only consists of cycles, and at least one of them is (12), then the word

$$\underbrace{123123 \dots 123}_{c_{(123)}} \underbrace{132132 \dots 132}_{c_{(321)}} \underbrace{1313 \dots 13}_{c_{(13)}} 1 \underbrace{2323 \dots 23}_{c_{(23)}} \underbrace{2121 \dots 21}_{c_{(12)}}$$

gives a realization.

CASE 4. If the collection only consists of triangles, then the word

$$\underbrace{123123 \dots 123}_{c_{(123)}} \underbrace{132132 \dots 132}_{c_{(321)}} 1$$

gives a realization.

By symmetry, this proves that collections with $T - 1$ edges come from words. \square

Example 2.3. The word 123231323123 has the decomposition (13)(23)(23)(123)123.

Since the state graph can be reconstructed from its decomposition, there is one variable associated to each decomposition. If x, x', y, y' are variables from the decompositions A, A', B, B' and $xy - x'y' \in I_{S,T}$, then we get the *Markov step*

$$\begin{bmatrix} A \\ B \end{bmatrix} \rightarrow \begin{bmatrix} A' \\ B' \end{bmatrix}.$$

The convention is that only the parts of the decomposition that is changed is written out, that is, the step

$$\begin{bmatrix} AC \\ BD \end{bmatrix} \rightarrow \begin{bmatrix} AC' \\ BD' \end{bmatrix}$$

is written as

$$\begin{bmatrix} C \\ D \end{bmatrix} \rightarrow \begin{bmatrix} C' \\ D' \end{bmatrix}.$$

After one step it might be necessary to decompose the graphs in a new way. For example,

$$\begin{bmatrix} (123) \\ (321) \end{bmatrix} \rightarrow \begin{bmatrix} (321) \\ (123) \end{bmatrix}$$

could give

$$\begin{bmatrix} (123) \\ (321)(321) \end{bmatrix} \rightarrow \begin{bmatrix} (321) \\ (12)(13)(23) \end{bmatrix}.$$

Remark 2.4. The order of the cycles and paths in the decompositions does not matter. For example, (12)(23)13 is the same decomposition as 13(23)(12).

Definition 2.5. Let

$$I_{3,T}^{\leq} = \langle b \in I_{3,T} \mid b \text{ is a quadratic binomial whose Markov move changes at most 12 edges} \rangle.$$

The following normal form for monomials is useful.

Definition 2.6. A monomial n is *normal*, if

- (1) all triangles in n are oriented the same way;
- (2) and if two variables divide n , then the number of triangles in them differ by at most two;
- (3) and either
 - (a) all triangles and paths are oriented in the same way,
 - (b) or there is at most one triangle in each variable in n , and there is no monomial n' satisfying
 - (i) $n' - n \in I_{3,T}^{\leq}$,
 - (ii) and n' has fewer triangles than n , or n' has equally many triangles but fewer paths than n ,
that is normal.

Example 2.7. The monomial $x_{1231}x_{3213}$ is not normal as it breaks Condition 1. The monomial $x_{1231231231}x_{1212121212}$ is not normal as it breaks Condition 2. The monomial $n = x_{123}x_{321}$ is not normal as it breaks condition 3, the monomial $n' = x_{121}x_{323}$ is an example of a normal monomial illustrating this.

3. Proof of the main theorem

To prove that the ideals $I_{3,T}$ are generated by quadrics, five lemmas are needed.

Lemma 3.1. *From a monomial m , it is possible by degree two-moves to reach a normal monomial n .*

Proof. The first step is to get all the triangles of m oriented the same way.

