RAPID MIXING AND MARKOV BASES

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ABSTRACT. The mixing behaviour of random walks on lattice points of polytopes using Markov bases is examined. It is shown that under a dilation of the underlying polytope, these random walks do not mix rapidly when a fixed Markov basis is used. We also show that this phenomenon does not disappear after adding more moves to the Markov basis. Avoiding rejections by sampling applicable moves does also not lead to an asymptotic improvement. As a way out, a method of how to adapt Markov bases in order to achieve the fastest mixing behaviour is introduced.

1. Introduction

Random walks have been successfully used in various applications to explore combinatorial structures where a complete enumeration is computationally prohibitive [17, 21, 9]. In many of these applications, the underlying discrete objects correspond to the elements of a fiber $F_{A,b} := \{u \in \mathbb{N}^d : Au = b\}$ of a matrix $A \in \mathbb{Z}^{m \times d}$ with $\ker(\mathbb{Z}(A)) \cap \mathbb{N}^d = \{0\}$ and a right-hand side $b \in \mathbb{Z}^m$. The exploration of fibers with random walks requires to connect their elements by edges so that there is a path between any two of them. In their groundbreaking work [9], Diaconis and Sturmfels have shown how to endow $F_{A,b}$ with the structure of a connected graph in a computational way: For a finite set $M \subset \ker(\mathbb{Z}(A))$, the fiber graph $F_{A,b}(M)$ is the graph on $F_{A,b}$ in which two nodes $u, v \in F_{A,b}$ are adjacent if $u - v \in \pm M$. They have coined the term Markov basis, which denotes a finite set $M \subset \ker(\mathbb{Z}(A))$ such that $F_{A,b}(M)$ is connected for all $b \in \mathbb{Z}^m$. Their main result shows that a Markov basis can be obtained by a Gröbner basis computation in a polynomial ring [9, Theorem 3.1]. Markov bases can be used to enumerate locally the neighborhood of a node in the fiber graph, which makes them a general machinery to approximate any probability distribution on any fiber of a matrix. The number of steps needed to approximate a given distribution sufficiently is the mixing time of the random walk. Even though the computation of Markov bases received a lot of attention in the last decade [14, 18, 30, 28, 29], mixing results on fiber graphs are still rare. It was shown in [6] that the mixing time of random walks on two-way contingency tables with the same row and column sums using a minimal Markov basis is quadratic in the diameter of the underlying fiber graph and a similar result is true...
for random walks on lattice points of polytopes that use the unit vectors as Markov basis vectors [7, 33].

In this paper, we study the mixing behaviour of the simple walk on fiber graphs, whose stationary distribution is the uniform distribution on \( \mathcal{F}_{A,b} \). Our main result concerns the mixing behaviour of fiber graph sequences that use a fixed Markov basis:

**Theorem 1.1.** Let \( A \in \mathbb{Z}^{m \times d} \), let \( \mathcal{M} \subset \ker_{\mathbb{Z}}(A) \) be a Markov basis for \( A \), and let \((b_i)_{i \in \mathbb{N}}\) a dominated sequence in \( \mathbb{N}A \). Then \((\mathcal{F}_{A,b_i}(\mathcal{M}))_{i \in \mathbb{N}}\) is no expander. If additionally \((b_i)_{i \in \mathbb{N}}\) has a meaningful parametrization, then \((\mathcal{F}_{A,b_i}(\mathcal{M}))_{i \in \mathbb{N}}\) is not rapidly mixing.

Surprisingly, walking randomly on a fiber with a larger Markov basis (Remark 3.24) or avoiding rejections by sampling only applicable moves (Remark 3.27) does not improve the asymptotic mixing behaviour. The conclusion we draw from these results is that an adaption of the Markov basis has to take place depending on the right-hand side \( b \in \mathbb{Z}^m \). In Section 4, we adapt the Markov basis so that the underlying graph becomes the complete graph with additional loops. Adding more moves to a Markov basis increases the rejection rate, i.e. the number of loops, on every node of the fiber. Thus, it is a fine line to find the proper number of moves to add without slowing down the random walk. The fastest mixing behaviour is obtained for expander graphs [16] and we show how to obtain expanders on fibers under mild assumptions on the diameter (Corollary 4.3). The idea of constructing expanders on fiber is due to Alexander Engström who used the zig-zag product to obtain expanders [13]. Our method is different and yields for fixed \( n \in \mathbb{N} \) an expanding family for \( n \times n \) contingency tables where all row and column sums are equal. Our adapted Markov basis can become arbitrarily large and a priori it is not easy to draw a move from it uniformly at random. It remains an interesting problem – both from a combinatorial and statistical side – to understand the structure of the adapted Markov basis and how one can draw from it efficiently.

**Conventions and Notation.** The natural numbers are \( \mathbb{N} := \{0, 1, 2, \ldots\} \). For any \( n \in \mathbb{N} \), we set \([n] := \{m \in \mathbb{N} : 1 \leq m \leq n\}\) and we use \( \mathbb{N}_{>n} \) and \( \mathbb{N}_{\geq n} \) to denote the subsets of \( \mathbb{N} \) whose elements are strictly greater and greater than \( n \) respectively. A graph is always undirected and can multiple loops. Let \( G = (V, E) \) be a graph. If there is \( d \in \mathbb{N} \) such that all the nodes of \( G \) are incident to \( d \) edges, then \( G \) is \( d \)-regular. The distance \( d_G(v, w) \) of two nodes \( v, w \in V \) is the number of edges in a shortest path connecting \( v \) and \( w \). The diameter \( \text{diam}(G) \) of \( G \) is the maximal distance that appears between any pair of its nodes. Here, it is assumed that all fiber-defining matrices \( A \in \mathbb{Z}^{m \times d} \) fulfill \( \ker_{\mathbb{Z}}(A) \cap \mathbb{N}^d = \{0\} \). The affine semigroup in \( \mathbb{Z}^m \) generated by the column vectors of \( A \) is denoted by \( \mathbb{N}A \). Let \((a_i)_{i \in \mathbb{N}}\) and \((b_i)_{i \in \mathbb{N}}\) be two sequences in \( \mathbb{Q} \), then \((a_i)_{i \in \mathbb{N}} \in \mathbb{O}(b_i)_{i \in \mathbb{N}}\) if there exist \( i_0 \in \mathbb{N} \) and \( C \in \mathbb{Q}_{>0} \) such that \( |a_i| \leq C \cdot |b_i| \) for all \( i \geq i_0 \). Similarly, we define \((a_i)_{i \in \mathbb{N}} \in \mathbb{Q}(b_i)_{i \in \mathbb{N}}\) if there exist \( i_0 \in \mathbb{N} \) and \( C \in \mathbb{Q}_{>0} \) such that \( |a_i| \geq C \cdot |b_i| \) for all \( i \geq i_0 \). The sequence \((a_i)_{i \in \mathbb{N}}\) is a subsequence of \((b_i)_{i \in \mathbb{N}}\) if there is a strongly increasing sequence \((i_k)_{k \in \mathbb{N}}\) in \( \mathbb{N} \) such that \( a_{i_k} = b_k \) for all \( k \in \mathbb{N} \).
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2. Markov chains on fiber graphs

Let $G = (V, E)$ be an undirected graph with $V = \{v_1, \ldots, v_n\}$. For $v_i, v_j \in V$, let $A^G_{ij}$ be the number of edges in $E$ with endpoints $v_i$ and $v_j$, then the matrix $A^G \in \mathbb{N}_{\geq 0}^{n \times n}$ is the adjacency matrix of $G$. For $v \in V$, let $\deg_G(v)$ be the number of edges incident to $v$ in $G$. The simple walk on $G$ has transition probabilities

$$S^G_{ij} = \begin{cases} \frac{A^G_{ij}}{\deg_G(v)}, & \text{if } \{v_i, v_j\} \in E \\ 0, & \text{otherwise} \end{cases}.$$

The simple walk on $G$ comes along with a discrete-time Markov chain whose state space is the node set $V$ of the graph [3]. Let $\pi_0 \in [0,1]^n$ be an initial distribution on $V$. For any $t \in \mathbb{N}$, let $\pi_t := \pi_0 \cdot (S^G)^t \in [0,1]^n$, then $\pi_t(i)$ is the probability that the simple walk with initial distribution $\pi_0$ is at $v_i$ at time $t$. The Markov chain on $G$ is aperiodic if for all $i \in [n]$, $\gcd\{t \in \mathbb{N}_{>0} : (S^G)^t_{i,i} > 0\} = 1$, symmetric if $S^G$ is symmetric, and irreducible if for all $i, j \in [n]$ there exists $t \in \mathbb{N}$ such that $(S^G)^t_{i,j} > 0$. An aperiodic and irreducible Markov chain converges towards a unique stationary distribution $\pi \in [0,1]^n$ [20, Theorem 4.9] and the second largest eigenvalue modulus (SLEM) $\lambda$ of $S^G$, is a measurement of the convergence rate [16, Section 3]: $(\|\pi_t - \pi\|)_{t \in \mathbb{N}} \in O(\lambda^t)_{t \in \mathbb{N}}$.

