Markov chains, CAT(0) cube complexes, and enumeration: monotone paths in a strip mix slowly

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Abstract

We prove that two natural Markov chains on the set of monotone paths in a strip mix slowly. To do so, we make novel use of the theory of non-positively curved (CAT(0)) cubical complexes to detect small bottlenecks in many graphs of combinatorial interest. Along the way, we give a formula for the number $c_m(n)$ of monotone paths of length n in a strip of height m. In particular we compute the exponential growth constant of $c_m(n)$ for arbitrary m, generalizing results of Williams for m = 2, 3.

1 Introduction

This paper uses tools from geometric group theory and enumerative combinatorics to derive probabilistic consequences about random walks of a combinatorial nature. Our methods have wide applicability, but we focus on one example of interest, which we carry out in detail: a random walk on the set of monotone paths in a strip.

A monotone path of length n in a strip of height m is a lattice paths that start at (0,0), takes steps N = (0,1), S = (0,-1) and E = (1,0), never retraces steps, and stays within the strip, as shown in Figure 1 for n = 15 and m = 3.



Figure 1: A monotone path of length 15 in a strip of height 3.

All monotone paths can be connected to each other by two kinds of local moves, illustrated in Figure 2.

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• switch corners: two consecutive steps that go in different directions exchange directions.

• flip the end: the last step of the path rotates 90°.





(b) Flipping the end.

This model was introduced by Abrams and Ghrist [AG04], who thought of this as a model for a robotic arm in a tunnel. They showed that the graph $S_{m,n}$ of possible configurations of the robotic arm connected by these local moves is a *cubical complex* $S_{m,n}$: a polyhedral complex made of unit cubes of varying dimensions. Ardila, Bastidas, Ceballos, and Guo [ABCG17a] proved that the space $S_{m,n}$ is non-positively curved, or CAT(0), and used this to give an algorithm to move the robotic arm optimally between any two configurations. They also derived a formula for the diameter of the graph $S_{m,n}$.

We revisit this combinatorial model, with new goals in mind. A central idea, relying on Ardila, Owen, and Sullivant's one-to-one correspondence between CAT(0) cube complexes and posets with inconsistent pairs (PIPs) [AOS12], is the following:

Idea 1.1. When the transition kernel of a Markov chain M is a CAT(0) cube complex, one can use the corresponding poset with inconsistent pairs (PIP) P_M to find bottlenecks (vertex separators) in the kernel, and obtain upper bounds on the mixing time of M.

This idea applies quite generally. In this paper we illustrate it in a detailed example: two random walks on the set of monotone paths in a strip. We make three main contributions, which we now describe. For precise definitions and statements, we refer the reader to the corresponding sections of the paper.

A. In Section 2 we study the number $c_m(n)$ of monotone paths of length n in a strip of height m. The generating functions for $c_2(n)$ and $c_3(n)$ were first computed by Williams [Wil96]. We give a general formula for the generating function of $c_m(n)$ for any height m. In particular, we are able to compute the *exponential growth constant* or *connective constant* $r_m = \lim_{n\to\infty} \sqrt[n]{c_m(n)}$ for any m.

Theorem 1.2. For each $m \ge 0$ there are constants q_m and r_m such that

$$c_m(n) \sim q_m \cdot r_m^n,$$

where $1 = r_0 < r_1 < r_2 < \cdots$, and $\lim_{m \to \infty} r_m = 1 + \sqrt{2} \approx 2.4142 \dots$ The growth constant r_m is the largest real root of the polynomial

$$a_m(x) = \alpha_+(x)\beta_+(x)^m + \alpha_-(x)\beta_-(x)^m,$$

where

$$\alpha_{\pm}(x) = \pm \frac{x^4 - 2x^3 - 1}{2\sqrt{(x^4 - 1)(x^2 - 2x - 1)}} + \frac{1 - x}{2},$$

$$\beta_{\pm}(x) = \frac{-x^3 + x^2 - x - 1 \pm \sqrt{(x^4 - 1)(x^2 - 2x - 1)}}{2}$$

This theorem allows us to use computer software to easily compute r_m for concrete values of m. This description of the growth constant r_m is the most explicit possible, because Galois theory tells us that there is no exact formula for it.

B. In Section 3 we find a small bottleneck in the transition kernel $S_{m,n}$ of monotone paths, connected by the local moves described above. We prove:

Theorem 1.3. For each $m \ge 2$, the transition kernel $S_{m,n}$ has a small bottleneck of n+1 vertices, whose removal separates the graph into two components $(S_{m,n})_a$ and $(S_{m,n})_b$ of sizes

$$|(S_{m,n})_a| \sim (1 - C_m)|S_{m,n}| \qquad |(S_{m,n})_b| \sim C_m|S_{m,n}|$$

where $C_m = 1/(r_m^2(r_m - 1)^2)$. These constants satisfy $0.345... \approx C_2 > C_3 > C_4 \ge \cdots$ and $\lim_{m \to \infty} C_m = 1.5 - \sqrt{2} \approx 0.0858...$

C. In Section 4 we use the results of A. and B. above to show that two natural Markov chains on the space of monotone paths, which we call the "symmetric" and "lazy simple" Markov chains, mix slowly. In each step of the symmetric Markov chain $M_{m,n}$, we choose a vertex of the path uniformly at random, and perform a local move there if it is available. In each step of the lazy simple Markov chain $N_{m,n}$, at each step we first decide whether to move with probability p, and if we do, we perform one of the available moves uniformly at random.

Theorem 1.4. Let $m \ge 2$. For the symmetric Markov chain $M_{m,n}$, the stationary distribution is uniform, and the mixing time grows exponentially with n:

$$au_{M_{m,n}}(\varepsilon) \ge C \cdot r_m^n \ln(\varepsilon^{-1})$$

For the lazy simple Markov chain $N_{m,n}^p$, the stationary distribution is proportional to the degree – with $\pi(x) \propto \deg(x)$ for each lattice path x – and the mixing time grows exponentially with n:

$$au_{N_{m,n}^p}(\varepsilon) \ge D \cdot \frac{1}{n} r_m^n \ln(\varepsilon^{-1}).$$

Here $0 < \varepsilon < 1$ is arbitrary, C and D are constants, and $r_m > 1$ is the constant of Theorem 1.2.

2 Enumeration of monotone paths in a strip

Let S_m be the strip of height *m* that extends infinitely to the right:

$$S_m = \{(x, y) \mid x \ge 0, \ 0 \le y \le m\}.$$

Definition 2.1. A monotone path in a strip is a lattice path that starts at (0,0), takes steps N = (0,1), S = (0,-1) and E = (1,0), never retraces steps, and stays within the strip.

In this section we study the enumeration of monotone paths in a strip.

2.1 The transfer-matrix method: monotone paths as walks in a graph

To enumerate monotone paths in a strip, we use the *transfer-matrix method*, which we now briefly recall. For a thorough treatment of the transfer-matrix method, including the relevant proofs, see for example [Sta11, Chapter 4.7]

Suppose we are interested in a certain family of combinatorial objects, and we wish to find the number a_n of objects of "size" n. The idea is to construct a directed graph G = (V, E) such that the objects of size n can be encoded as – that is, they are in bijection with – the walks of length n in G. If we succeed, then the enumeration problem becomes a linear algebra problem. If we let A be the $V \times V$ adjacency matrix of G, given by

 $A_{uv} =$ number of edges from u to v for $u, v \in V$

then the key observation of the transfer-matrix method [Sta11, Theorem 4.7.1] is that

 A_{uv}^n = number of paths of length *n* from *u* to *v* for $u, v \in V$.

