Degree bounds for a minimal Markov basis for the three-state toric homogeneous Markov chain model

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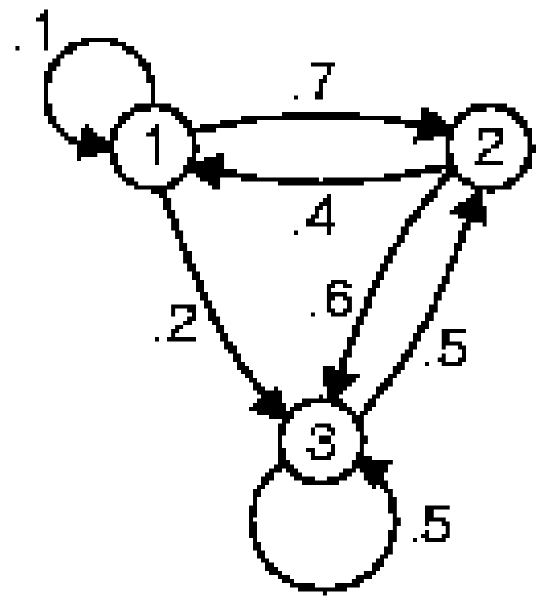
Discrete time Markov chain

we consider a discrete time Markov chain X_t, with $t = 1, \ldots, T$ $(T \geq 3)$, over a finite space of states $[S] = \{1, \ldots, S\}$.



Toric homogeneous Markov chain

Let $\mathbf{w} = (s_1, \ldots, s_T)$ be a path of length T on states $[S]$, which is sometimes written as $\omega = (s_1 \cdots s_T)$ or simply $\omega = s_1 \cdots s_T$. We are interested in Markov bases of toric ideals arising from the following statistical models

$$p(\omega) = c\gamma_{s_1}\beta_{s_1,s_2} \cdots \beta_{s_{T-1},s_T}. \tag{1}$$

where c is a normalizing constant, γ_{s_i} indicates the probability of the initial state, and β_{s_i,s_j} are the transition probabilities from state s_i to s_j. The model (1) is called a toric homogeneous Markov chain (THMC) model.

Problem We want to understand a **Markov basis** under THMC model as $T \to \infty$.

Recall Markov basis

Suppose $P = \{x \in \mathbb{R}^d | Ax = b,\ x \geq 0\} \neq \emptyset$ and let M be a finite set such that $M \subset \{x \in \mathbb{Z}^d | Ax = 0\}$.

We define the graph G_b such that:

- Nodes of G_b are all the lattice points inside of P.
- We draw an undirected edge between a node u and a node v iff $u - v \in M$.

Definition :

M is called a **Markov basis** if G_b is a connected graph for all b.

Example

				Total
	? ? ?	? ? ?	? ? ?	6
	? ? ?	? ? ?	? ? ?	6
Total	4	4	4	

Table 1: 2×3 tables with 1-marginals.

There are 19 tables with these marginals.

$\pm$

1	-1	0
-1	1	0

$\pm$

0	1	-1
0	-1	1

$\pm$

1	0	-1
-1	0	1

There are 3 elements in a Markov basis modulo signs.

4	0	2
0	4	2

+

-1	0	1
1	0	-1

=

3	0	3
1	4	1

A table with the marginals plus an element of a Markov basis is also a table with the given marginals.

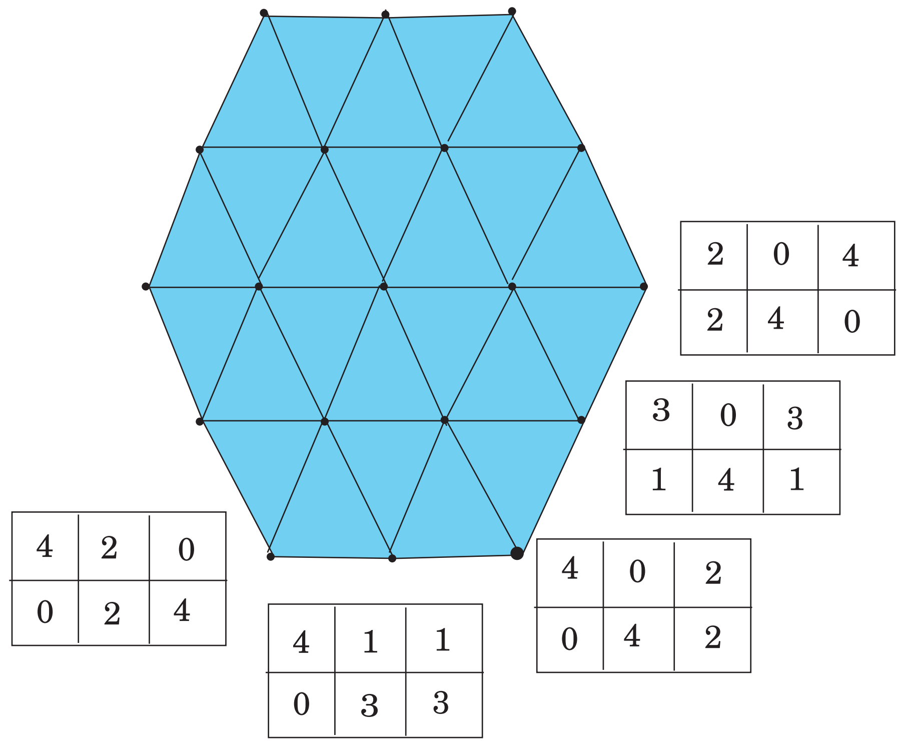


Figure 1: A Markov basis for 2×3 tables. An element of the Markov basis is a undirected edge between integral points in the polytope.