If the monomial m has variables with triangles oriented differently, and a variable with more than one triangle, then the move

$$\begin{bmatrix} (123) \\ (321) \end{bmatrix} \rightarrow \begin{bmatrix} (321) \\ (123) \end{bmatrix}$$

decreases the number of triangles, since (123)(321) becomes (12)(13)(23) in the decomposition. After possible repetitions, either all triangles have the same orientation or the

variables have at most one triangle. If there is a pair of variables with opposite oriented triangles, then there are two cases depending on if anyone of them have a path. If one of them have a path P , then it has the triangle, say (123) , with the same orientation. The step

$$\begin{bmatrix} (123)P \\ (321) \end{bmatrix} \rightarrow \begin{bmatrix} (321)P \\ (123) \end{bmatrix},$$

reduce the number of triangles. If neither of them have a path, then the move

$$\begin{bmatrix} (123) \\ (321) \end{bmatrix} \rightarrow \begin{bmatrix} (12)31 \\ (23)13 \end{bmatrix}$$

reduces the number of triangles. Now all triangles can be assumed to have the same orientation, and Condition 1 is satisfied.

The second step is to reduce the difference between the number of triangles in the variables. If one variable contains at least three more triangles T_1, T_2, T_3 than another variable, then the other one contains at least three two-cycles C_1, C_2 and C_3 . The move

$$\begin{bmatrix} T_1T_2 \\ C_1C_2C_3 \end{bmatrix} \rightarrow \begin{bmatrix} C_1C_2C_3 \\ T_1T_2 \end{bmatrix}$$

reduces the difference. After repetitions, Condition 2 is satisfied.

If all paths and triangles have the same orientation, then the monomial is normal, since Condition 3.a is satisfied.

To show that Condition 3.b is satisfied we first find moves to a monomial with at most one triangle in each variable.

If there are no triangles, then we are done. Otherwise, there is a triangle and a path P with opposite orientations. The path P is not in a variable with a triangle, and thus no variable contains more than two triangles due to that Condition 2 is satisfied. If there is a variable with two triangles and a path Q , then P and Q are equally long, and the step

$$\begin{bmatrix} P \\ Q \end{bmatrix} \rightarrow \begin{bmatrix} Q \\ P \end{bmatrix}$$

reduce the number of triangles. From now on, we assume that no variables with two triangles have a path. If there are no variables with two triangles and no paths, then all variables have at most one triangle. Now assume that there is a variable with two triangles, say (123) , and no path. By parity the path P have two edges, and is of opposite orientation, say 321 . The move

$$\begin{bmatrix} 321 \\ (123) \end{bmatrix} \rightarrow \begin{bmatrix} (12) \\ (23)31 \end{bmatrix}$$

reduces the number of triangles. This procedure can be repeated as long as there are variables with more than one triangle, and there are triangles and paths of opposite orientation. Thus, we either get everything oriented in the same way, and satisfy Condition 3.a, or get at most one triangle in each variable. Using quadratic Markov moves changing at most 12 edges, minimize according to satisfy Condition 3.b. \square

Definition 3.2. The ij -spin of a variable x is $s_{ij}(x) = c_{ij} - c_{ji}$ where c_{kl} is the number of kl edges in the state graph of x . The ij -spin of a monomial $m = x_1 \cdots x_d$ is $s_{ij}(m) = \sum_{k=1}^d s_{ij}(x_k)$. The *spin-vector* of a monomial m is the vector $(s_{12}(m), s_{31}(m), s_{23}(m))$. The *total spin* of a monomial m is $s_{12}(m) + s_{23}(m) + s_{31}(m)$.

Although there are homotopy and valuation theoretic interpretations of spin, we only use it for combinatorial calculations.

Example 3.3. The state graph of $m = x_{123}x_{212}$ has two 12 edges and one 21 edge and one 23 edge. This give that the spin vector of m is $(1, 0, 1)$.

Lemma 3.4. *Let m and n be normal monomials with $m - n \in I_{3,T}$. If m has all paths and triangles oriented the same way, then so does n .*

Proof. The proof is divided into four cases: Whether or not n has triangles in any of the variables and parity of T . By symmetry, we can assume m has orientation (123) . For contradiction, assume that n has a path or triangle with orientation (321) .