Remark 2.1. If $G$ is $d$-regular, then $S^G = \frac{1}{d} A^G$ and hence $S^G$ is symmetric. If $G$ is also connected, then the simple walk is irreducible and converges towards the uniform distribution $\pi = \frac{1}{|V|} \cdot (1, \ldots, 1)^T \in [0,1]^{|V|}$ on $V$.

The closer the second largest eigenvalue of a random walk is to 1, the slower the convergence to its stationary distribution. The next definition states under which conditions we still have a polynomial bound on the mixing time.

Definition 2.2. For any $i \in \mathbb{N}$, let $G_i = (V_i, E_i)$ be a graph and let $\lambda_i$ be the second largest eigenvalue modulus of $S^{G_i}$. The sequence $(G_i)_{i \in \mathbb{N}}$ is rapidly mixing if there is a polynomial $p \in \mathbb{Q}_{\geq 0}[t]$ such that for all $i \in \mathbb{N}$, $\lambda_i \leq 1 - \frac{1}{p(\log |V_i|)}$. The sequence $(G_i)_{i \in \mathbb{N}}$ is an expander if there exists $\epsilon > 0$ such that for all $i \in \mathbb{N}$, $\lambda_i \leq 1 - \epsilon$.

Expander graphs are highly demanded in computer science because of their good mixing behaviour. Their name relates to the fact that their edge-expansion (Definition 3.6) can strictly bounded away from zero (Proposition 3.8). The mixing time of
rapidly mixing Markov chains can be bounded by a polynomial in the logarithm of the size of the state space (see [25, Section 2.3] or [3, Section 1.1.2]) and thus only logarithmically many nodes have to be visited by the random walk to converge. The key player of this paper is the simple walk on the following type of graph:

**Definition 2.3.** Let \( F, M \subset \mathbb{Z}^d \) be finite sets. The fiber graph \( F(M) \) is the graph on \( F \) where two nodes \( u, v \in F \) are adjacent if \( u - v \in \pm M \) and where every node \( w \in F \) gets a loop for every \( m \in \pm M \) that satisfies \( w + m \notin F \).

Recall that graphs can have multiple loops. The edges incident to a node \( v \in F \) correspond precisely to elements in \( \pm M \) and thus the graph \( F(M) \) is \( |\pm M| \)-regular. If \( 0 \in M \), then \( v - v \in \pm M \) and thus every node has at least one loop. In order to run irreducible Markov chains on fiber graphs, these graphs have to be connected.

**Definition 2.4.** Let \( F, M \subset \mathbb{Z}^d \) be finite sets, then \( M \) is a Markov basis for \( F \) if the graph \( F(M) \) is connected. Let \( I \) be a set of indices, \( d_i \in \mathbb{N} \) be natural numbers and \( F_i \subset \mathbb{Z}^{d_i} \) and \( M_i \subset \mathbb{Z}^{d_i} \) be finite sets for any \( i \in I \). A sequence \( (M_i)_{i \in I} \) is a Markov basis for \( (F_i)_{i \in I} \) if \( M_i \) is a Markov basis for \( F_i \) for all \( i \in I \). A finite set \( M \subset \mathbb{Z}^d \) is a Markov basis for \( F \) if \( F_i \subset \mathbb{Z}^d \) if \( (M_i)_{i \in \mathbb{N}} \) is a Markov basis for \( (F_i)_{i \in \mathbb{N}} \).

In many applications, \( F \subset \mathbb{Z}^d \) is given implicit by \( \mathbb{Z} \)-linear equations and inequalities and thus its complete structure is unfeasible. In algebraic statistics for instance, \( F \) equals \( F_{A,b} \) for a matrix \( A \in \mathbb{Z}^{m \times d} \) and a right-hand side \( b \in \mathbb{Z}^m \) [10]. Note that our general assumption \( \ker_\mathbb{Z}(A) \cap \mathbb{N}^d = \{0\} \) makes \( F_{A,b} \) finite for all \( b \in \mathbb{N}A \). We thus call a set \( M \subset \mathbb{Z} \) a Markov basis for \( A \) if \( M \) is a Markov basis for \( (F_{A,b})_{b \in \mathbb{N}A} \). If one can efficiently verify whether \( v \in \mathbb{Z}^d \) is contained in \( F \) or not, as for \( F = F_{A,b} \), then it is possible to explore \( F \) with the simple walk using \( M \) as follows: At a given node \( v \in F \), select uniformly an element \( m \in \pm M \) and walk along the edge given by \( m \in \mathbb{N} \), which either points to \( v \) or to a different node \( v \neq v + m \in F \).

**Lemma 2.5.** Let \( F \subset \mathbb{Z}^d \) be a finite and non-empty set and \( M \subset \mathbb{Z}^d \) a Markov basis for \( F \). The simple walk on \( F(M) \) is irreducible, aperiodic, symmetric, reversible, and its stationary distribution is the uniform distribution on \( F \).

**Proof.** The random walk is irreducible and symmetric since \( F(M) \) is connected and \( |\pm M| \)-regular (Remark 2.1). Thus, it suffices to show that \( F(M) \) has one aperiodic state to show that all states are aperiodic. Choose \( v \in F \) and \( m \in M \) arbitrarily. Since \( F \) is finite, let \( \mu \in \mathbb{N} \) be the largest natural number such that \( v + \mu m \in F \). Then \( m \) cannot be applied on \( v + \mu m \) and thus \( v + \mu m \) has a loop. The reversibility follows immediately and since the transition matrix of the simple walk is symmetric, the uniform distribution is the unique stationary distribution. \( \square \)

**Remark 2.6.** The Metropolis-Hastings-methodology allows to modify the simple walk so that it converges to any given probability distribution on \( F \) [20, Section 3].
3. Expanding in fixed dimension

Let \( A \in \mathbb{Z}^{m \times d} \) and \( \mathcal{M} \subset \ker_{\mathbb{Z}}(A) \) be a Markov basis for \( A \). In this section, we study the mixing behaviour of \((\mathcal{F}_{A,b_i}(\mathcal{M}))_{i \in \mathbb{N}}\) for sequences \((b_i)_{i \in \mathbb{N}}\) in \( NA \) that are almost rays (Definition 3.2). Roughly speaking, our strategy is to show that the sequence of second largest eigenvalues \((\lambda_i)_{i \in \mathbb{N}}\) of this graph sequence satisfies \( \lambda_i \geq 1 - \frac{C}{i} \) for a constant \( C \in \mathbb{Q}_{>0} \) and sufficiently many \( i \in \mathbb{N} \). This leads, together with an assumption on the growth of the fiber (Definition 3.17), to a slow mixing result (Theorem 1.1). Our proof uses the well-known connection between the second largest eigenvalue modulus of the simple walk and the edge-expansion of the underlying graph (Proposition 3.8). Thus, our goal is to bound the edge-expansion of \((\mathcal{F}_{A,b_i}(\mathcal{M}))_{i \in \mathbb{N}}\) from above appropriately.

Here, we use a particular property of \((b_i)_{i \in \mathbb{N}}\), namely that we can translate a smaller fiber into a larger fiber \( u + \mathcal{F}_{A,b_i} \subseteq \mathcal{F}_{A,b_j} \). It is then left to count the number of Markov moves that leave the subset \( u + \mathcal{F}_{A,b_i} \) in \( \mathcal{F}_{A,b_j}(\mathcal{M}) \), which is done by Lemma 3.11 and Ehrhart’s theory. To start with, let us make precise the properties of sequences in \( NA \) that are crucial in the proof of Theorem 1.1.

**Definition 3.1.** Let \( A \in \mathbb{Z}^{m \times d} \) and let \((b_i)_{i \in \mathbb{N}}\) be a sequence in \( NA \). The sequence \((b_i)_{i \in \mathbb{N}}\) is a *ray* in \( NA \) if there is \( b \in NA \) such that \((b_i)_{i \in \mathbb{N}} = (i \cdot b)_{i \in \mathbb{N}}\).

We need the following terminology for our next definition: For \( b \in NA \), the \( \mathbb{Q} \)-relaxation of \( \mathcal{F}_{A,b} \) is the polytope \( \mathcal{R}_{A,b} := \{ x \in \mathbb{Q}^d_{\geq 0} : Ax = b \} \).

**Definition 3.2.** Let \( A \in \mathbb{Z}^{m \times d} \). A sequence \((b_i)_{i \in \mathbb{N}}\) is *dominated* if there exists \( b \in NA \) with \( \dim(\mathcal{R}_{A,b}) > 0 \) such that \( b_i - i \cdot b \in NA \) for all \( i \in \mathbb{N} \) and if there is \( u \in \mathcal{F}_{A,b} \) and \( w_i \in \mathcal{F}_{A,b_i - i \cdot b} \) with \( \text{supp}(w_i) \subseteq \text{supp}(u) \) for all \( i \in \mathbb{N} \).