Our enumeration problem then reduces to computing powers of the adjacency matrix. In particular, the eigenvalues of A^0, A^1, A^2, \ldots control the growth of the sequence a_0, a_1, a_2, \ldots

Let us now apply this philosophy to the problem that interests us.

A failed encoding of monotone paths as walks in a graph. A natural first idea is to encode a path by keeping track of the height h_i of each node i. For example, the monotone path in Figure 1 has node heights 0, 0, 0, 1, 1, 2, 2, 3, 3, 3, 2, 2, 1, 1, 2, 3. This sequence of heights can be viewed as a walk in the graph F_m with vertices $0, 1, \ldots, m$ and edges $i \to i - 1$, $i \to i$, $i \to i + 1$ whenever those vertices are in the range $\{0, \ldots, m\}$. Each monotone paths gives rise to a different walk in this graph F_m starting at 0. However, not every such walk arises from a monotone path: a monotone path cannot contain an edge $i \to i + 1$ (resp. $i \to i - 1$) followed by the reverse edge $i + 1 \to i$ (resp. $i - 1 \to i$). For this reason, the graph F_m does not provide the necessary bijective encoding.

A successful encoding of monotone paths as walks in a graph. To resolve the issue above, we redundantly insert some memory into the bookkeeping procedure. We encode a path as a sequence of pairs: for the *i*th node, we keep track of the *height pair* (h_{i-1}, h_i) of heights of nodes i - 1 and i. (We define $h_{-1} = 0$.) For example, the monotone path in Figure 1 is recorded by the successive height pairs 00, 00, 01, 11, 12, 22, 23, 33, 33, 32, 22, 21, 11, 12, 23.¹

Now we consider the directed graph whose vertices are the possible height pairs, and whose edges are the possible transitions between two consecutive height pairs.

Definition 2.2. Let m be a positive integer. The transfer graph G_m is the directed graph with

- vertices: (i, i 1), (i, i), (i, i + 1) whenever the indices are between 0 and m, and
- edges: $(i, j) \rightarrow (j, k)$ unless $j = i \pm 1$ and k = i.



Figure 3: The graph G_2 and its adjacency matrix A_2 ...

The graph G_2 is illustrated in Figure 3.

Lemma 2.3. The number $c_m(n)$ of monotone paths of length n in a strip of height m equals the number of walks of length n in the transfer graph G_m that start at vertex (0,0).

Proof. For a monotone path of length n, let $0 = h_0, h_1, h_2, \ldots, h_n$ be the heights of the nodes. Since the path cannot retrace steps, the sequence above cannot contain a consecutive subsequence h, h + 1, h or h + 1, h, h + 1. Therefore $(0, 0) \rightarrow (0, h_1) \rightarrow (h_1, h_2) \rightarrow \cdots \rightarrow (h_{n-1}, h_n)$ is a walk of length n in G_m . Conversely, every walk of length n starting at (0, 0) corresponds to such a monotone path.

2.2 The characteristic polynomial

Having established the encoding of monotone paths as walks in a transfer graph G_m , we proceed with the linear algebraic analysis. Let A_m be the $(3m+1) \times (3m+1)$ adjacency matrix of G_m ; its non-zero entries are:

$$(A_m)_{(i,j),(j,k)} = 1$$
 unless $j = i \pm 1$ and $i = k$

all other entries equal 0. Let its characteristic polynomial be

$$a_m(x) = \det(A_m - xI).$$

The adjacency matrix A_2 is shown in Figure 3, and its characteristic polynomial is $a_2(x) = -x^7 + 3x^6 - 3x^5 + x^4 + 2x^3 - 2x^2 + x + 1$.

Lemma 2.4. The characteristic polynomial $a_m(x) = \det(A_m - xI)$ of the adjacency matrix of the graph G_m is given by the recurrence

$$a_m(x) = \begin{cases} 1-x & m=0\\ x^4 - 2x^3 + x^2 - 1 & m=1\\ (-x^3 + x^2 - x - 1)a_{m-1}(x) - x^4 a_{m-2}(x) & m \ge 2. \end{cases}$$

¹We write ij for the pair (i, j) when it introduces no confusion.

Proof. Consider the 3×3 matrices

$$X = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad Y = \begin{bmatrix} -x & 0 & 0 \\ 1 & 1 - x & 1 \\ 0 & 0 & -x \end{bmatrix}, \qquad Z = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$

For a matrix S, let $\overline{S}_{i,j}, \overline{S}_{j,j}$ and $\overline{S}_{i,j}$ respectively denote the matrix S with its *i*-th row, *j*-th column or the *i*-th row and *j*-th column deleted. Then one can verify that $A_m - xI$ is the $(3m + 1) \times (3m + 1)$ matrix with block format given below.

$$A_m - xI = \begin{bmatrix} Y_{1,1} & Z_1, & 0 & 0 & \cdots & 0 & 0 & 0 \\ \overline{X}_{,1} & Y & Z & 0 & \cdots & 0 & 0 & 0 \\ 0 & X & Y & Z & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & Y & Z & 0 \\ 0 & 0 & 0 & 0 & \cdots & X & Y & \overline{Z}_{,3} \\ 0 & 0 & 0 & 0 & \cdots & 0 & \overline{X}_3, & \overline{Y}_{3,3} \end{bmatrix}$$

Expanding by cofactors,

$$\begin{array}{rcl} a_m(x) & = & \det(A_m - xI) \\ & = & \begin{vmatrix} 1 - x & 1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & -x & 0 & 1 & 1 & 0 & \cdots \\ 1 & 0 & -x & 0 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 1 - x & 1 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \ddots \end{vmatrix}$$

$$= & (1 - x) \begin{vmatrix} & & & & & & & \\ -x & 0 & 1 & 1 & 0 & \cdots \\ 0 & -x & 0 & 0 & 0 & \cdots \\ 0 & 1 & 1 - x & 1 & 0 & \cdots \\ 0 & 0 & 0 & -x & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix}$$

$$= & (1 - x)(-x) \begin{vmatrix} & & & & & & \\ -x & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix}$$

$$- & & & & & \\ -x & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix}$$

$$- & & & & & & \\ -x & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix}$$

where $b_m(x) = \det(B_m(x))$ for the $(3m+2) \times (3m+2)$ matrix

$$B_m(x) = \begin{bmatrix} W & Z & \cdots & 0 \\ X & Y & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \overline{Y}_{3,3} \end{bmatrix} \quad \text{where} \quad W = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 - x & 1 \\ 0 & 0 & -x \end{bmatrix}.$$

Therefore we have

$$a_m(x) = x^2(1-x)a_{m-1}(x) + b_{m-1}(x)$$

Now, subtracting row 1 of $B_m(x)$ from row 2 and expanding by cofactors, we obtain the following:

$$b_{m}(x) = \det B_{m}(x)$$

$$= \begin{vmatrix} 0 & 1 & 1 & 0 & 0 & 0 & \cdots \\ 1 & 1 - x & 1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & -x & 0 & 1 & 1 & \cdots \\ 1 & 1 & 0 & -x & 0 & 0 & \cdots \\ 0 & 0 & 0 & 1 & 1 - x & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix} = \begin{vmatrix} 0 & 1 & 1 & 0 & 0 & 0 & \cdots \\ 1 & -x & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & -x & 0 & 1 & 1 & \cdots \\ 1 & 1 & 0 & -x & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & -x & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix}$$

$$= (-1) \begin{vmatrix} 1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & -x & 0 & 1 & 1 & \cdots \\ 1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & -x & 0 & 1 & 1 & \cdots \\ 1 & 0 & -x & 0 & 0 & \cdots \\ 0 & 0 & 1 & 1 - x & 1 & \cdots \\ 0 & 0 & 1 & 1 - x & 1 & \cdots \\ 0 & 0 & 0 & 0 & -x & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix} + (1) \begin{vmatrix} 1 & -x & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 1 & 1 & \cdots \\ 1 & 1 & -x & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & -x & \cdots \\ 0 & 0 & 0 & 0 & -x & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix}$$

Subtracting the first (non-grayed) row from the third (non-grayed) row in the second

matrix above, we obtain that $b_m(x)$ equals



Thus we have the recursion formulas

$$a_m(x) = (x^2 - x^3)a_{m-1}(x) + b_{m-1}(x)$$

$$b_m(x) = -x^2a_{m-1}(x) - (1+x)b_{m-1}(x)$$

The first equation gives a formula for each term of the *b*-sequence in terms of the *a*-sequence. Substituting that formula for b_m and b_{m-1} in the second equation gives the desired recurrence for $a_m(x)$.