CASE A. There are no triangles in n .

CASE A.1. Let T be even.

By assumption, n contains a path with (321) orientation. This path has an odd number of edges as there is an odd number of edges in the state graph of each variable. Every variable in m has a triangle or a path. In m , everything has the same orientation, so the total spin is at least the degree of m . In n , all variables contribute 1 or -1 to the total spin, and at least one of the variables contributes -1 . Thus, n has total spin strictly less than its degree, contradicting that m and n have the same total spin.

CASE A.2. Let T be odd.

By assumption, n contains a path with (321) orientation. This path has an even number of edges as there is an even number of edges in the state graph of the variable. By symmetry, we can assume n contains the path 321 . Now, n cannot contain the path 123 since n is normal and that would allow a move reducing the number of paths:

$$\begin{bmatrix} 321 \\ 123 \end{bmatrix} \rightarrow \begin{bmatrix} (12) \\ (23) \end{bmatrix}.$$

To cancel the negative 23-spin from a 321 path, n must contain a 23 edge outside a two-cycle. That edge must be in a path since there are no triangles in n . The only path of the right length and orientation is 231 since 123 is excluded. The same argument for 12 gives that n contains a 312 path for every path 321. Since n is normal, the only type of path oriented as (321) in n is 321. All spin in n is from the paths 312, 231, 312, so the 31-spin is strictly greater than the sum of the 12-spin and 23-spin in n . The only way to get a similar contribution to 31-spin in m is from 31 paths without triangles, but that is impossible since m is normal and T is odd.

CASE B. There are triangles in n .

CASE B.1. Let T be even.

If all triangles in n have orientation (321), then there are variables with paths 12, 23 and 31 in n . If there is a variable in n with a triangle and no path, then the move

$$\left[\begin{array}{c} (321) \\ 12 \end{array} \right] \rightarrow \left[\begin{array}{c} (12)32 \\ 13 \end{array} \right]$$

reduces the number of triangles in n , contradicting normality. If there is a path on the variable with a triangle, then moves of the type

$$\left[\begin{array}{c} 321 \\ 12 \end{array} \right] \rightarrow \left[\begin{array}{c} (12) \\ 32 \end{array} \right]$$

reduce the number of paths.

Next, we consider the case that all triangles in n have orientation (123). By assumption, there is a variable in n with a (321) oriented path. This variable does not contain a triangle since it is oriented differently and n is normal. This is a single edge path since T is even. By symmetry, let the path be 21. If n contains the path 123, then the move

$$\left[\begin{array}{c} 21 \\ 123 \end{array} \right] \rightarrow \left[\begin{array}{c} 23 \\ (12) \end{array} \right]$$

reduces the number of paths, contradicting normality. If n contains a variable with a triangle and no path, then the move

$$\left[\begin{array}{c} 21 \\ (123) \end{array} \right] \rightarrow \left[\begin{array}{c} 23 \\ (12)31 \end{array} \right]$$

reduces the number of triangles, again contradicting normality. The variables in n with triangles have exactly one triangle since n is normal. Furthermore, they have a path on two edges since T is even. The only such path with correct orientation is 231. The path 12 cannot occur in n since the move

$$\left[\begin{array}{c} 12 \\ 231 \end{array} \right] \rightarrow \left[\begin{array}{c} 31 \\ 123 \end{array} \right]$$

creates a variable with the path 123, yielding a contradiction as earlier. If n contains a 32 path, then the move

$$\left[\begin{array}{c} 32 \\ 231 \end{array} \right] \rightarrow \left[\begin{array}{c} 31 \\ (23) \end{array} \right]$$

reduces the number of paths, contradicting normality. Likewise, the move

$$\left[\begin{array}{c} 13 \\ 231 \end{array} \right] \rightarrow \left[\begin{array}{c} 23 \\ (13) \end{array} \right]$$

contradicts that n contains the path 13. The set of spin vectors $(s_{12}(x), s_{31}(x), s_{23}(x))$ of variables x potentially occurring in n is:

$$\{(-1, 0, 0), (0, 1, 0), (0, 0, 1), (1, 2, 2)\},$$

and $(-1, 0, 0)$ occurs. The spins then satisfy $s_{23}(n) + s_{31}(n) - 3s_{12}(n) - d > 0$ where d is the degree of n . All d variables x in m satisfy $s_{23}(x) + s_{31}(x) - 3s_{12}(x) - 1 \leq 0$ since m is normal and oriented (123).