On the one hand, being dominated is a sufficient, though technical, condition on \((b_i)_{i \in \mathbb{N}}\) that is crucial in our proof of the asymptotic growth of the second largest eigenvalue modulus of \((\mathcal{F}_{A,b_i}(\mathcal{M}))_{i \in \mathbb{N}}\). The prime example of a dominated sequence the reader should have in mind is a ray in the semigroup \( NA \):

**Remark 3.3.** The ray \((i \cdot b)_{i \in \mathbb{N}}\) with \( b \in NA \) and \( \dim(\mathcal{R}_{A,b}) > 0 \) is dominated by \( b \).

Dominated sequences appear, for instance, as subsequence of sequences whose distance to the facets of \( NA \) becomes arbitrarily large. Let \( H_A(b) := \min\{\text{dist}(b,F) : F \text{ facet of } NA\} \), where \( \text{dist}(b,F) \in \mathbb{Q}_{\geq 0} \) denotes the distance between \( b \) and \( F \subseteq NA \).

**Proposition 3.4.** Let \( A \in \mathbb{Z}^{m \times d} \) with non-trivial kernel. Let \((b_i)_{i \in \mathbb{N}}\) be a sequence in \( NA \) with \( \lim \sup_{i \in \mathbb{N}} H_A(b_i) = \infty \), then \((b_i)_{i \in \mathbb{N}}\) has a dominated subsequence.

**Proof.** Let \( a_1, \ldots, a_d \in \mathbb{Z}^m \) be the columns of \( A \) and let \( c := a_1 + \cdots + a_d \). First, we show the following: For every \( k \in \mathbb{N} \) there exists \( m_k \in \mathbb{N} \), such that any \( b \in NA \) with \( H_A(b) \geq m_k \) is contained in \( k \cdot c + NA \). The set \( NA \setminus (k \cdot c + NA) \) is contained in finitely many hyperplanes parallel to the facets of \( NA \). Hence, choosing \( m_k \in \mathbb{N} \) large enough, every \( b \in NA \) with \( H_A(b) \geq m_k \) cannot be in \( NA \setminus (k \cdot c + NA) \). The
statement of the lemma follows immediately because \( \limsup_{i \in \mathbb{N}} H_A(b_i) = \infty \) implies that there is \( i_k \in \mathbb{N} \) such that \( H_A(b_i) \geq m_k \). Hence, for all \( k \in \mathbb{N} \), \( b_{i_k} \in k \cdot c + NA \). In particular, \( (b_{i_k})_{k \in \mathbb{N}} \) is dominated by \( c \) since \( F_{A,c} \) has an element with full support and since \( \dim(R_{A,c}) = \dim(\ker_Z(A)) > 0 \). \( \square \)

**Remark 3.5.** The reverse of Proposition 3.4 is not true. For instance, take the matrix

\[
A = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\]

and \( b = (2, 0)^T \in \mathbb{Z}^2 \). The ray \((i \cdot b)_{i \in \mathbb{N}}\) is dominated since \( \dim(R_{A,b}) > 0 \). However, since \( \{i \cdot b : i \in \mathbb{N}\} \) is contained in a facet of \( NA \), \( H_A(i \cdot b) = 0 \) for all \( i \in \mathbb{N} \).

To put hands on the second largest eigenvalue of the simple walk, we use the following connecting piece between statistics and combinatorics.

**Definition 3.6.** Let \( G = (V, E) \) be a graph and \( S \subseteq V \). Then \( E_G(S) \subseteq E \) denotes the set of all edges with endpoints in \( S \) and \( V \setminus S \). The edge-expansion of \( G \) is

\[
h(G) := \min \left\{ \frac{|E_G(S)|}{|S|} : S \subset V, 0 < 2|S| \leq |V| \right\}. \]

**Remark 3.7.** The invariant \( h(G) \) has many names in the literature, like **Cheeger constant** [4] or **isoperimetric number** [22]. Also, the conductance \( \Phi \) of the simple walk on a \( d \)-regular graph \( G \) fulfills \( \Phi \cdot d = h(G) \) [26].

**Proposition 3.8.** Let \( G = (V, E) \) be a connected and \( d \)-regular graph and let \( \lambda \) be the second largest eigenvalue modulus of \( S^G \), then \( \lambda \geq 1 - \frac{2}{d} \cdot h(G) \).

**Proof.** This is [16, Theorem 4.11]. \( \square \)

**Example 3.9.** For any \( d \in \mathbb{N} \), let \( A_d = (1, \ldots, 1) \in \mathbb{Z}^{1 \times d} \) and let \( e_k \in \mathbb{Z}^d \) be the \( k \)-th unit vector of \( \mathbb{Z}^d \), then the set \( M_d := \{e_1 - e_k : 2 \leq k \leq d\} \) is a Markov basis for \( A_d \). The graph \( F_{A_{2,i}}(M_2) \) is isomorphic to the path graph on \([i + 1]\) for any \( i \in \mathbb{N} \) and hence its edge-expansion is \( \frac{2}{i + 1} \) if \( i \) is odd and \( \frac{2}{i} \) when \( i \) is even [22, Section 2]. Since \( |\pm M_2| = 2 \), the second largest eigenvalue modulus \( \lambda_i \) of the simple walk on \( F_{A_{2,i}}(M_2) \) satisfies \( \lambda_i \geq 1 - \frac{1}{i} \) by Proposition 3.8. Hence, the sequence \( (F_{A_{2,i}}(M_2))_{i \in \mathbb{N}} \) is neither an expander and because of \( \log |F_{A_{2,i}}| = \log(i + 1) \) nor rapidly mixing.

The edge-expansion of a graph can be bounded from above by dividing the number of edges leaving a fixed subset by the size of this particular subset. For certain subsets of fibers, it is possible to give a description of the nodes that are incident to edges which leave this set. Intuitively, those nodes lie on the **boundary** of this set.

**Definition 3.10.** Let \( A \in \mathbb{Z}^{m \times d} \), \( b \in NA \), and \( M \subset \ker_Z(A) \). For \( u \in \mathbb{N}^d \), the \( u \)-boundary of \( F_{A,b} \) is \( \partial^u_M(F_{A,b}) := \{v \in u + F_{A,b} : \exists m \in \pm M : v + m \in \mathbb{N}^d \setminus (u + F_{A,b})\} \).
Figure 1. Let $A_3$ be as in Example 3.9. The white points represent the nodes of the sets $\partial^{(3,0,0)^T}_{M_3}(F_{A_3,3})$, $\partial^{(3,0,0)^T}_{M_3\cup M_3}(F_{A_3,3})$, and $\partial^{(1,1,1)^T}_{M_3}(F_{A_3,3})$ in $F_{A_3,6}$ (from left to right).

Figure 1 justifies in a way that $\partial^u_M(F_{A,b})$ can indeed be regarded as a boundary. With this, the number of outgoing edges in a translated fiber $u + F_{A,b}$ within a larger fiber can be bounded from above:

**Lemma 3.11.** Let $A \in \mathbb{Z}^{m \times d}$ and $b, b' \in \mathbb{N}^A$ with $2|F_{A,b}| \leq |F_{A,b'+b}|$. Then for any finite set $\mathcal{M} \subset \ker Z(A)$ and all $u \in F_{A,b}$,

$$h(F_{A,b'+b}(\mathcal{M})) \leq \frac{2|M| \cdot |\partial^u_M(F_{A,b})|}{|F_{A,b}|}.$$ 

**Proof.** By assumption, $u + F_{A,b} \subset F_{A,b'+b}$ and since $2|u + F_{A,b}| = 2|F_{A,b}| \leq |F_{A,b'+b}|$,

$$h(F_{A,b'+b}(\mathcal{M})) \leq \frac{|E_{F_{A,b'+b}(\mathcal{M})}(u + F_{A,b})|}{|u + F_{A,b}|}.$$ 

The edges leaving the set $u + F_{A,b}$ in $F_{A,b'+b}(\mathcal{M}) \subset \mathbb{N}^d$ are precisely those with endpoints in $\partial^u_M(F_{A,b})$. Every node of $F_{A,b'+b}(\mathcal{M})$ has at most $|\pm \mathcal{M}|$ incident edges and hence $|E_{F_{A,b'+b}(\mathcal{M})}(u + F_{A,b})|$ is bounded from above by $2|M| \cdot |\partial^u_M(F_{A,b})|$. \qed

The size of the entries in a Markov basis is crucial to determine the size of the boundary. The larger those entries are, the more nodes are in the boundary (Lemma 3.13) since more nodes in the shifted fiber $u + F_{A,b}$ are adjacent to nodes outside of $u + F_{A,b}$. The next definition should not be mixed up with the Markov complexity [24].

**Definition 3.12.** The complexity of a finite set $\mathcal{M} \subset \mathbb{Z}^d$ is $C(\mathcal{M}) := \max_{m \in \mathcal{M}} \|m\|_{\infty}$.