The first few characteristic polynomials $a_m(x)$ are shown in Table 1. We now give an explicit formula for them.

Proposition 2.5. The polynomial $a_m(x)$ is given explicitly by the formula

$$a_m(x) = \alpha_+(x)\beta_+(x)^m + \alpha_-(x)\beta_-(x)^m$$

for all $m \geq 0$, where

$$\alpha_{\pm}(x) = \pm \frac{x^4 - 2x^3 - 1}{2\sqrt{(x^4 - 1)(x^2 - 2x - 1)}} + \frac{1 - x}{2},$$

$$\beta_{\pm}(x) = \frac{-x^3 + x^2 - x - 1 \pm \sqrt{(x^4 - 1)(x^2 - 2x - 1)}}{2}$$

for any $x \notin \{\pm 1, \pm i, 1 \pm \sqrt{2}\}.$

Proof. The relation

$$a_m(x) = (-x^3 + x^2 - x - 1)a_{m-1}(x) - x^4 a_{m-2}(x)$$
 for $m \ge 2$

is a linear recurrence with constant coefficients in the field of power series in x. To solve it, we need to compute the characteristic polynomial of the recurrence:

$$\beta^2 + (x^3 - x^2 + x + 1)\beta + x^4 = 0,$$

whose discriminant is

$$\gamma(x) := (x^3 - x^2 + x + 1)^2 - 4x^4 = x^6 - 2x^5 - x^4 - x^2 + 2x + 1 = (x^4 - 1)(x^2 - 2x - 1);$$

its roots are $\pm 1, \pm i, 1 \pm \sqrt{2}$.

For $\gamma(x) \neq 0$, this polynomial has two different roots β^{\pm} , given in the statement of the proposition. The general theory of recurrences tells us that there must exist constants α_{\pm} such that

$$a_n = \alpha_+ \beta_+^n + \alpha_- \beta_-^n$$

for all natural numbers n. Substituting n = 0, 1 gives the system of equations

$$1 - x = \alpha_{+} + \alpha_{-}$$
$$x^{4} - 2x^{3} + x^{2} - 1 = \alpha_{+}\beta_{+} + \alpha_{-}\beta_{-}$$

whose solution for α_+ and α_- is as given.

It feels like a small miracle that the discriminant $\gamma(x)$ arising in this problem has such a nice factorization; it would be interesting to explain this conceptually.

Proposition 2.6. The number $c_m(n)$ of monotone paths of length n in the strip of height m is the sum of the entries in row 00 of A_m^n ; equivalently,

$$c_m(n) = [10 \cdots 0] A_m^n [11 \cdots 1]^T.$$

Proof. The number $c_m(n)$ equals the number of paths of length n in the transfer graph G_m that start at 00, so it is the sum of the entries in the first row of A_m^n , which is given by $[10\cdots 0]A^n[11\cdots 1]^T$.

For any fixed height m, Proposition 2.6 may be used to give an explicit formula for the function $c_m(n)$ as n varies. To do so, one computes the Jordan normal form J_m of A_m , so that if $A_m = K J_m K^{-1}$ then $A_m^n = K J_m^n K^{-1}$, where the powers of J_m are easily computed; see for example [GVL13, (9.1.4)]. We get an even nicer answer for the generating function of this sequence.

Theorem 2.7. Let m be a fixed positive integer. The generating function for the number $c_m(n)$ of monotone paths of length n in the strip of height m is

$$\sum_{n\geq 0} c_m(n)x^n = \frac{\det(I - xA_m; 00)}{\det(I - xA_m)}$$

where $(I - xA_m; 00)$ is the matrix obtained from $I - xA_m$ by replacing every entry in the first column 00 with a 1.

Proof. For any $N \times N$ matrix A we have

$$\sum_{n \ge 0} A_{ij}^n x^n = \left(\sum_{n \ge 0} (Ax)^n \right)_{ij} = \left((I - Ax)^{-1} \right)_{ij} = \frac{(-1)^{i+j} \det(I - xA \, : \, j, i)}{\det(I - xA)}$$

where (K : j, i) denotes the matrix K with row j and column i removed. Therefore

$$\sum_{j=1}^{N} \sum_{n \ge 0} A_{ij}^{n} x^{n} = \sum_{j=1}^{N} \frac{(-1)^{j+i} \det(I - xA : j, i)}{\det(I - xA)},$$
$$= \frac{\det(I - xA ; j)}{\det(I - xA)},$$

where (K; j) denotes the matrix K with every entry in row j replaced by a 1; in the last step we use the expansion of det(I - xA) by cofactors along the jth row. Applying this formula to Proposition 2.6 gives the desired result.

Remark 2.8. Using Theorem 2.7 for the transition matrix A_2 of Figure 3, we readily obtain the generating function for monotone paths in a strip of height 2:

$$\sum_{n\geq 0} c_2(n)x^n = \frac{1-x+x^2+x^3-x^4+x^5+x^6}{1-3x+3x^2-x^3-2x^4+2x^5-x^6-x^7}$$
$$= \frac{1+x^2+x^3}{1-2x+x^2-x^3-x^4}$$
$$= 1+2x+4x^2+8x^3+15x^4+28x^5+53x^6+101x^7+\cdots$$

This matches the computation of Williams in [Wil96, (3)] and Ardila, Bastidas, Ceballos, and Guo in [ABCG17a, Corollary 3.6]; Williams also computed the generating function for $c_3(n)$. Their methods require a careful analysis for each fixed height m, and the complexity of that analysis grows with m. The advantage of our method is that it works uniformly for any height m.

2.3 Asymptotic analysis

Theorem 2.7 shows that for any fixed n, the generating function for $c_m(n)$ is a rational function in x. This implies that the asymptotic growth of $c_m(n)$ is controlled by the roots of the denominator of that rational function. Let us make that precise.