Four models

We refer to them as Model (a), Model (b), Model (c), and Model (d), according to the following:

(a) THMC model (1)

(b) THMC model without initial parameters: when $\gamma_1 = \cdots = \gamma_S$

(c) THMC model without self-loops: $\beta_{s_i,s_j} = 0$ whenever $s_i = s_j$.

(d) THMC model without initial parameters and without self-loops, i.e., both (b) and (c) are satisfied

Design matrix for Model (a)

Ordering $[S] \cup [S]^2$ and $[S]^T$ lexicographically, the matrix $A^{(a)}$ is:

	1111	1112	1121	1122	1211	1212	1221	1222	2111	2112	2121	2122	2211	2212	2221	2222
1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1
11	3	2	1	1	1	0	0	0	2	1	0	0	1	0	0	0
12	0	1	1	1	1	2	1	1	0	1	1	1	0	1	0	0
21	0	0	1	0	1	1	1	0	1	1	2	1	1	1	1	0
22	0	0	0	1	0	0	1	2	0	0	0	1	1	1	2	3

Design matrix for Model (b)

Ordering $[S]^2$ and $[S]^T$ lexicographically with $S = 2$ and $T = 4$ the matrix $A^{(b)}$ is:

	1111	1112	1121	1122	1211	1212	1221	1222	2111	2112	2121	2122	2211	2212	2221	2222
11	3	2	1	1	1	0	0	0	2	1	0	0	1	0	0	0
12	0	1	1	1	1	2	1	1	0	1	1	1	0	1	0	0
21	0	0	1	0	1	1	1	0	1	1	2	1	1	1	1	0
22	0	0	0	1	0	0	1	2	0	0	0	1	1	1	2	3

Good news

Let $P^{(d)}$ be the **design polytope** for Model (d).

Theorem Let $S = 3$. The number of vertices of $P^{(d)}$ is bounded by some constant C which does not depend on T.

Given the above theorem and our normality conjecture for Model (d), one can prove the following conjecture:

Conjecture We consider Model (d). Then for $S = 3$ and for any $T \geq 4$, a minimum Markov basis for the toric ideal $I_{A^{(d)}}$, where $A^{(d)}$ is the design matrix under Model (d), consists of binomials of degree less than or equal to $d = 6$. Moreover, there are only finitely many moves up to a certain shift equivalence relation.

Bad news

For Model (a),

Theorem The **semigroup** generated by the columns of the design matrix $A^{(a)}$ is not normal for $S \geq 3$ and $T \geq 4$.

For Model (b),

Theorem The semigroup generated by the columns of the design matrix $A^{(b)}$ is not normal for $S \geq 2$ and $T \geq 3$.

So it is very hard to understand a Markov basis for $T \to \infty$.

We also think the semigroup generated by the columns of the design matrix $A^{(b)}$ is not normal for $S = 3$ and $T \geq 4$. But no proof.

Actually we are very close

For Model (d) with $S = 3$ we can go a bit further.

A. Takemura, D. Haws, A. Martín del Campo, and I are still working on this more. Now we have an explicit hypoer plane representations of the design polytope $P^{(d)}$. Also from using this representation we "think" we can show the normality of the semigroup generated by the columns of the design matrix $A^{(d)}$.

By computation $(d \leq 120)$ we can show that the semigroup generated by the columns of the design matrix $A^{(d)}$ is normal.

“Conjecture”

Using Theorem 13.14 in [Sturmfels 1996].

Theorem 13.14 in [Sturmfels 1996] Let $A \subset \mathbb{Z}^d$ be a graded set such that the semigroup generated by the elements in A is normal. Then the toric ideal I_A associate with the set A is generated by homogeneous binomials of degree at most d.

Using this theorem and our “conjecture” we can show that

Conjecture We consider Model (d). Then for $S = 3$ and for any $T \geq 4$, a Markov basis for the toric ideal $I_{A^{(d)}}$ consists of binomials of degree less than or equal to $d = 6$. Moreover, there are only finitely many moves up to a certain shift equivalence relation.

Big conjecture

On the experimentations we ran, we found evidence that more should be true.

Conjecture Fix $S \geq 3$; then, for every $T \geq 4$, there is a Markov basis for the toric ideal $I_{A^{(d)}}$ consisting of binomials of degree at most $S-1$, and there is a Gröbner basis with respect to some term ordering consisting of binomials of degree at most S.

Despite the computational limitations (the number of generators grows exponentially when T grows,) we were able to test this conjecture using the software `4ti2` for $T = 4, 5, 6$ with $S = 3$ and $T = 4, 5$ with $S = 4$.

Question??

For downloading our paper please go to

`http://arxiv.org/abs/1108.0481`.

Thank you!