**Lemma 3.13.** Let $A \in \mathbb{Z}^{m \times d}$, let $\mathcal{M} \subset \ker Z(A)$ be a finite set, and let $b \in \mathbb{N}^A$. Then for all $u \in \mathbb{N}^d$,

$$\partial^u_M(F_{A,b}) \subseteq u + \bigcup_{j \in \text{supp}(u)} \bigcup_{r=0}^{C(\mathcal{M})} \{w \in F_{A,b} : w_j = r\}.$$
Proof. Let \( v \in \partial_M(\mathcal{F}_{A,b}) \), then there is \( m \in \pm \mathcal{M} \) such that \( v + m \in \mathbb{N}^d \), but \( v + m \not\in u + \mathcal{F}_{A,b} \). Since \( v \in u + \mathcal{F}_{A,b} \), there is \( w \in \mathcal{F}_{A,b} \) such that \( v = u + w \). The vector \( w + m \) must have a negative entry, since otherwise \( w + m \in \mathbb{N}^d \), that is \( w + m \in \mathcal{F}_{A,b} \) which implies \( v + m = u + w + m \in u + \mathcal{F}_{A,b} \). Hence, there is \( j \in [d] \) such that \((w + m)_j < 0\). Suppose \( j \notin \text{supp}(u) \). Then \((u + w + m)_j = (w + m)_j < 0\), which contradicts \( u + w + m = v + m \in \mathbb{N}^d \). Thus, \( j \in \text{supp}(u) \) and \( w_j < -m_j \). Since that means \( w_r \leq C(\mathcal{M}) \), the statement follows.

Lemma 3.11 allows to measure edge-expansion by essentially comparing the growth of fibers with the growth of their boundary. The idea is to show that the boundary grows asymptotically slower than the fiber itself. Counting the number of integer points in a polytope is the subject of Ehrhart theory [12]. Let \( P \subset \mathbb{Q}^d \) be a polytope and consider the map \( L_P : \mathbb{N} \to \mathbb{N} \) which counts the integer points in the \( i \)-th dilation \( iP := \{i \cdot x \in \mathbb{Q}^d : x \in P\} \), i.e.

\[
L_P(i) := |(iP) \cap \mathbb{Z}^d|.
\]

According to Ehrhart’s theorem (cf. [2, Theorem 3.23]), \( L_P \) is a quasi-polynomial of degree \( r := \dim(P) \), that is there exist periodic functions \( c_0, \ldots, c_r : \mathbb{N} \to \mathbb{Z} \) with integral periods such that

\[
L_P(t) = c_r(t)t^r + c_{r-1}(t)t^{r-1} + \ldots + c_0(t)
\]

with \( c_r \) not identically zero. Here, the dimension of a set is the dimension of its affine space. This applies to rays in affine semigroups: Since for any \( i \in \mathbb{N} \), the integer points of \( \mathcal{R}_{A,ib} \) are precisely the elements of \( \mathcal{F}_{A,ib} \), \( L_{\mathcal{R}_{A,ib}}(i) = |\mathcal{F}_{A,ib}| \) for all \( i \in \mathbb{N} \) and hence \( |\mathcal{F}_{A,ib}| \) grows in \( i \) (quasi-)polynomial of degree \( \dim(\mathcal{R}_{A,ib}) \).

Remark 3.14. For any integer matrix \( A \) and \( b \in \mathbb{N}A \), \( \dim(\mathcal{R}_{A,b}) \geq \dim(\mathcal{F}_{A,b}) \). In particular, if \( \dim(\mathcal{F}_{A,b}) > 0 \), then \(|\mathcal{F}_{A,ib}|_{i \in \mathbb{N}}\) is unbounded. If \( A \) is totally unimodular, then \( \mathcal{R}_{A,b} = \text{conv}(\mathcal{F}_{A,b}) \) and hence the dimensions of \( \mathcal{R}_{A,b} \) and \( \mathcal{F}_{A,b} \) coincide.

The sets appearing in Lemma 3.13 are not precisely dilates of polytopes and Ehrhart theory does not apply directly. Nevertheless, their growth can be bounded as well in terms of their dimension.

Lemma 3.15. Let \( A \in \mathbb{Z}^{m \times d} \), \( b \in \mathbb{Z}^m \), and fix integers \( j \in [d] \) and \( l \in \mathbb{N} \). If for all \( i \in \mathbb{N}_{>0} \), \( \mathcal{R}_{A,ib} \) is not completely contained in the hyperplane \( H := \{x \in \mathbb{Q}^d : x_j = l\} \), then there is \( C \in \mathbb{N} \) such that the number of integer points in \( \mathcal{R}_{A,ib} \cap H \) is bounded from above by \( C \cdot i^{\dim(\mathcal{R}_{A,ib})-1} \).

Proof. Write \( P := \mathcal{R}_{A,b} \) and \( r := \dim(P) \). For \( i \) large enough, the dimension of \((iP) \cap H\) stabilizes, i.e. there are \( r', N \in \mathbb{N} \) such that \( r' := \dim(iP \cap H) \) for all \( i \geq N \). The affine space of \( iP \cap H \) is completely contained in \( H \) whereas the affine space of \( iP \) has elements outside of \( H \). That implies \( r' < r \). Let \( A = (a_1, \ldots, a_d) \) and \( A' \) be
submatrix of $A$ omitting the $j$-th column, then the (bijective) projection of $iP \cap H$ onto all coordinates different from $j$ is

$$Q_i := \{ x \in \mathbb{Q}^{d-1} : A'x = ib - la_j \}.$$  

By [32, Proposition 1], there exists finitely many sets $C_1, \ldots, C_k$ covering $\mathbb{N}$ such that for $i \in C_j$, the number of integer points in $Q_i$ is a quasi-polynomial of degree at most $r'$. □

Lemma 3.16. Let $p(t) = \sum_{s=0}^{r} c_s(t)t^s$ be a quasi-polynomial of degree $r > 0$ and let $k \in \mathbb{N}$ such that $c_r(k) > 0$. There exists $n \in \mathbb{N}_{>0}$ and $N \in \mathbb{N}$ such that for all $i \in k+n \cdot N$ with $i \geq N$, $2p(i) < p(i+ni)$.

Proof. Let $n \geq 2$ such that $c_r(i+ni) = c_r(i)$ for all $i \in \mathbb{N}$ (i.e. if $c_r$ is not a constant, let $n \geq 2$ be the period of $c_r$). For all $i \in k+n \cdot N$, $c_r(i+ni) = c_r(i) = c_r(k) > 0$ and

$$p(i+ni) - 2 \cdot p(i) = c_r(k) ((1+n)^r - 2) i^r + \sum_{s=0}^{r-1} (c_s(i+ni)(1+n)^s - 2c_s(i)) i^s.$$  

The sum in the term on the right-hand side of this equation is a quasi-polynomial of degree at most $r-1$ and the left term on the right-hand side is a polynomial of degree $r > 0$ whose leading coefficient is positive due to $n \geq 2$ and $r > 0$. Thus, there is $N \in \mathbb{N}$ such that for all $i \in k+n \cdot N$ with $i \geq N$,

$$c_r(k) ((1+n)^r - 2) i^r > -\sum_{s=0}^{r-1} (c_s(i+in)(1+n)^s - 2c_s(k)) i^s,$$

that is $2p(i) < p(i+ni)$.

The growth of the state space needs to be compared with the growth of the second largest eigenvalue modulus to disprove rapid mixing, as demonstrated in Example 3.9. With the following property of a sequences $(b_i)_{i \in \mathbb{N}}$ in $\mathbb{N}A$, however, a lower bound the second largest eigenvalue in terms of the parameter $(i)_{i \in \mathbb{N}}$ instead of $(|F_{A,b_i}|)_{i \in \mathbb{N}}$ suffices:

Definition 3.17. A sequence $(b_i)_{i \in \mathbb{N}}$ in $\mathbb{N}A$ has a meaningful parametrization if there exists a polynomial $q \in \mathbb{Q}[t]$ such that $|F_{A,b_i}| \leq q(i)$ for all $i \in \mathbb{N}$.

Example 3.18. Consider $A_2$ from Example 3.9, then $|F_{A_2,b_i}| = i + 1$. The sequence $(2^i)_{i \in \mathbb{N}}$ in $\mathbb{N}A_2 = \mathbb{N}$ is not meaningfully parametrized. However, it is a subsequence of the sequence $(i)_{i \in \mathbb{N}}$, which has a meaningful parametrization.

Proposition 3.19. Let $A \in \mathbb{Z}^{m \times d}$ and let $(b_i)_{i \in \mathbb{N}}$ be a sequence in $\mathbb{N}A$ satisfying $(\|b_i\|)_{i \in \mathbb{N}} \in \mathcal{O}(i^r)_{i \in \mathbb{N}}$ for some $r \in \mathbb{N}$. Then $(b_i)_{i \in \mathbb{N}}$ has a meaningful parametrization.