Theorem 2.9. [Sta11, Theorem 4.1.1] Let $\alpha_1, \ldots, \alpha_d$ be a fixed sequence of complex numbers, $d \ge 1$ and $\alpha_d \ne 0$. Let $Q(x) = 1 + \alpha_1 x + \cdots + \alpha_d x^d = \prod_{i=1}^k (1 - \lambda_i x)^{d_i}$ where the λ_i s are distinct and $d_1 + \cdots + d_k = d$. The following conditions on a function $f : \mathbb{N} \to \mathbb{C}$ are equivalent:

1. There is a polynomial P(x) of degree less than d and polynomials $p_i(x)$ with $\deg p_i(x) < d_i$ for i = 1, ..., k such that

$$\sum_{n \ge 0} f(n)x^n = \frac{P(x)}{Q(x)} = \sum_{i=1}^k \frac{p_i(x)}{(1 - \lambda_i x)^{d_i}}$$

2. For all $n \geq 0$,

$$f(n+d) + \alpha_1 f(n+d-1) + \alpha_2 f(n+d-2) + \dots + \alpha_d f(n) = 0$$

3. There exist polynomials P_i with deg $P_i(x) < d_i$ for i = 1, ..., k such that, for all $n \ge 0$,

$$f(n) = \sum_{i=1}^{k} P_i(n)\lambda_i^n.$$

If one is interested in the asymptotic growth of f(n), one needs to pay attention to the dominant terms of the expression in Theorem 2.9.3. This can be a subtle matter, because our polynomial Q(x) can have complex roots $1/\lambda_i$, which can occur with multiplicites. If we are in the fortunate situation where a simple real root dominates the others, the situation is simpler, as follows.

Say two sequences $(f(n))_{n\geq 0}$ and $(g(n))_{n\geq 0}$ are asymptotically equivalent, and write

$$f(n) \sim g(n)$$
 if $\lim_{n \to \infty} \frac{f(n)}{g(n)} = 1$

Lemma 2.10. Assume that the conditions of Theorem 2.9 hold, and that $\lambda = \lambda_1 \in \mathbb{R}_{>0}$ has the property that $d_1 = 1$ and $|\lambda_i| < \lambda$ for i = 2, ..., k. Then

$$f(n) \sim a \cdot \lambda^n$$
 where $a = \frac{-\lambda P(1/\lambda)}{Q'(1/\lambda)}$

Proof. Since $d_1 = 1$ the corresponding polynomial $p_1(x) = a$ is a constant, and the Taylor expansion of

$$\sum_{n \ge 0} f(n)x^n = \frac{P(x)}{Q(x)} = \frac{a}{1 - \lambda x} + \sum_{i=2}^k \frac{p_i(x)}{(1 - \lambda_i x)^{d_i}}$$

gives $f(n) \sim a \cdot \lambda^n$. To identify the constant a, notice that

$$a = \lim_{x \to 1/\lambda} \frac{P(x)}{Q(x)} (1 - x\lambda)$$

=
$$\lim_{x \to 1/\lambda} \frac{-\lambda P(x) + P'(x)(1 - x\lambda)}{Q'(x)}$$

=
$$\frac{-\lambda P(1/\lambda)}{Q'(1/\lambda)}$$

by L'Hôpital's rule.

Now let us apply this framework to the monotone paths that interest us. Let $\lambda_1, \ldots, \lambda_k$ be the eigenvalues of our transition matrix A_m with respective multiplicities d_1, \ldots, d_k , so that

$$\det(I - A_m x) = \prod_{i=1}^k (1 - \lambda_i x)^{d_i}$$

Theorem 2.7 tells us that Theorem 2.9 applies to the sequence $c_m(n)$. We can use it to immediately read off a linear recurrence relation for $c_m(n)$, as well as an explicit formula:

$$c_m(n) = \sum_{i=1}^k P_i(n)\lambda_i^n \tag{1}$$

For a fixed height m, the polynomials P_i – and hence the exact formula for $c_m(n)$ – can be computed explicitly: this is done by writing down the partial fraction decomposition of the right hand side of Theorem 2.7, and then computing its Taylor series.

Additionally, we are in the fortunate situation where a single real eigenvalue of A_m dominates the others and Lemma 2.10 applies, as we now explain.

Definition 2.11. A square matrix A is primitive if it is entrywise non-negative and some positive power A^k is entrywise positive.

Theorem 2.12 (Perron-Frobenius). Every primitive matrix A has a Perron eigenvalue r: this is a positive eigenvalue r > 0 such that $r > |\lambda|$ for any other eigenvalue λ of A. Furthermore, r is a simple eigenvalue of A – that is, it has multiplicity 1 – and it is between the minimum and the maximum column sums of A.

Lemma 2.13. The matrix A_m is primitive and its Perron eigenvalue $r_m = \lambda(A_m)$ satisfies $1 \le r_m \le 3$.

Proof. Our matrix A_m is clearly non-negative. By inspecting the graph G_m , we see that for any vertices u and v there is a walk from u to v of length at most 2m + 1. This walk must use at least one vertex (i, i), and adding loops $(i, i) \rightarrow (i, i)$ to the walk, one can extend it to have length exactly 2m + 1. Therefore A_m^{2m+1} is positive. The first claim follows, and the second one follows readily from the Perron-Frobenius theorem and the observation that the indegree and outdegree of any vertex of G_m is at least 1 and at most 3.

m	$a_m(x) = \det(A_m - xI)$	r_m
0	-x + 1	1
1	$x^4 - 2x^3 + x^2 - 1$	1.6180
2	$-x^7 + 3x^6 - 3x^5 + x^4 + 2x^3 - 2x^2 + x + 1$	1.8971
3	$x^{10} - 4x^9 + 6x^8 - 4x^7 - 2x^6 + 6x^5 - 5x^4 + 2x^2 - 2x - 1$	2.0507
4	$-x^{13} + 5x^{12} - 10x^{11} + 10x^{10} - x^9 - 11x^8 + 15x^7 - 7x^6 - 4x^5 + 8x^4 - 3x^3 - x^2 + 3x + 1$	2.1444
\downarrow		↓ ↓
∞		$1 + \sqrt{2}$

Table 1: Characteristic polynomial $a_m(x)$ and Perron eigenvalue r_m of the transition matrix A_m . The number r_m is the exponential growth constant of the number $c_m(n)$ of monotone paths of length n in a tunnel of height m.

Corollary 2.14. The Perron eigenvalue If $r_m := \lambda(A_m)$ of the matrix A_m , that is, the largest positive root of the polynomial $a_m(x)$ of Proposition 2.5, is the exponential growth rate constant for monotone paths in a strip of height m; more precisely,

$$c_m(n) \sim q_m \cdot r_m^n$$

for a constant q_m .

Proof. This follows readily from Lemma 2.10 and Lemma 2.13.

Table 1 shows the growth constants r_m for monotone paths in height m; that is, the Perron eigenvalues of the transition matrices A_m , for the first few values of m. We note that our description of the growth constant r_m as the largest real root of the polynomial $a_m(x)$ in Proposition 2.5 is the most explicit possible, because Galois theory tells us that there is no exact formula for it. For example, $a_3(x)$ factors into two irreducible quintics, and the quintic $x^5 - 2x^4 + x^2 - 2x - 1$ that has r_3 as a root has full Galois group S_5 .

We now offer an optimal upper bound for the growth constants r_m as the height m of the tunnel grows.

Proposition 2.15. The Perron eigenvalues r_0, r_1, r_2, \ldots of the matrices A_0, A_1, A_2, \ldots satisfy

$$1 = r_0 < r_1 < r_2 < \cdots$$
, and $\lim_{m \to \infty} r_m = 1 + \sqrt{2}$.

Proof. If we had $r_{m+1} < r_m$ for some m, Corollary 2.14 would imply

$$\lim_{n \to \infty} \frac{c_{m+1}(n)}{c_m(n)} = \lim_{n \to \infty} \frac{a_{m+1}}{a_m} \left(\frac{r_{m+1}}{r_m}\right)^n = 0,$$

contradicting the fact that $c_m(n) \leq c_{m+1}(n)$. Also, if we had $r_{m+1} = r_m$, then this would be a common root of the polynomials $a_{m+1}(x)$ and $a_m(x)$, and the recurrence of Lemma 2.4 would imply that it is also a root of $a_{m-1}(x), a_{m-2}(x), \ldots, a_0(x)$. However a_0 and a_1 don't have a root in common. This proves the first claim.