CASE B.2. Let T be odd.

First, we consider the case that all triangles are oriented (321). Since n is normal, every variable contains at most one triangle. With every triangle comes a single edge path since T is odd. By symmetry, we assume that 13 is a path in n . To get a non-negative 31-spin, the edge 13 is compensated by a path with 31. This path is not in a variable with a triangle since they would have different orientation. The path with 31 contains two edges since T is odd. There are two options: 231 and 312.

However, the moves

$$\left[\begin{array}{c} (321)13 \\ 312 \end{array} \right] \rightarrow \left[\begin{array}{c} (12)(13) \\ 132 \end{array} \right] \quad \text{and} \quad \left[\begin{array}{c} (321)13 \\ 231 \end{array} \right] \rightarrow \left[\begin{array}{c} (12)(23) \\ 213 \end{array} \right]$$

reduce the number of triangles, contradicting that n is normal.

Now, we consider the case of all triangles oriented (123). By assumption, there is a path in n with the orientation (321) and this variable has no triangle since n is normal. The path has two edges since T is odd. By symmetry, we assume that n contains the path 321. All variables with triangles in n have a path with one edge since n is normal. If that path is not 31, then the moves

$$\left[\begin{array}{c} (123)12 \\ 321 \end{array} \right] \rightarrow \left[\begin{array}{c} (12)312 \\ (23) \end{array} \right] \quad \text{or} \quad \left[\begin{array}{c} (123)23 \\ 321 \end{array} \right] \rightarrow \left[\begin{array}{c} (23)231 \\ (12) \end{array} \right]$$

decrease the number of triangles, contradicting normality. Thus, all paths with the (321) orientation have to be 321 and all variables with triangles have the path 31. The set of spin vectors $(s_{12}(x), s_{31}(x), s_{23}(x))$ of variables x potentially occurring in n is

$$\{(0, 0, 0), (0, 1, 1), (-1, 0, -1), (1, 1, 0), (1, 2, 1)\},$$

and $(-1, 0, -1)$ occurs. The spins satisfy $s_{12}(n) - s_{13}(n) + s_{23}(n) < 0$ while the variables x in m all satisfy $s_{12}(x) - s_{13}(x) + s_{23}(x) \geq 0$. \square

Lemma 3.5. *Let m and n be normal monomials with $m - n \in I_{3,T}$. The maximal number of triangles in a variable in m cannot be less than the minimal number of triangles in a variable in n .*

Proof. If m has variables with different orientation, then so does n by Lemma 3.4. In this case, both monomials have at most one triangle in each variable and both monomials have variables with no triangles.

Now, we consider the case that both monomials have all variables oriented the same way. The total spin is different for m and n if the maximal number of triangles in a variable in m is less than the minimal number of triangles in a variable in n . \square

Lemma 3.6. *If m and n are normal monomials such that $m - n \in I_{3,T}$ and m and n have all paths and triangles oriented in the same way, then it is possible to use degree two-steps to go from m to n .*

Proof. By symmetry, we can assume that the orientation of the monomials is (123). The proof is structured as follows: We start with two monomials m and n of degree d and no common variables. Then, a sequence of steps is presented from m to m' and from n to n' so that they share a variable. By induction on d , it is then possible to go between m and n by degree two steps. The base case is trivial. The induction step is split into two cases: A. There is a variable x in m and a variable y in n that have the same number of triangles; B. Otherwise.