Proof. Denote by $a_1, \ldots, a_m \in \mathbb{Z}^d$ the rows of $A$. Since $\ker_\mathbb{Z}(A) \cap \mathbb{N}^d = \{0\}$, there exist coefficients $\lambda_1, \ldots, \lambda_m \in \mathbb{Q}$ such that $w := \sum_{i=1}^{m} \lambda_i a_i \in \mathbb{Q}^d$. In particular, for any $b \in \mathbb{N}A$ and for any $u \in F_{A,b}$, $\|u\|_{\infty} \cdot \min_{i \in \mathbb{N}} w_i \leq w^T u \leq m \cdot \|\lambda\|_{\infty} \cdot \|b\|_{\infty}$. Thus,

$$|F_{A,b}| \leq \left( \frac{m \cdot \|\lambda\|_{\infty} \cdot \|b\|_{\infty}}{\min_{i \in \mathbb{N}} w_i} \right)^d.$$
Hence, if $\|b_i\| \leq C \cdot i^\epsilon$ for all $i \in \mathbb{N}$, then $(b_i)_{i \in \mathbb{N}}$ has a meaningful parametrization. \qed

For sequences with a meaningful parametrization, it suffices to bound the edge-expansion appropriately from above to show a slow mixing behaviour.

Lemma 3.20. Let $A \in \mathbb{Z}^{m \times d}$, $\mathcal{M} \subset \ker_{\mathbb{Z}}(A)$ be a finite set, and let $(b_i)_{i \in \mathbb{N}}$ be a sequence in $\mathbb{N}A$ with meaningful parametrization. If there is an infinite subset $\mathcal{I} \subseteq \mathbb{N}$ and $C \in \mathbb{N}$ such that $h(\mathcal{F}_{A,b_i}(\mathcal{M})) \leq \frac{C}{i}$ for all $i \in \mathcal{I}$, then $(\mathcal{F}_{A,b_i}(\mathcal{M}))_{i \in \mathbb{N}}$ is not rapidly mixing.

Proof. Let $\lambda_i \in [0, 1]$ be the second largest eigenvalue modulus of the simple walk on $\mathcal{F}_{A,b_i}(\mathcal{M})$ and assume that the sequence mixes rapidly. Then there exists a polynomial $p \in \mathbb{Q}_{\geq 0}[t]$ such that for all $i \in \mathcal{I}$,

$$1 - \frac{1}{p(\log |\mathcal{F}_{A,b_i}|)} \geq \lambda_i \geq 1 - \frac{C}{|\mathcal{M}| \cdot i}$$

where we have used the assumption on the edge-expansion and Proposition 3.8 to obtain the lower bound. This implies that for all $i \in \mathcal{I}$, $\frac{1}{i} \cdot p(\log |\mathcal{F}_{A,b_i}|) \geq \frac{|\mathcal{M}|}{C}$. However, since the parametrization is meaningful, there exists a polynomial $q \in \mathbb{Q}[t]$ such that $|\mathcal{F}_{A,b_i}| \leq q(i)$ and thus $p(\log |\mathcal{F}_{A,b_i}|) \leq p(\log q(i))$ for $i$ sufficiently large, which gives a contradiction since $\mathcal{I}$ is an infinite subset and hence unbounded. \qed

We are now ready to prove our main theorem:

Proof of Theorem 1.1. Since $(b_i)_{i \in \mathbb{N}}$ is dominated, there is $b \in \mathbb{N}A$ with $\dim(\mathcal{R}_{A,b}) > 0$ such that $b'_i := b_i - i \cdot b \in \mathbb{N}A$ for all $i \in \mathbb{N}$. Moreover, there is $u \in \mathcal{F}_{A,b}$ and a sequence $(w_i)_{i \in \mathbb{N}}$ in $\mathbb{N}^d$ such that for all $i \in \mathbb{N}$, $w_i \in \mathcal{F}_{A,b'_i}$ and $\supp(w_i) \subseteq \supp(u)$. Clearly, it suffices to show the theorem for the subsequence $(b_{(C(M)+1)i})_{i \in \mathbb{N}}$ which inherits the properties of being dominated and being meaningfully parametrized from $(b_i)_{i \in \mathbb{N}}$ due to the linear re-parametrization. Thus, we replace $b_i$ with $b_{(C(M)+1)i}$, $b$ with $(C(M) + 1) \cdot b$, and $b'_i$ with $b'_{(C(M)+1)i}$. Additionally, we replace $w_i$ with $w_{(C(M)+1)i}$ and $u$ with $(C(M) + 1) \cdot u$, which does not change the support of $u$. After these changes, we have $u_i > C(M)$ for all $i \in \supp(u)$, which is needed later in the proof. The Ehrhart quasi-polynomial $L_{\mathcal{R}_{A,b}}$ has degree $r := \dim(\mathcal{R}_{A,b})$ and by the definition of being dominated, $r > 0$. Write $L_{\mathcal{R}_{A,b}}(i) = \sum_{s=0}^r c_s(i) i^s$ with $c_s$ not identically zero. Since $L_{\mathcal{R}_{A,b}}(i) = |\mathcal{F}_{A,ib}| > 0$, there exists $k \in \mathbb{N}$ such that $c_s(k) > 0$. By Lemma 3.16, there exists $n \in \mathbb{N}_{>0}$ and $N \in \mathbb{N}$ such that $2|\mathcal{F}_{A,ib}| \leq |\mathcal{F}_{A,(i+ni)b}|$ for all $i \in (k + n \cdot N) \cap \mathbb{N}_{> N} =: \mathcal{I}$. By the choice of $w_i$ and $u$, $A \cdot (w_{i+ni} + ni \cdot u) = b'_{i+ni} + ni \cdot b = b_{i+ni} - ib$ for all $i \in \mathcal{I}$ and hence $w_{i+ni} + ni \cdot u + \mathcal{F}_{A,ib} \subseteq \mathcal{F}_{A,b_{i+ni}}$. In particular, for any $i \in \mathcal{I}$

$$2|\mathcal{F}_{A,ib}| \leq |\mathcal{F}_{A,(i+ni)b}| = |w_{i+ni} + \mathcal{F}_{A,(i+ni)b}| \leq |\mathcal{F}_{A,b_{i+ni}}|.$$ 

For any $i \in \mathcal{I}$, set $u_i := w_{i+ni} + ni \cdot u$, then Lemma 3.13 gives

$$|\partial_M^n(\mathcal{F}_{A,ib})| \leq \sum_{j \in \supp(u_i)} \sum_{l=0}^{C(M)} |\{v \in \mathcal{F}_{A,ib} : v_j = l\}|.$$
Since $2|\mathcal{F}_{A,b}| \leq |\mathcal{F}_{A,b_{i+n}}|$ and $u_i \in \mathcal{F}_{A,b_{i+n}+ni-b}$ for all $i \in \mathcal{I}$, an application of Lemma 3.11 yields the upper bound on the edge-expansion of the graph $\mathcal{F}_{A,b_{i+n}}(\mathcal{M})$:

$$h(\mathcal{F}_{A,b_{i+n}}(\mathcal{M})) \leq 2|\mathcal{M}| \cdot \frac{\partial_{A,b}^u(\mathcal{F}_{A,b})}{|\mathcal{F}_{A,b}|} \leq 2|\mathcal{M}| \cdot \frac{\sum_{l=0}^{C(\mathcal{M})} L_{j,l}(i)}{|\mathcal{F}_{A,b}|},$$

where equation (3.1) and $\text{supp}(u_i) \subseteq \text{supp}(u)$ was used in the first and second inequality respectively. For any $j \in \text{supp}(u)$ and $l \in [C(\mathcal{M})] \cup \{0\}$, let $H_{j,l} = \{x \in \mathbb{Q}^d : x_j = l\}$ be a hyperplane in $\mathbb{Q}^d$, then for all $i \in \mathcal{I}$, the integer points in $(i \cdot \mathcal{R}_{A,b}) \cap H_{j,l}$ are precisely $L_{j,l}(i) := |\{w \in \mathcal{F}_{A,b} : w_j = l\}|$. Since $u_j > C(\mathcal{M})$ for all $j \in \text{supp}(u)$, the vector $i \cdot u \in \mathcal{R}_{A,b}$ is not contained in $(i \cdot \mathcal{R}_{A,b}) \cap H_{j,l}$ for all $l \in [C(\mathcal{M})] \cup \{0\}$ and all $i \in \mathcal{I}$. Lemma 3.15 then implies that for all $j \in \text{supp}(u)$ and $l \in [C(\mathcal{M})] \cup \{0\}$, there is a constant $C_j \in \mathbb{N}$ such that $L_{j,l}(i) \leq C_j \cdot l^{-1}$ for all $i \in \mathbb{N}$. Let $C \in \mathbb{N}$ be the maximum of all $C_j$'s, then

$$h(\mathcal{F}_{A,b_{i+n}}(\mathcal{M})) \leq 2|\mathcal{M}| \cdot \frac{\sum_{l=0}^{C(\mathcal{M})} L_{j,l}(i)}{L_{R_{A,b}}(i)} = 2|\mathcal{M}| \cdot \frac{|\text{supp}(u)| \cdot (C(\mathcal{M}) + 1) \cdot C \cdot l^{-1}}{c_r(k) l + \sum_{s=0}^{r-1} c_s(i) l^s}.$$

Since $|\mathcal{M}|, C(\mathcal{M}), n, C$, and $\text{supp}(u)$ are constants which are independent of $i \in \mathcal{I}$ and since $c_r(k) > 0$, $(h(\mathcal{F}_{A,b_{i+n}}(\mathcal{M})))_{i \in \mathcal{I}} \in \mathcal{O}\left(\frac{1}{(n+1)}\right)_{i \in \mathcal{I}}$. It follows from Proposition 3.8 that the sequence is no expander and if $(b_i)_{i \in \mathbb{N}}$ has a meaningful parametrization, then Lemma 3.20 implies that the sequence cannot mix rapidly.