For the second part, notice that the Perron eigenvalues are increasing and bounded above by 3 by Lemma 2.13, so the sequence does converge. Let the limit be

$$\lim_{m \to \infty} r_m = r$$

and assume, for the sake of contradiction, that $r \neq 1 + \sqrt{2}$.

Since r_m is an eigenvalue for A_m , it is a root of $a_m(x)$, so Proposition 2.5 gives

$$0 = a_m(r_m) = \alpha_+(r_m)\beta_+(r_m)^m + \alpha_-(r_m)\beta_-(r_m)^m$$

Let us write $\alpha(x) = \alpha_+(x)/\alpha_-(x)$ and $\beta(x) = \beta_-(x)/\beta_+(x)$; these are well defined and non-zero for all but a finite number of values x. Thus for all sufficiently large m we have

$$-\alpha(r_m) = \beta(r_m)^m$$

and

$$\frac{1}{m}\log(-\alpha(r_m)) = \log\beta(r_m).$$
(2)

We now wish to take limits, but since the discriminant $\gamma(x) = (x^4 - 1)(x^2 - 2x - 1)$ – whose square root arises in α_{\pm} and β_{\pm} – can be negative, we need to regard these as complex functions. Making a branch cut along the ray spanned by 1 + i gives rise to two branches of the square root function $\pm \sqrt{z}$, each of which is continuous in the domain

$$D = \mathbb{C} \setminus (1+i) \mathbb{R}_{>0}.$$

Now $r_m \to r$ implies $\gamma(r_m) \to \gamma(r)$. This limit is real and non-zero, since r > 1 and we assumed $r \neq 1 + \sqrt{2}$. Thus \sqrt{z} is continuous at $\gamma(r)$, so $\sqrt{\gamma(r_m)} \rightarrow \sqrt{\gamma(r)}$. This implies that $\alpha(r_m) \to \alpha(r)$ and $\beta(r_m) \to \beta(r)$.

One may verify computationally that $\alpha_+, \alpha_-, \beta_+, \beta_-$ have no real roots. Furthermore, α_{-} and α_{+} only have two positive poles, located at x = 1 and $x = 1 + \sqrt{2}$, the positive roots of the polynomial $\gamma(x)$. Thus we can choose a branch of the logarithm function that is continuous at $-\alpha(r)$ and $\beta(r)$. Since $\alpha(r) \neq 0$, the left hand side of (2) converges to 0, while the right hand side converges to $\log \beta(r)$; this means that $\beta(r) = 1$. Thus $\beta_{-}(r) = \beta_{+}(r)$, which implies that $\gamma(r) = 0$, a contradiction.

We conclude that indeed $r = 1 + \sqrt{2}$ as desired.

We note that these results are consistent with the observation, recorded by Janse van Rensburg, Prellberg, and Rechnitzer in [JVRPR08, Lemma 2.1], that the growth constant for the monotone paths in the first quadrant. equals $1 + \sqrt{2}$. Remarkably, they showed that the growth constant still equals $1 + \sqrt{2}$ when considering monotone paths in the wedges bound by lines y = 0 and y = mx, or bound by lines y = -mx and y = mx, for any integer slope m. It would be interesting to generalize our results to those settings.

3 Using CAT(0) cube complexes to find a small bottleneck

For many Markov chains M, the transition kernel is the skeleton of a CAT(0) cube complex. When that is the case, Ardila, Owen, and Sullivant [AOS12] showed how to associate a poset with inconsistent pairs (PIP) P_M to M. The central idea, which bears repeating, that gave rise to this paper is the following:



Figure 4: The transition kernel $G_{2,6}$ of length 6 monotone paths in a strip of height 2.

Idea 3.1. When the transition kernel of a Markov chain M is a CAT(0) cube complex, one can use the corresponding poset with inconsistent pairs (PIP) P_M to find bottlenecks (vertex separators) in the kernel, and obtain upper bounds on the mixing time of M.

In this section we make this statement precise, and in the next section we will use it to bound the mixing time of the Markov chain $M_{m,n}$.

3.1 The cube complex of monotone paths in a strip

There are numerous contexts where a discrete system moves according to local, reversible moves. Abrams, Ghrist, and Peterson introduced the formalism of *reconfigurable systems* to model a very wide variety of such contexts. In particular, they showed how a reconfigurable system X leads to a *cube complex* S(X). Ardila, Bastidas, Ceballos, and Guo described the complex $S_{m,n}$ of monotone paths in a strip, using the language of robotic arms in a tunnel. We now give their description, and refer the reader to [AG04, ABY14, GP07] for the general framework.

Definition 3.2. Let $S_{m,n}$ be the transition kernel of the Markov chain $M_{m,n}$. Its vertices correspond to the $c_m(n)$ monotone paths of length n in a strip of height m. Two vertices are connected to each other if the corresponding paths can be obtained from one another by one of the following moves:

- switch corners: two consecutive steps that go in different directions exchange directions,
- flip the end: the last step of the path rotates 90°.

These moves are illustrated in Figure 2. The transition kernel $G_{2,6}$ is shown in Figure 4. It feels natural, and is very useful, to "fill in the cubes" in this graph; let us make this precise.

Definition 3.3. Given a path P and two moves available at P, say these two moves are compatible if no step of the path is involved in both of them.

Intuitively, two moves M_1 and M_2 on a path P are compatible when they are "physically independent" from each other in P. Performing M_1 and then M_2 gives the same result as performing M_2 and then M_1 , so we can imagine that M_1 and M_2 can be performed simultaneously if desired.

For a path P and k moves of P that are pairwise compatible, we can obtain 2^k different paths by performing any subset of these k moves to P. These 2^k vertices form the graph of a k-dimensional cube in $S_{m,n}$.

Definition 3.4. Let $S_{m,n}$ be the transition cube complex of the Markov chain $M_{m,n}$. Its vertices correspond to the $c_m(n)$ monotone paths of length n in a strip of height m. Its k-dimensional cubes correspond to the k-tuples of pairwise compatible moves.

This cube complex is naturally a metric space, where each individual cube is a unit cube with the standard Euclidean metric.

3.2 CAT(0) cube complexes and posets with inconsistent pairs

The cube complex S(X) of a reconfigurable system is always locally non-positively curved [AG04, ABY14, GP07] and sometimes globally non-positively curved, or $CAT(\theta)$. The reader may consult the definitions in the references above. When a cube complex is CAT(0), Ardila, Owen, and Sullivant [AOS12] showed how to find geodesic between any two points under various metrics. This has consequences for robotic motion planning, among others [ABCG17b, AM20]. As we stated in Idea 3.1, this also has implications for the mixing times of Markov chains.

3.2.1 CAT(0) cube complexes: how to define them

The CAT(0) property is the metric property of being non-positively curved, as witnessed by the fact that triangles are "thinner" than in Euclidean space. Let us make this precise for completeness, although we will not use this definition in what follows.

Definition 3.5. Let X be a metric space where there is a unique geodesic (shortest) path between any two points. Consider a triangle T in X of side lengths a, b, c, and build a comparison triangle T_0 with the same side lengths in Euclidean plane. Consider a chord of length d in T that connects two points on the boundary of T; there is a corresponding comparison chord in T_0 , say of length d_0 . If for every triangle T in X and every chord in T we have $d \leq d_0$, we say that X is CAT(0).