CASE A. There is a variable x in m and variable y in n that have the same number of triangles.

By parity, there can not be paths in x and y of different lengths. This case is split into four different subcases: 1. The variables x and y have the same path; 2. The variables x and y have different one edge paths; 3. The variables x and y have different two edge paths; 4. The variable x has no path and y has a path with two edges.

CASE A.1. The variables x and y have the same path.

The state graphs of m and n are the same. All edges with orientation (321) are in two-cycles since all variables in m and n have the orientation (123). All two cycles contain an edge with orientation (321). This proves that the collection of two cycles in m is the same as the collection of two-cycles in n . Now it is possible to do a sequence of moves

$$\begin{bmatrix} (i_1 i_2) \\ (i_3 i_4) \end{bmatrix} \rightarrow \begin{bmatrix} (i_3 i_4) \\ (i_1 i_2) \end{bmatrix}$$

to m', n' that share a variable since any subcollection of two-cycles from m and n can be picked and moved to these variables.

CASE A.2. The variables x and y have different paths with one edge.

By symmetry, let the path on x be 12 and let the edge on y be 23. If the monomial m contains the paths 23 or 231, then the moves

$$\begin{bmatrix} 12 \\ 23 \end{bmatrix} \rightarrow \begin{bmatrix} 23 \\ 12 \end{bmatrix} \text{ or } \begin{bmatrix} 12 \\ 231 \end{bmatrix} \rightarrow \begin{bmatrix} 23 \\ 312 \end{bmatrix}$$

create a monomial m' that contains a variable x' with the same number of edges as y and the same path. This reduces to Case 1.

If m does not contain 23 or 231, then any edge 23 not in a two-cycle or a triangle is in a path 123. In particular, the 12-spin of m and n is strictly greater than the 23-spin of m and n . By a similar argument for n , the steps

$$\begin{bmatrix} 23 \\ 12 \end{bmatrix} \rightarrow \begin{bmatrix} 12 \\ 23 \end{bmatrix} \text{ or } \begin{bmatrix} 23 \\ 312 \end{bmatrix} \rightarrow \begin{bmatrix} 12 \\ 231 \end{bmatrix},$$

give either a reduction to Case 1 or that the 23-spin of n and m is greater than the 12-spin of n and m , a contradiction.

CASE A.3. The variables x and y have different two edge paths.

By symmetry, let x have the path 123 and let y have the path 231. If m contains the path 231 or n contains the path 123, then Case 1 applies after a swap of paths. If both m and n contain the path 312, then, after the moves

$$\begin{bmatrix} 123 \\ 312 \end{bmatrix} \rightarrow \begin{bmatrix} 312 \\ 123 \end{bmatrix} \text{ and } \begin{bmatrix} 231 \\ 312 \end{bmatrix} \rightarrow \begin{bmatrix} 312 \\ 231 \end{bmatrix},$$

Case 1 applies. If n contains a path 12 or m contains the path 31, then the steps

$$\begin{bmatrix} 231 \\ 12 \end{bmatrix} \rightarrow \begin{bmatrix} 123 \\ 31 \end{bmatrix} \text{ and } \begin{bmatrix} 123 \\ 31 \end{bmatrix} \rightarrow \begin{bmatrix} 231 \\ 12 \end{bmatrix}$$

reduce to Case 1.

Neither n nor m contain 312. If n contains no 312-path, then the 31-spin of n and m is strictly greater than the 12-spin of n and m while in m , all 31-edges not in two-cycles are in triangles or paths containing 12. This is a contradiction.

Similarly, if m contains no 312, then the 12-spin of m and n is strictly greater than the 31-spin of m and n while in n , all 12-edges not in two-cycles are in triangles or paths containing 31. This is also a contradiction.

CASE A.4. The variable x has no path and y has a path with two edges.