**Remark 3.21.** Basically, Theorem 1.1 shows the existence of $C, C' \in \mathbb{N}_{>1}$ such that the second largest eigenvalue modulus $\lambda_i$ of the simple walk on $\mathcal{F}_{A,b_i}(\mathcal{M})$ satisfies $\lambda_i \geq 1 - \frac{C}{i}$ for all $i \in C' \cdot \mathbb{N}$. Here, the constant $C'$ is due to the many boundary effects and the fluctuations in Ehrhart quasi-polynomials. For instance, when $(b_i)_{i \in \mathbb{N}}$ is a ray instead of a dominated sequence and when $A$ is totally unimodular, then $\lambda_i \geq 1 - \frac{C}{i}$ holds for all $i \in \mathbb{N}_{>C'}$ for a constant $C' \in \mathbb{N}$. Also, when $(b_i)_{i \in \mathbb{N}}$ is a sequence with $\limsup_{i \in \mathbb{N}} H_A(b_i) = \infty$, then $\limsup_{i \in \mathbb{N}} \lambda_i = 1$ due to Theorem 1.1 and Proposition 3.4.

**Corollary 3.22.** Let $A \in \mathbb{Z}^{n \times d}$ and let $\mathcal{M} \subset \ker(\mathcal{A})$ be a Markov basis for $A$. Let $(b_i)_{i \in \mathbb{N}}$ from $\text{NA}$ have a meaningful parametrization and suppose there is $p \in \mathbb{Q}[t]$ with $p(\mathbb{N}) \subseteq \mathbb{N}$ such that $(b_{p(i)})_{i \in \mathbb{N}}$ is dominated. Then $(\mathcal{F}_{A,b_i}(\mathcal{M}))_{i \in \mathbb{N}}$ is not rapidly mixing.

**Proof.** Clearly, there exists $C \in \mathbb{N}_{>0}$ such that $p(C \cdot (i+1)) > p(C \cdot i)$ for all $i$ sufficiently large. Let $b'_i := b_{p(C \cdot i)}$, then $(b'_i)_{i \in \mathbb{N}}$ is a subsequence of $(b_i)_{i \in \mathbb{N}}$ and hence it suffices to show that $(\mathcal{F}_{A,b'_i}(\mathcal{M}))_{i \in \mathbb{N}}$ is not rapidly mixing. Since $|\mathcal{F}_{A,b'_i}| = |\mathcal{F}_{A,b_{p(C \cdot i)}}| \leq q(p(C \cdot i))$ for a polynomial $q \in \mathbb{Q}[t]$, $(b'_i)_{i \in \mathbb{N}}$ has a meaningful parametrization. By assumption, there exists $b \in \text{NA}$ such that $b_{p(i)} - i \cdot b \in \text{NA}$ for all $i \in \mathbb{N}$ and hence $b'_i - i \cdot C \cdot b \in \text{NA}$ for all $i \in \mathbb{N}$. Theorem 1.1 then implies that $(\mathcal{F}_{A,b'_i}(\mathcal{M}))_{i \in \mathbb{N}}$ is not rapidly mixing. □
Corollary 3.23. Let $A \in \mathbb{Z}^{n \times d}$, $\mathcal{M} \subset \ker_{\mathbb{Z}}(A)$ a Markov basis for $A$, and $b \in NA$ with $\dim(R_{A,b}) > 0$. Suppose that $(b_i)_{i \in \mathbb{N}}$ has $(p(k) \cdot b)_{k \in \mathbb{N}}$ as subsequence for some non-constant $p \in \mathbb{Q}[t]$. Then $(F_{A,b}(\mathcal{M}))_{i \in \mathbb{N}}$ is not rapidly mixing.

Proof. Let $C, N \in \mathbb{N}$ such that $p(C \cdot k) \geq k$ for $k \geq N$. Then $(p(C \cdot k) - k) \cdot b \in NA$ for $k \geq N$ and hence $(p(C \cdot k) \cdot b)_{k \in \mathbb{N} \geq N}$ is dominated. Clearly, $(p(C \cdot k) \cdot b)_{k \in \mathbb{N} \geq N}$ is meaningfully parametrized because of Proposition 3.19 and hence the statement is a consequence of Theorem 1.1.

Remark 3.24. Let $\mathcal{M} = \{m_1, \ldots, m_r\} \subset \ker_{\mathbb{Z}}(A)$ be a Markov basis for $A$. Extending $\mathcal{M}$ by adding a finite number of $\mathbb{Z}$-linear combinations $\sum_{i=1}^{k} \lambda_i m_i$ may improve the mixing behaviour in one particular fiber, but since the complexity of the new set of moves is still finite, this cannot lead to rapid mixing asymptotically due to Theorem 1.1. For instance, this implies that the Graver basis of $A$ has the same asymptotic mixing behaviour than any other finite Markov basis for $A$.

Example 3.25. Let $A_{n|m}$ be the constraint matrix of the $n \times m$-independence model [10]. Elements in the kernel of $A_{n|m}$ can be written as $n \times m$ contingency tables whose row and column sums are zero and the basic moves $\mathcal{M}_{n|m}$ are a minimal Markov basis for $A_{n|m}$. These are all moves in the orbit of

$$
\begin{bmatrix}
1 & -1 & 0 & \cdots & 0 \\
-1 & 1 & 0 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0
\end{bmatrix}
\in \mathbb{Z}^{n \times m}
$$

under the group action of $S_n \times S_m$ on the rows and columns. Using this Markov basis to explore the set of contingency tables was suggested in [9]. Elements in the same fiber of $A_{n|m}$ have the same $\| \cdot \|_1$-norm, namely $\frac{1}{2}\|b\|_1$, since the row-space of $A_{n|m}$ contains the vector $(1, \ldots, 1) \in \mathbb{R}^{n \times m}$. Observe that the invariant $\frac{1}{2}\|b\|_1$ is precisely the sample size of goodness-of-fit tests for the independence model [10, Chapter 1.1]. Thus, we obtain sequences $(b_i)_{i \in \mathbb{N}}$ with a meaningful parametrization whenever the sample size grows polynomial in $i$ by Proposition 3.19. Assume that $n \geq m$ and that $b_i \geq \frac{s}{t} \cdot i \cdot (1, \ldots, 1)^T$ for fixed $s, t \in \mathbb{N}$, then $b_{i-t,n} - i \cdot s \cdot (n, \ldots, n, m, \ldots, m)^T \in NA_{n|m}$ (where $n, \ldots, n$ denotes the $m$ column sums and $m, \ldots, m$ denotes the $n$ row sums) and it follows that $(b_{i-t,n})_{i \in \mathbb{N}}$ is dominated since the fiber of $(n, \ldots, n, m, \ldots, m)^T$ contains an element with full support. Corollary 3.22 shows that the simple fiber walk on $(F_{A_{n|m},b_i}(\mathcal{M}_{n|m}))_{i \in \mathbb{N}}$ is not rapidly mixing. These assumptions hold for instance when $n = m$ and $b_i := (i, \ldots, i) \in \mathbb{N}^{2n}$, even though the node-connectivity under the basic moves $\mathcal{M}_{n|m}$ is best-possible due to [23, Theorem 2.9].

Using Markov chain comparison methods as in [11], Theorem 1.1 can be used to show that related random walks on fibers are not rapidly mixing as well. We show that...
the random walk on a fiber where we sample uniformly from the full Markov basis has asymptotically the same mixing behaviour than the random walk which samples from the set of applicable moves locally.

**Proposition 3.26.** Let $G = (V, E)$ be a connected $d$-regular graph and let $G'$ be the graph obtained from $G$ after removing all its loops. Let $\lambda$ and $\lambda'$ be the second largest eigenvalues of $S^G$ and $S^{G'}$ respectively, then $(1 - \lambda') \leq d \cdot (1 - \lambda)$.

**Proof.** Let $m$ be the number of edges and $\delta$ be the minimal degree in $G'$ respectively. If $G'$ is bipartite, then $\lambda' = 1$ and the claim holds. Assume differently, the stationary distribution $\pi'$ of $S^{G'}$ is the uniform distribution on $V$ whereas the stationary distribution of $S^G$ is $\pi' : V \rightarrow [0, 1]$, $\pi'(u) = \deg_{G'}(u) \cdot (2m)^{-1}$. We use [31, Lemma 2.5]. For any $u \in V$,

$$\frac{\pi'(u)}{\pi(u)} = \frac{|V| \cdot \deg_{G'}(u)}{2m} \geq \frac{|V| \cdot \delta}{2m}$$

and for any distinct $w, v \in V$,

$$\frac{\pi'(w) \cdot S^{G'}_{w,v}}{\pi(w) \cdot S^G_{w,v}} = \frac{|V| \cdot d}{2m}.$$ 

Since the diagonal entries of $S^{G'}$ are zero, [31, Lemma 2.5] implies $(1 - \lambda') \leq d \cdot \delta^{-1} \cdot (1 - \lambda)$. Since $G$ is connected, $G'$ has no isolated nodes and hence $\delta^{-1} \leq 1$. 