3.2.2 CAT(0) cube complexes: how to recognize them topologically

Testing whether a general metric space is CAT(0) is quite subtle. However, Gromov [Gro87] proved that this is easier to do this if the space is a cubical complex. In a cubical complex, the link of any vertex is a simplicial complex. We say that a simplicial

complex Δ is *flag* if it has no empty simplices; that is, any d + 1 vertices which are pairwise connected by edges of Δ form a *d*-simplex in Δ .

Theorem 3.6. (Gromov, [Gro87]) A cubical complex is CAT(0) if and only if it is simply connected and the link of any vertex is a flag simplicial complex.

If one has a reasonably small cubical complex, one can easily use this criterion to determine whether it is CAT(0). Roughly speaking, the first property says that the space should be connected and have no holes. The second one says that if we stand at a vertex and see that our complex contains all the 2-faces of a *d*-cube that contain v, then in fact it also contains that *d*-cube. For example we see, by inspection, that the cube complex of monotone paths $S_{2,6}$ in Figure 4 is CAT(0). More generally $S_{m,n}$ is always CAT(0); see Theorem 3.12.

3.2.3 CAT(0) cube complexes: how to describe and build them combinatorially

Most relevantly to us, Ardila, Owen, and Sullivant [AOS12] gave a combinatorial criterion to determine whether a cube complex is CAT(0). They showed that rooted CAT(0) cube complexes are in bijection with *posets with inconsistent pairs* (PIPs). Thus, if we wish to prove that a cube complex is CAT(0), it is sufficient to choose a root for it, and identify the corresponding PIP. Let us describe this carefully now.

Definition 3.7. A poset with inconsistent pairs (PIP) is a finite poset P, together with a collection of inconsistent pairs $\{p,q\}$ – denoted $p \nleftrightarrow q$ – such that:

- 1. If p and q are inconsistent, then there is no r such that $r \ge p$ and $r \ge q$.
- 2. If p and q are inconsistent and $p' \ge p$ and $q' \ge q$, then p' and q' are inconsistent.

The Hasse diagram of a PIP is obtained by drawing the poset, and connecting each minimal inconsistent pair with a dotted line. An inconsistent pair $p \nleftrightarrow q$ is minimal if there is no other inconsistent pair $p' \nleftrightarrow q'$ with $p' \leq p$ and $q' \leq q$. The left panel of Figure 5 shows a PIP.

Recall that $I \subseteq P$ is an order ideal or downset of poset P if $a \leq b$ and $b \in I$ imply $a \in I$. A consistent downset is one which contains no inconsistent pairs.

Definition 3.8. Let P be a poset with inconsistent pairs. The rooted cube complex of P, denoted S(P), is defined as follows:

• vertices: The vertices of $\mathcal{S}(P)$ are identified with the consistent order ideals of P.

• edges: There is an edge joining two vertices if the corresponding order ideals differ by a single element.

• cubes: More generally, there is a cube C(I, L) for each pair (I, L) of a consistent order ideal I and a subset $L \subseteq I_{max}$, where I_{max} is the set of maximal elements of I. This cube has dimension |L|, and its vertices are obtained by removing from I the $2^{|L|}$ possible subsets of L.

The cubes are naturally glued along their faces according to their labels. The root of S(P) is the vertex corresponding to the empty order ideal.

We denote the corresponding graph S(P). The right panel of Figure 5 shows the rooted cube complex $\mathcal{S}(P)$ (rooted at \emptyset) corresponding to the PIP on the left panel.

Theorem 3.9 (Ardila, Owen, Sullivant). [AOS12] The map $P \mapsto S(P)$ is a bijection between finite posets with inconsistent pairs and finite rooted CAT(0) cube complexes.



Figure 5: A PIP $P \cong C_{2,4}$ and the corresponding CAT(0) cubical complex $\mathcal{S}(P) \cong \mathcal{S}_{2,4}$.

When a cube complex is CAT(0), Ardila, Owen, and Sullivant [AOS12] showed how to find geodesic paths between any two points under various metrics. This has consequences for robotic motion planning, among others [ABCG17b, AM20]. We will see here that it also has implications for the mixing times of Markov chains.

3.3 The bottleneck lemma for CAT(0) cube complexes

Definition 3.10. Let G be a connected graph, we say that a set of vertices $T \subset V(G)$ is a vertex separator or bottleneck if the removal of T and the edges incident to T disconnects the graph.

Lemma 3.11. Let P be a poset with inconsistent pairs and S(P) be the graph of the corresponding CAT(0) cubical complex. Let $p \nleftrightarrow q$ be an inconsistent pair of P, and

 $S(P)_{p \leftrightarrow q} = vertices of S(P)$ whose consistent order ideals contain neither p nor q.

$$S(P)_p$$
 = vertices of $S(P)$ whose consistent order ideals contain p

 $S(P)_q$ = vertices of S(P) whose consistent order ideals contain q

Then $S(P)_{p \leftrightarrow q}$ is a bottleneck for S(P) that separates the sets $S(P)_p$ and $S(P)_q$ from each other.

Proof. Because $p \nleftrightarrow q$ form an inconsistent pair of P, every vertex of S(P) lies in exactly one of these three sets. Thus it suffices to show that there cannot be an edge of S(P)connecting a vertex $v \in S(P)_p$ to vertex $w \in S(P)_q$. But vertex v corresponds to an order ideal I containing p (and hence not containing q) and vertex w corresponds to an order ideal J containing q (and hence not containing p). It follows that the ideals Iand J differ by at least two elements, so there cannot be an edge between v and w, as desired.

3.4 The cube complex $S_{m,n}$ of monotone paths in a strip is CAT(0)

Recall that $S_{m,n}$ is the cube complex of monotone paths of length n in a strip of height m. For example, for m = 2 and n = 4, Figure 6 shows the 10 possible paths, labeled to match Figure 5. This labeling shows that in fact $S_{2,4}$ is the CAT(0) cube complex in that figure. Ardila, Bastidas, Ceballos, and Guo [ABCG17a] proved that this is an instance of a general phenomenon:

Theorem 3.12. [ABCG17a] For any positive integers m and n, the cube complex $S_{m,n}$ of monotone paths of length n in a strip of height m is CAT(0).



Figure 6: The monotone paths of length 4 in a tunnel of height 2.

3.4.1 The coral PIP

To prove that $S_{m,n}$ is CAT(0), [ABCG17a] introduced and used the technique shown in Section 3.2.3: the authors introduced the *coral PIP* $C_{m,n}$, and showed that its corresponding CAT(0) cube complex is $S(C_{m,n}) \cong S_{m,n}$. To describe the coral PIP, we need to introduce the notion of a *coral snake*.

Definition 3.13. A coral snake λ of height at most m is an oriented path of unit squares, colored alternatingly black and red (starting with black), inside the strip of height m such that:

(i) The snake λ starts with the bottom left square of the strip, and takes unit steps up, down, and right.

(ii) Suppose λ turns from a vertical segment V_1 to a horizontal segment H to a vertical segment V_2 at corners C_1 and C_2 . Then V_1 and V_2 face the same direction if and only if C_1 and C_2 have the same color. (Note: we consider the first column of the snake a vertical segment going up, even if it consists of a single cell.)



Figure 7: Illustration of condition (ii) in Definition 3.13.

The length $l(\lambda)$ is the number of unit squares of λ , the height $h(\lambda)$ is the number of rows it touches, and the width $w(\lambda)$ is the number of columns it touches. We say that μ contains λ , in which case we write $\lambda \leq \mu$, if λ is an initial sub-snake of μ obtained by restricting to the first k cells of μ for some k. We write $\lambda \prec \mu$ if $\lambda \leq \mu$ and $\lambda \neq \mu$. For technical reasons, sometimes we will also consider the empty snake \emptyset .