By symmetry, we can assume that y has the path 123. If m contains any variable with a path on two edges, then swapping that path to x with a two-cycle gives a reduction to Case 1 or 3. If m contains a variable with a triangle and a path with one edge, then moves of type

$$\begin{bmatrix} (i_1 i_2) \\ (ijk)ij \end{bmatrix} \rightarrow \begin{bmatrix} ijk \\ (i_1 i_2)kij \end{bmatrix}$$

give a reduction to Case 1 or 3.

If m contains a variable other than x that has a triangle with no path, then the move

$$\begin{bmatrix} (i_1 i_2) \\ (ijk) \end{bmatrix} \rightarrow \begin{bmatrix} ijk \\ (i_1 i_2)ki \end{bmatrix}$$

gives a reduction to Case 1 or 3.

The remaining case is that all variables in m except x contain no triangles and no paths of length two. If T is odd, then the other variables contain no paths and if T is even, then the other variables have paths with one edge. The variable x contains fewer edges outside two-cycles than y and the other variables in m contain the lowest possible number of edges outside two-cycles. Thus, the total spin of m and n cannot be the same, a contradiction.

CASE B. There are no variables in m and n that have the same number of variables.

By Lemma 3.5 and symmetry, we have that for some integer t : The variables in n have t or $t+2$ triangles; the variables in m have $t-1$ or $t+1$ triangles; there are variables with $t, t+1$, and $t+2$ triangles. By parity, there are two subcases: 1. The variables in m have paths with one edge; 2. The variables in y have paths with one edge.

CASE B.1. The variables in m have paths with one edge.

If all paths on the variables are the same, then this edge would get d higher spin than any other edge. This is a contradiction because the paths in n all have two edges and the edge spins are more evenly distributed. Thus, there are different paths in m . By symmetry, we can assume the paths are 12 and 23. The move

$$\begin{bmatrix} (123)12 \\ (i_1 i_2)23 \end{bmatrix} \rightarrow \begin{bmatrix} (i_1 i_2)123 \\ (123) \end{bmatrix}$$

almost gives a reduction to Case A. It is possible that the new monomial needs to be normalized first by swapping two triangles for three two-cycles, but then Case A applies. If 12 is not on a variable with a triangle to start off with, we can swap it that way.

CASE B.2. The variables in n have paths with one edge.

The same type of argument as in Case 1 applies, with m and n switched. \square

Lemma 3.7. *If m and n are normal monomials, both with paths and triangles in different orientations, and if $m - n \in I_{3,T}$, then it is possible to go from m to n using degree two steps.*

Proof. Divide into four cases: By parity of T , and whether or not m has triangles in any of the variables.

CASE A. Let T be even.

CASE A.1. There are triangles in m .

By symmetry, let the triangles in m have orientation (123). By assumption, m have a path of orientation (321), and by parity and symmetry one of these paths is 21. If a triangle has the paths 123 or 312, then the moves

$$\begin{bmatrix} 123 \\ 21 \end{bmatrix} \rightarrow \begin{bmatrix} (12) \\ 23 \end{bmatrix} \text{ or } \begin{bmatrix} 312 \\ 21 \end{bmatrix} \rightarrow \begin{bmatrix} (12) \\ 31 \end{bmatrix}$$

reduce the number of paths, contradicting normality. If there is a triangle with no path, then the move

$$\begin{bmatrix} (123) \\ 21 \end{bmatrix} \rightarrow \begin{bmatrix} (12)23 \\ 31 \end{bmatrix}$$

reduce the number of triangles, again contradicting normality. Thus, every triangle in m has the path 231. We assumed that there is a triangle in m , so the path 231 is in m . Using that path and moves similar to those above, we exclude the existence of paths 13 and 32. Furthermore, if the path 12 exists, then the move

$$\begin{bmatrix} 231 \\ 12 \end{bmatrix} \rightarrow \begin{bmatrix} 123 \\ 31 \end{bmatrix}$$

leads to a contradiction, as one of the earlier moves demonstrated.