**Remark 3.27.** Fix a constraint matrix $A \in \mathbb{Z}^{m \times d}$ and Markov basis $\mathcal{M}$ of $A$ and consider the random walk $S'$ on $\mathcal{F}_{A,b}(\mathcal{M})$ which samples for any $v \in \mathcal{F}_{A,b}$ uniformly from the set of all applicable moves $\{m \in \pm \mathcal{M} : v + m \in \mathbb{N}^d\}$ to explore the fiber. This modified random walk is precisely the simple walk on the graph obtained from $\mathcal{F}_{A,b}(\mathcal{M})$ after removing all its loops. In particular, this random walk has no rejections. However, Proposition 3.26 implies that whenever $(\mathcal{F}_{A,b}(\mathcal{M}))_{i \in \mathbb{N}}$ is not rapidly mixing, this modified random walk is not rapidly mixing as well.

4. **Constructing expander graphs on fibers**

The message from the previous section is that the moves in a Markov bases do not suffice to provide a good mixing behaviour asymptotically. A possible way out is to adapt the Markov basis appropriately so that its complexity grows with the size of the right-hand entries. This can be achieved by adding a varying number of $\mathbb{Z}$-linear combinations of the moves in a way that the edge-expansion of the resulting graph can be controlled. However, a growth of the set of allowed moves comes along with an increase of the number of loops, i.e. an increase of the rejection rate of the walk. Let $A \in \mathbb{Z}^{m \times d}$ be a matrix, $\mathcal{M} = \{m_1, \ldots, m_k\} \subset \ker_{\mathbb{Z}}(A)$ be a Markov basis for $A$, and $b \in \mathbb{N}A$. For $l \in \mathbb{N}$, let

$$\mathcal{M}(l) = \left\{ \sum_{j=1}^{k} \lambda_j m_j : \lambda_1, \ldots, \lambda_k \in \mathbb{Z}, \sum_{j=1}^{k} |\lambda_j| \leq l \right\}$$
and define $d_{A,b}^M := \text{diam}(\mathcal{F}_{A,b}(\mathcal{M}))$ and $\mathcal{M}^b := \mathcal{M}(d_{A,b}^M)$. Using $\mathcal{M}^b$ instead of $\mathcal{M}$ as a set of allowed moves, the corresponding fiber graph $\mathcal{F}_{A,b}(\mathcal{M}^b)$ is the complete graph on $\mathcal{F}_{A,b}$. We discuss in Remark 4.4 how moves from $\mathcal{M}^b$ can be sampled uniformly. The transition matrix of the simple walk on $\mathcal{F}_{A,b}(\mathcal{M}^b)$ is

$$
\begin{bmatrix}
1 & 1 & \cdots & 1 & 1 \\
1 & \ddots & & \vdots & \vdots \\
\vdots & \ddots & \ddots & \vdots & \vdots \\
1 & \cdots & \cdots & 1 & 1
\end{bmatrix} + \frac{1}{|\mathcal{M}^b|} \begin{bmatrix}
|\mathcal{M}^b| - |\mathcal{F}_{A,b}| & 0 & \cdots & 0 & 0 \\
0 & \ddots & & \vdots & \vdots \\
\vdots & \ddots & \ddots & \vdots & \vdots \\
0 & \cdots & \cdots & 0 & |\mathcal{M}^b| - |\mathcal{F}_{A,b}|
\end{bmatrix}
$$

In particular, its second largest eigenvalue modulus is $1 - \frac{|\mathcal{F}_{A,b}|}{|\mathcal{M}^b|}$ and hence the next proposition is immediate.

**Proposition 4.1.** Let $A \in \mathbb{Z}^{m \times d}$, $\mathcal{M} \subset \ker(A)$ be a Markov basis for $A$ and $(b_i)_{i \in \mathbb{N}}$ a sequence in $\mathbb{N}A$. Suppose there exists $r \in \mathbb{N}$ such that $(|\mathcal{F}_{A,b_i}|)_{i \in \mathbb{N}} \in \mathcal{O}(i^r)_{i \in \mathbb{N}}$ and $(|\mathcal{M}^b_i|)_{i \in \mathbb{N}} \in \mathcal{O}(i^r)_{i \in \mathbb{N}}$, then $(\mathcal{F}_{A,b_i}(\mathcal{M}^b_i))_{i \in \mathbb{N}}$ is an expander.

To make use of Proposition 4.1, the growths of the fibers and the adapted Markov bases have to be compared. Again, Ehrhart’s theory applies to compute the growth of certain fiber sequences. The asymptotic growth of $\mathcal{M}^b_i$ depends on the growth of the diameter of $\mathcal{F}_{A,b_i}(\mathcal{M})$. Hence, we first want to understand how the number of elements in $\mathcal{M}(l)$ grows as a function of $l \in \mathbb{N}$.

**Lemma 4.2.** Let $\mathcal{M} = \{m_1, \ldots, m_k\} \subset \mathbb{Z}^d$, then $(|\mathcal{M}(l)|)_{l \in \mathbb{N}} \in \mathcal{O}(l^{\dim(\mathcal{M})})_{l \in \mathbb{N}}$.

**Proof.** We identify the finite set $\mathcal{M}$ with the integer matrix $(m_1, \ldots, m_k) \in \mathbb{Z}^{d \times k}$. Denote the $k$-dimensional cross-polytope by $\mathcal{P} := \{x \in \mathbb{Q}^k : \|x\| \leq 1\}$ and let $\mathcal{P}' := \{\mathcal{M} \cdot x : x \in \mathcal{P}\}$ be its image in $\mathbb{Q}^d$ under $\mathcal{M}$. With this, we can write $\mathcal{M}(l) = \{\mathcal{M} \cdot x : x \in (l \cdot \mathcal{P}) \cap \mathbb{Z}^k\}$ and hence $\mathcal{M}(l) \subseteq (l \cdot \mathcal{P}') \cap \mathbb{Z}^d$. Since $\mathcal{P}'$ is a polytope, Ehrhart’s theorem [2, Theorem 3.23] gives $|(l \cdot \mathcal{P}') \cap \mathbb{Z}^d| \leq C \cdot l^{\dim(\mathcal{P}')}$ for some $C \in \mathbb{Q}_{>0}$ and since $\dim(\mathcal{P}') = \dim(\mathcal{M})$, the claim follows.

**Corollary 4.3.** Let $A \in \mathbb{Z}^{m \times d}$ and let $\mathcal{M} \subset \ker\mathbb{Z}(A)$ be a Markov basis for $A$. Let $(b_i)_{i \in \mathbb{N}}$ be a sequence in $\mathbb{N}A$ such that $(|\mathcal{F}_{A,b_i}|)_{i \in \mathbb{N}} \in \Omega(i^{d - \dim(\mathcal{A})})$ and $(d_{A,b_i}^M)_{i \in \mathbb{N}} \in \mathcal{O}(i)_{i \in \mathbb{N}}$. Then $(\mathcal{F}_{A,b_i}(\mathcal{M}^b_i))_{i \in \mathbb{N}}$ is an expander.

**Proof.** Let $r := \dim(\ker\mathbb{Z}(A))$. It suffices to show that $|\mathcal{M}^b_i| \leq C \cdot i^r$ for a constant $C \in \mathbb{Q}_{>0}$ since the statement follows then from Proposition 4.1. Since $\mathcal{M}$ is a Markov basis for $A$, $\dim(\mathcal{M}) = r$ and thus Lemma 4.2 implies that $|\mathcal{M}(l)| \leq C_1 \cdot l^r$ for a constant $C_1 \in \mathbb{Q}_{>0}$. The assumption implies that there exists $C_2 \in \mathbb{Q}_{>0}$ such that $d_{A,b_i}^M \leq C_2 \cdot i$ for all $i \in \mathbb{N}$. Then, $|\mathcal{M}^b_i| = |\mathcal{M}(d_{A,b_i}^M)| \leq |\mathcal{M}(C_2 \cdot i)| \leq C_1 \cdot C_2^r \cdot i^r$. □
Expanders are not per se fast, and Corollary 4.3 is an asymptotic statement. That means, for a given matrix $A \in \mathbb{Z}^{m \times d}$, a given Markov basis $M \subset \ker_{\mathbb{Z}}(A)$, and a right-hand side $b \in \mathbb{N}A$, we know by Theorem 1.1 that the second largest eigenvalue modulus of the simple walk that uses $M$ can be arbitrarily close to 1. On the other hand, since $(d^M_{A,i,b})_{i \in \mathbb{N}} \in O(i)_{i \in \mathbb{N}}$ by [27], the second largest eigenvalue modulus of the simple walk that uses the adapted Markov basis $M^{i-b}$ can be bounded away from 1 strictly. Thus, there exists a threshold $i_0 \in \mathbb{N}$ such that the adapted Markov basis is faster than the conventional Markov basis on $F_{A,i,b}$ for $i \geq i_0$. The exact value of $i_0$ depends on the hidden constants in the asymptotic formulations of Corollary 4.3 and can be quite small, as in Figure 2, but also very large so that the advantages of the adapted Markov bases may pay off only for large right-hand sides.