Figure 8: A coral snake λ of length $l(\lambda) = 11$, height $h(\lambda) = 3$, and width $w(\lambda) = 7$. We encourage the reader to check condition (*ii*).

Although the colors of a coral snake are a useful visual aid, we sometimes omit them since they are uniquely determined by the shape of the snake.

Definition 3.14. Define the coral PIP $C_{m,n}$ as follows:

- Elements: pairs (λ, s) consisting of a coral snake $\lambda \neq \emptyset$ with $h(\lambda) \leq m$ and an integer $0 \leq s \leq n l(\lambda) w(\lambda) + 1$.
- Order: $(\lambda, s) \leq (\mu, t)$ if $\lambda \leq \mu$ and $s \geq t$.
- Inconsistency: $(\lambda, s) \nleftrightarrow (\mu, t)$ if neither λ nor μ contains the other.

For simplicity, we call the elements (λ, s) of the coral PIP numbered snakes. We write them by placing the number s in the first cell of λ .

The left panel of Figure 9 shows the coral PIP $C_{2,9}$. The right panel shows how $C_{2,8}, C_{2,7}, \ldots$ are subPIPs of $C_{2,9}$; they are obtained from it by removing one colored layer at a time.

Theorem 3.15. [ABCG17a] The monotone paths of length n in a strip of height m are in bijection with the order ideals of the coral PIP $C_{m.n}$.



Figure 9: (a) The coral PIP $C_{2,9}$ with its numbered snakes. (b) The coral PIPs $C_{2,8}, C_{2,7}, \ldots$ are obtained from $C_{2,9}$ by removing one colored layer at a time.

3.4.2 Using the coral PIP to find a small bottleneck in $S_{m,n}$

We now use Bottleneck Lemma 3.11 to find a small bottleneck in $S_{m,n}$. Figure 9 shows us the way: there is a natural choice of an inconsistent pair in the coral PIP $C_{m,n}$.

Definition 3.16. Let the low inconsistent pair of the coral PIP $C_{m,n}$ consist of:

$$a = \boxed{\begin{array}{c} & & \\$$

Let the backbone of $C_{m,n}$ be the consistent order ideal

$$B = \left\{ \boxed{n-1} < \boxed{n-2} < \dots < \boxed{0} \right\} \subset C_{m,n}.$$

Notice that a and b have the largest possible indices among the tableaux of their respective shapes. This inconsistent pair decomposes the set of consistent order ideals into three subsets $\mathcal{S}(C_{m,n}) = \mathcal{S}(C_{m,n})_{a \leftrightarrow b} \sqcup \mathcal{S}(C_{m,n})_a \sqcup \mathcal{S}(C_{m,n})_b$, depending on whether an order ideal contains neither a nor b, only a, or only b.

As an example, in Figure 5, a = 3, b = 5, and

$$\begin{aligned} \mathcal{S}(C_{2,4})_{3 \nleftrightarrow 5} &= \{ \emptyset, 1, 12, 124, 1247 \}, \\ \mathcal{S}(C_{2,4})_3 &= \{ 123, 1234, 12347, 12346, 123467, 1234679, 12346710 \}, \\ \mathcal{S}(C_{2,4})_5 &= \{ 1245, 12457, 124578 \}. \end{aligned}$$

Each one of these order ideals corresponds to a path shown in Figure 6. The reader may wish to compare the lists above with those paths, to motivate the following lemmas.

The statements of the following two lemmas can be understood independently, but the proofs assume familiarity with the details of the bijection $\mathcal{S}(C_{m,n}) \to \mathcal{S}_{m,n}$ of Theorem 3.15, as explained in Lemma 5.9 and Theorem 5.5 of [ABCG17b].

Lemma 3.17. The bijection $\mathcal{S}(C_{m,n}) \to \mathcal{S}_{m,n}$ of Theorem 3.15 restricts to a bijection

 $\mathcal{S}(C_{m,n})_{a \nleftrightarrow b} \rightarrow \text{ paths containing at most one vertical step.}$

There are n + 1 such paths.

Proof. We claim that the order ideals I in $S(C_{m,n})_{a \leftrightarrow b}$ are precisely those that only contain numbered snakes of length 1. Indeed, assume $I \in S(C_{m,n})_{a \leftrightarrow b}$. We claim that I only contains numbered snakes of length 1. Indeed, if I contained a numbered snake (λ, s) of length at least 2, then it would also contain the numbered snake $(\lambda_2, s) \leq (\lambda, s)$, where λ_2 consists of the first two squares of λ . If λ_2 consists of two vertically arranged squares, then $s \leq n - 2 - 1 + 1 = n - 2$ by the definition of $C_{m,n}$, so I also contains $a = (\lambda_2, n - 2) \leq (\lambda_2, s)$, a contradiction. Similarly, if λ_2 consists of two horizontally arranged squares, then $s \leq n - 2 - 2 + 1 = n - 3$, so I also contains $b = (\lambda_2, n - 3) \leq (\lambda_2, s)$, a contradiction. The converse is clear.

It follows that $S(C_{m,n})_{a \leftrightarrow b}$ consists of the empty ideal – which corresponds to the horizontal path – and for $0 \leq k \leq n-1$, the order ideal generated by (\Box, k) , which corresponds to the path that takes k horizontal steps, then one vertical step, and then n-1-k horizontal steps, as desired.

Lemma 3.18. The bijection $\mathcal{S}(C_{m,n}) \to \mathcal{S}_{m,n}$ of Theorem 3.15 restricts to a bijection

 $\mathcal{S}(C_{m,n})_b \rightarrow$ paths that contain a second vertical step, which points down.

The number of such paths is

$$u_m(n) := c_m(n-4) + 2c_m(n-5) + 3c_m(n-6) + \dots + (n-3)c_m(0).$$

Proof. First consider an order ideal I in $\mathcal{S}(C_{m,n})_b$. Then $b = (\Box, n-2) \in I$, so the first two steps of the *coral snake tableaux* T corresponding to I in [ABCG17b, Lemma 5.9] are horizontally arranged. In the corresponding monotone path, the first and second vertical steps point up and down, respectively.

Conversely, consider a monotone path P whose first two vertical steps are the *j*th and *k*th, which point up and down, respectively for some $1 \le j < k \le n$. The corresponding coral snake tableaux T and its decomposition into join-irreducibles – as described in the proof of [ABCG17b, Theorem 5.5], starts:

$$T = \underbrace{j_{-1}}_{k-2} \cdots = \underbrace{j_{-1}}_{k-3} \lor \underbrace{k_{-3}}_{k-2} \lor \cdots$$

The second join-irreducible above corresponds to element $(\Box, k-3)$ of $C_{m,n}$, which must be in the ideal I corresponding to P. But then $(\Box, k-3) \ge (\Box, n-3) = b$ implies that the ideal I contains b as well, as desired.

Now let us count the number of arm configurations for a given choice of $k \ge 3$. There are k-2 choices for the value of j, and this choice entirely determines the first k steps of the path. Step k+1 must be horizontal, and there are $c_m(n-k-1)$ choices for the rest of the path. It follows that $u_m(n) = \sum_{k\ge 3} (k-2)c_m(n-k-1)$, as desired. \Box

These combinatorial considerations allows us to show that the small bottleneck of n+1 vertices in $\mathcal{S}(C_{m,n})_{a \leftrightarrow b}$ separates the cube complex $\mathcal{S}(C_{m,n})$ into two parts $\mathcal{S}(C_{m,n})_a$ and $\mathcal{S}(C_{m,n})_b$ that each contain roughly a constant fraction of the (exponentially many) vertices.