The only paths left are 21, 23, 31, and 231. Thus, the only possible spin vectors of variables in m are $(-1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, and $(1, 2, 2)$ with $(1, 2, 2)$ and $(-1, 0, 0)$ occurring.

If n has triangles, then the same argument gives six possible sets of spin vectors, due to symmetry break. However, only one of the six have the two last coordinates positive and larger than the first coordinate and that is the same as for m . The variables m and n contain paths and triangles of the same type. To match up the spins, they have to be equally many of each type. It suffices to swap two-cycles using degree two steps.

If n does not contain triangles, then $|s_{12}(n)| + |s_{23}(n)| + |s_{31}(n)|$ is at most the degree of n . From the list of paths in m , we know that the same expression for m is larger than the degree of m , a contradiction.

CASE A.2. There are no triangles in m .

If there are triangles in n , then this is Case 1, so assume that n does not contain triangles. Using the steps

$$\begin{bmatrix} (i_1 i_2) k_1 k_2 \\ (j_1 j_2) k_2 k_1 \end{bmatrix} \rightarrow \begin{bmatrix} (i_1 i_2) j_1 j_2 \\ (k_1 k_2) j_2 j_1 \end{bmatrix} \text{ and } \begin{bmatrix} (ij) \\ (kl) \end{bmatrix} \rightarrow \begin{bmatrix} (kl) \\ (ij) \end{bmatrix}$$

we get from m to n by degree two moves.

CASE B. Let T be odd.

CASE B.1. There are triangles in m .

By symmetry, the triangles have the orientation (123) and m contains the path 321. If m contain a variable with the path 12 or 23, then the moves

$$\begin{bmatrix} 321 \\ (123)23 \end{bmatrix} \rightarrow \begin{bmatrix} 231 \\ (12)(23) \end{bmatrix} \text{ or } \begin{bmatrix} 321 \\ (123)12 \end{bmatrix} \rightarrow \begin{bmatrix} 312 \\ (12)(23) \end{bmatrix}$$

reduce the number of triangles, contradicting normality. All paths on variables with triangles have to be 31. If the paths 132 or 213 occur, then the moves

$$\begin{bmatrix} 132 \\ 31 \end{bmatrix} \rightarrow \begin{bmatrix} (13) \\ 32 \end{bmatrix} \text{ or } \begin{bmatrix} 213 \\ 31 \end{bmatrix} \rightarrow \begin{bmatrix} (13) \\ 21 \end{bmatrix}$$

reduce the number of paths, contradicting normality. All paths with orientation (321) are 321. If the path 123 occurs, then the move

$$\begin{bmatrix} 123 \\ 321 \end{bmatrix} \rightarrow \begin{bmatrix} (12) \\ (23) \end{bmatrix}$$

reduces the number of paths and contradicts normality. If there is a variable with no triangle and no path, then the move

$$\begin{bmatrix} (123)31 \\ (ij) \end{bmatrix} \rightarrow \begin{bmatrix} (ij)312 \\ 231 \end{bmatrix}$$

reduces the number of triangles, contradicting normality. The paths that occur are 321, 31, 231 and 312. Now proceed exactly as in Case A.1.

CASE B.2. There are no triangles in m .

If there are triangles in n , then this is Case 1, so assume that there are no triangles in n .

The steps

$$\begin{bmatrix} ijk \\ kji \end{bmatrix} \rightarrow \begin{bmatrix} (ij) \\ (jk) \end{bmatrix}$$

give that the monomials cannot contain both orientations of a path. If both the paths 123 and 231 are more common in m than in n , then the 23-spin cannot be equal for both monomials. Thus, there is at most one type of path in any orientation that is more common in m than in n . By symmetry, there is one path in each orientation for which the monomials m and n have an equal number. These paths have one undirected edge ij in common. The ij -spin gives that the other paths containing directed ij are equally common. Then the total spin gives that both monomials m and n have the same number of each path. The collection of paths and two-cycles are the same. In this situation swapping two-cycles is enough to go between m and n . \square