Remark 4.4. Running the simple walk on $F_{A,b}(M(l))$ for some $l \in \mathbb{N}$ requires to sample from $M(l)$ uniformly and hence a good understanding of this set is necessary. Basically, we shift the problem of sampling from $F_{A,b}$ for all $b \in \mathbb{N}A$ where $F_{A,b}(M)$ has diameter $l$ to the problem of sampling from $M(l)$, which can be seen as some kind of rejection sampling from a larger set $u + M(l) \supseteq F_{A,b}$. For large fibers, one applicable move $m \in M(l)$ suffices to obtain a sample $u + m \in F_{A,b}$ that is very close to uniform. Write $M = \{m_1, \ldots, m_k\}$ and $r := \text{rank}(M)$. When $r = k$, then an element $\lambda$ picked uniformly from $\{u \in \mathbb{Z}^k : \|u\|_1 \leq l\}$ gives rise to an element $M \cdot \lambda$ that is uniformly generated from $M(l)$. This is not the case when $r > k$. One approach to sample from $M(l)$ uniformly in this case is to first compute a lattice basis $B := \{b_1, \ldots, b_r\} \subset \mathbb{Z}^d$ of $M \cdot \mathbb{Z}^k$ in order to get rid of relations among the moves from $M$. Then, we compute for every $i \in [k]$ coefficients $\lambda_1^i, \ldots, \lambda_r^i$ such that $m_i = \sum_{j=1}^r \lambda_j^i b_j$. For $C := \sum_{j=1}^r \max_{i \in [k]} |\lambda_j^i|$, we have $M(l) \subseteq B(C \cdot l)$. Thus, after sampling coefficients $\lambda$ from $\{u \in \mathbb{Z}^r : \|u\|_1 \leq C \cdot l\}$ uniformly, we obtain a move $B \cdot \lambda$ that is sampled uniformly from a superset of $M(l)$. Since $|B(C \cdot l)|$ grows as $O(l^r)_{i \in \mathbb{N}}$, Proposition 4.1 remains valid. Sampling from the cross-polytope $\{u \in \mathbb{Z}^r : \|u\|_1 \leq C \cdot l\}$ can be done with the heat-bath method as studied in [27], which is fast for $l \to \infty$.

Example 4.5. The constraint matrix $A_{n|n}$ of the independence model (Example 3.25) is totally unimodular and hence $\dim(R_{A_{n|n},1_n}) = \dim(F_{A_{n|n},1_n})$ where $1_n \in \mathbb{Z}^{n+n}$ is the vector with all entries equal to 1. It was shown in [23, Proposition 2.10] that the diameter of $F_{A_{n|n},M_{n|n}}(i \cdot 1_n)$ is $(n-1)i$. In particular, for fixed $n \in \mathbb{N}$, the diameter grows linearly in $i$ and hence Corollary 4.3 yields that the sequence $(F_{A_{n|n},i \cdot 1_n}(M_{n|n}^{i+1}))_{i \in \mathbb{N}}$ is an expander.

Example 4.6. Assume $d > 2$ and consider $A_d$ and $\mathcal{M}_d$ from Example 3.9. It is not hard to see that the graph-distance between any two nodes $u, v \in F_{A_d,i}$ is at most $\|u - v\|_1$. Since the maximal $\|\cdot\|_1$-distance of two elements in $F_{A_d,i}$ is $2i$, the diameter of $F_{A_d,i}(\mathcal{M}_d)$ is $2i$. Hence, $(F_{A_d,i}(\mathcal{M}_d))_{i \in \mathbb{N}}$ is an expander.
Example 4.7. For $k \in \mathbb{N}$, let $I_k$ be the identity matrix in $\mathbb{Z}^{k \times k}$, $1_k$ be the $k$-dimensional vector with all entries equal to 1 and define the matrix

$$H_k := \begin{bmatrix} I_k & I_k & 0 & 0 & -1_k & 0 \\ 0 & 0 & I_k & I_k & 0 & -1_k \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \in \mathbb{Z}^{(2k+1) \times (4k+2)}.$$  

It was shown in [15, Theorem 2] that the reduced lexicographic Gröbner basis $G_k$ of $H_k$ is $\{e_i - e_{k+i} : i \in \{1, \ldots, k, 2k+1, \ldots, 3k\}\}$ together with the move 

$$(0, \ldots, 0, 1, \ldots, 1, 0, \ldots, 0, -1, \ldots, -1, 1, -1)^T.$$  

With [15, Section 4], it is easy to show that for any $k \in \mathbb{N}$, the diameter of $\mathcal{F}_{H_k, i \cdot e_{2k+1}}(G_k)$ is $(2k+1)i$. Thus, $(\mathcal{F}_{H_k, i \cdot e_{2k+1}}(G_k((2k+1)i)))_{i \in \mathbb{N}}$ is is an expander.

5. Scaling the Dimension

Markov bases of constraint matrices coming from statistical problems are often parametrized and they can be stated explicitly for any parameter. For instance, the basic moves $\mathcal{M}_{n|n}$ of the independence model (Example 3.25) form a Markov basis for $A_{n|n}$ for every $n \in \mathbb{N}$. Thus, varying the parameter $n$ provides fiber graphs where the set of moves is adapted canonically.

Remark 5.1. Let $b_n := (1, \ldots, 1) \in \mathbb{N}^{2n}$, then the elements of $\mathcal{F}_{A_{n|n}, b_n}$ can be identified with the elements of the symmetric group $S_n$ on $[n]$. Finding a set of generators such that the corresponding Cayley graph on $S_n$ is an expander is an active research field in group theory, see for instance [19]. In [8], it was shown that the simple walk on the Cayley graph of $S_n$ that uses the transpositions mixes rapidly in $\frac{1}{2}n \log n$ many steps. Inspired by shuffling a deck of $n$ cards, a random walk on $S_n$ that uses riffle shuffles was studied in [1] and shown to be rapidly mixing as well.
Parametric descriptions of Markov bases can be arbitrarily complicated in general, since by the Universality theorem [5], any integer vector appears as a subvector of a Markov basis element of the three-way no interaction model, when the parameters are large enough. Different than in fixed dimension, where the Markov basis is fixed, the size of the Markov basis is important in the convergence analysis when the dimension varies because the local sampling process of a move can be computationally challenging as the Markov basis becomes larger. The trade-off between an easily accessible set of moves and a corresponding random walk that has good mixing properties shows the realms of fiber walks in practice. The next proposition illustrates this for $H_k$ from Example 4.7, where the overwhelming number of moves in its parametric Graver basis $Gr_k$ slows the chain down for $k \to \infty$, despite the fact that the edge-connectivity of these fibers is best-possible [15, Theorem 4]. A description of $Gr_k$ is in [15, Theorem 2].

Proposition 5.2. The sequence $(F_{H_k,e_{2k+1}}(Gr_k))_{k \in \mathbb{N}}$ is not rapidly mixing.

Proof. According to [15, Section 4], $F_{H_k,e_{2k+1}}(Gr_k)$ is isomorphic to the graph on the nodes $\{0,1\}^{k+1}$ in which two nodes $(i_1, \ldots, i_k)$ and $(j_1, \ldots, j_k)$ are adjacent if either $i_{k+1} = j_{k+1}$ and $\|i - j\|_\infty = 1$, or if $i_{i+1} \neq j_{k+1}$. For any $k \in \mathbb{N}_{>0}$, let $S_k := \{(0, i, 0) : i \in \{0,1\}^{k-1}\} \cup \{(0, i, 1) : i \in \{0,1\}^{k-1}\}$, then $|S_k| = \frac{1}{2}|F_{A_k,e_{2k+1}}|$. Counting the edges leaving $S_k$, for any $(0, i, 0) \in S_k$ there are $k$ many with endpoints in $\{(1, i, 0) : i \in \{0,1\}^{k-1}\}$ and $2^{k-1}$ with endpoints in $\{(1, i, 1) : i \in \{0,1\}^{k-1}\}$. The same is true for any $(0, i, 1) \in S_k$. Hence, there are $(k + 2^{k-1}) \cdot 2 \cdot 2^{k-1}$ edges leaving $S_k$. The edge-expansion of $F_{A_k,e_{2k+1}}(Gr_k)$ is thus bounded from above by $k + 2^{k-1}$. Since $|Gr_k| = 2 \cdot (4^k + 4k)$ and $\log |F_{H_k,e_{2k+1}}| = k + 1$, the claim follows. 

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