Theorem 3.8. *The three-state toric Markov chain model is generated by quadrics.*

Proof. Let m', n' be two monomials with $m' - n' \in I_{3,T}$ and let m, n be the corresponding normal monomials from Lemma 3.1. According to Lemma 3.4, either both m and n have everything oriented in the same way or they have paths and triangles oriented differently. It is possible to go between m and n by Lemma 3.6 and Lemma 3.7. \square

Remark 3.9. In the Markov moves introduced, at most 12 edges were interchanged. This shows that the Markov moves, and the generating binomials, fall into a finite number of symmetry classes.

Remark 3.10. Using computer calculations we found a monomial order and a corresponding Gröbner basis of $I_{3,4}$ consisting of quadratic binomials. These monomial orders seem very rare and this explains why these quadratic bases have not been found before. For example the weight vector

$$(3276, 2143, 272, 3760, 8497, 5589, 4947, 9850, 4347, 2483, \\ 4517, 1124, 1610, 7287, 3128, 4608, 161, 8235, 9582, 7607)$$

for the variable ordered

$$(x_{3232}, x_{2323}, x_{3231}, x_{1323}, x_{3132}, x_{2313}, x_{3131}, x_{1313}, x_{2321}, x_{2132}, \\ x_{2131}, x_{1232}, x_{1231}, x_{1312}, x_{3212}, x_{2123}, x_{3121}, x_{1213}, x_{2121}, x_{1212})$$

produce a quadratic Gröbner basis. This was checked with the software 4ti2 [1].

Example 3.11. The Markov degree of $I_{4,T}$ is in general higher than 3. For example the binomial $x_{1414}x_{2323}x_{4142}x_{4232} - x_{1423}^2x_{3232}x_{4141}$ is indispensable in $I_{4,4}$ this proves that the conjecture is false in general.

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- [1] 4ti2 team. *4ti2 – A software package for algebraic, geometric and combinatorial problems on linear spaces*. Available at www.4ti2.de.
- [2] M. Drton, B. Sturmfels, and S. Sullivant. *Lectures on algebraic statistics*. Oberwolfach Seminars, 39. *Birkhäuser Verlag, Basel*, 2009. 171 pp.
- [3] A. Engström. Cut ideals of K_4 -minor free graphs are generated by quadrics. *Michigan Math. J.* **60** (2011), no. 3, 705–714.
- [4] A. Engström, T. Kahle and S. Sullivant. Multigraded Commutative Algebra of Graph Decompositions. [arxiv:1102.2601](https://arxiv.org/abs/1102.2601), preprint 2011, 38 pp.
- [5] A. Engström and P. Norén. Ideals of Graph Homomorphisms. *Ann. Comb.*, to appear, 34 pp.
- [6] P. Diaconis and B. Sturmfels. Algebraic algorithms for sampling from conditional distributions. *Ann. Statist.* **26** (1998), No. 1, 363–397.
- [7] H. Hara and A. Takemura. A Markov basis for two-state toric homogeneous Markov chain model without initial parameters. *J. Japan Statist. Soc.* **41** (2011) 33–49.
- [8] D. Haws, A. Martin del Campo and R. Yoshida. Degree bounds for a minimal Markov basis for the three-state toric homogeneous Markov chain model, pp. 63–98, in *Harmony of Gröbner Bases and the Modern Industrial Society*, edited by T. Hibi, World Scientific, 2012, 388 pp.
- [9] D. Haws, A. Martin del Campo, A. Takemura and R. Yoshida. Markov degree of the three-state toric homogeneous Markov chain model. [arXiv:1204.3070](https://arxiv.org/abs/1204.3070), preprint 2012, 20 pp.
- [10] B. Sturmfels and S. Sullivant. Toric geometry of cuts and splits. *Michigan Math. J.* **57** (2008), 689–709.