Lemma 3.19. For any fixed height $m \ge 2$ of the strip, there is a constant $0 < C_m < 1$ such that

$$\lim_{n \to \infty} \frac{\mathcal{S}(C_{m,n})_b}{\mathcal{S}(C_{m,n})} = \lim_{n \to \infty} \frac{u_m(n)}{c_m(n)} = C_m.$$

The constant C_m decreases with m, and approaches $1.5 - \sqrt{2} \approx 0.0858...$ as m goes to infinity.

Proof. We saw that the generating function for $c_m(n)$ is rational

$$\sum_{n\geq 0} c_m(n)x^n = \frac{p(x)}{q(x)}$$

and Lemma 3.18 shows that

$$\sum_{n\geq 0} u_m(n)x^n = (\sum_{n\geq 0} u_m(n)x^n)(x^4 + 2x^5 + 3x^6 + \dots) = \frac{p(x)}{q(x)}\frac{x^4}{(1-x)^2}$$

Furthermore, as discussed in Corollary 2.14, the denominators q(x) and $q(x)(1-x)^2$ have a simple factor $1 - r_m x$ that dominates the others, where $r_m > 1$ is the Perron eigenvalue of A_m , so that Corollary 2.14 then tells us that

$$c_m(n) \sim q_m \cdot r_m^n$$
 and $u_m(n) \sim v_m \cdot r_m^n$,

where

$$q_m = \frac{-r_m p(1/r_m)}{q'(1/r_m)}$$

and

$$v_m = \frac{-r_m [p(x)x^4]_{x=1/r_m}}{[q(x)(1-x)^2]'|_{x=1/r_m}}$$
$$= \frac{-r_m p(1/r_m)}{q'(1/r_m)(1-\frac{1}{r_m})^2 r_m^4}.$$

taking into account that $q(1/r_m) = 0$. It follows that

$$\lim_{n \to \infty} \frac{u_m(n)}{c_m(n)} = \frac{v_m}{q_m} = \frac{1}{r_m^2(r_m - 1)^2}.$$

Since the Perron eigenvalues r_m increase starting at 1.618... and converging to $1 + \sqrt{2}$ by Proposition 2.15, the constants $C_m = \frac{1}{r_m^2(r_m-1)^2}$ decrease starting at 0.345... and converge to $1.5 - \sqrt{2}$ as desired.

4 The Markov chains of monotone paths in a strip mix slowly.

We are finally ready to turn to the main goal of this paper: to investigate the mixing times of two natural Markov chains on the set of monotone paths of length n in a strip of height m, based on the local moves introduced in Section 1. We can think of these as random walks on the graph $S_{m,n}$.

4.1 **Preliminaries on Markov chains**

Let us review some basic facts about the mixing of Markov chains; for a more detailed account, see for example [LPW09].

Definition 4.1. A sequence of random variables $(X_0, X_1, ...)$ is a finite Markov chain with finite state space Ω and transition matrix P if for all $x, y \in \Omega$, all $t \ge 1$, and all events $H_{t-1} = \bigcap_{0 \le s \le t-1} (X_s = x_s)$ satisfying $P(H_{t-1} \cap (X_t = x)) > 0$, we have

$$\mathbf{P}(X_{t+1} = y \mid H_{t-1} \cap (X_t = x)) = \mathbf{P}(X_{t+1} = y \mid X_t = x) = P(x, y)$$

In words, the Markov property requires that the probability P(x, y) of moving from the current state $X_t = x$ to the next state $X_{t+1} = y$ does not depend on any earlier states.

A Markov chain is *irreducible* if for any $x, y \in \Omega$ there exists an integer $r \geq 0$ such that $P^r(x, y) > 0$. The *period* of a state x is the greatest common divisor of the *return* times t such that $P^t(x, x) > 0$. A Markov chain is *aperiodic* if every state x has period 1.

Definition 4.2. A probability distribution π over Ω is a stationary distribution for a Markov chain on Ω with transition matrix P if $\pi = \pi P$.

Theorem 4.3. If a Markov chain with transition matrix P is irreducible and aperiodic then it has a unique stationary distribution π . We have, for all $x, y \in \Omega$,

$$\lim_{t \to \infty} P^t(x, y) = \pi(y)$$

Proposition/Definition 4.4. [LPW09, Proposition 1.19] Suppose a Markov chain on Ω has transition matrix P. If a probability distribution π on Ω satisfies

$$\pi(x)P(x,y) = \pi(y)P(y,x) \qquad \forall x,y \in \Omega$$

the chain is said to be reversible with respect to π , and moreover, π is a stationary distribution for the Markov chain.

Consequently, if a Markov chain is irreducible, aperiodic, and reversible with respect to a distribution π , then π is the unique stationary distribution for the chain.

In order to quantify how quickly the chain converges to stationarity, we introduce the notions of total variation distance and mixing time.

Proposition/Definition 4.5. [LPW09, Proposition 4.2] The total variation distance between two probability distributions μ and ν on a state space Ω is:

$$\begin{aligned} ||\mu - \nu||_{TV} &:= & \max_{A \subseteq \Omega} |\mu(A) - \nu(A)| \\ &= & \frac{1}{2} \sum_{x \in \Omega} |\mu(x) - \nu(x)|. \end{aligned}$$

Definition 4.6. For a Markov chain $(X_0, X_1, ...)$ we define

$$d(t) \coloneqq \max_{x \in \Omega} ||P^t(x, \cdot) - \pi(\cdot)||_{TV}$$

The ε -mixing time of the Markov chain is defined to be

$$\tau(\varepsilon) \coloneqq \min\{t : d(t) \le \varepsilon\}.$$

The distance d(t) measures how far the farthest *t*-step distribution $P^t(x, \cdot)$ starting at an $x \in \Omega$ is from the stationary distribution π . The mixing time tells us how many steps we need to take until the *t*-step distribution starting at any state is within ε of the stationary distribution, measured in total variation distance.

The bottleneck ratio of a Markov chain is a geometric quantity that can provide upper as well as lower bounds on the mixing time. In our case, it is the lower bound which is relevant.

Definition 4.7. The bottleneck ratio or conductance of an irreducible and aperiodic Markov chain on Ω with transition matrix P is given by

$$\Phi := \min_{S \subset \Omega: 0 < \pi(S) \le \frac{1}{2}} \frac{\sum\limits_{x \in S, y \notin S} \pi(x) P(x, y)}{\pi(S)}.$$

In what follows in the rest of this section, we will always assume that the Markov chain in question is irreducible and aperiodic. Let the eigenvalues of its transition matrix be given by $1 = \lambda_0 > \lambda_1 \ge \cdots \ge \lambda_{|\Omega|-1} > -1$. Let $\lambda_{\max} = \max\{\lambda_1, |\lambda_{|\Omega|-1}|\}$. A lower bound in the mixing time can be established in two steps. The total variation distance to stationarity can be shown to be lower bounded below by the second largest eigenvalue in magnitude.

Theorem 4.8. $[MT^+06, Theorem 4.9]$ The mixing time of an irreducible Markov chain can be bounded as

$$\tau(\varepsilon) \ge \frac{|\lambda_{max}|}{1 - |\lambda_{max}|} \ln((2\varepsilon)^{-1}).$$

Secondly, the second largest eigenvalue in magnitude can be related to the conductance of the chain.

Theorem 4.9. [Sin93, Lemma 2.6] For an irreducible and reversible Markov chain with conductance Φ ,

$$\lambda_1 \ge 1 - 2\Phi$$

Since $\lambda_{\max} \geq \lambda_1$, the following is an immediate consequence.

Corollary 4.10. For an irreducible and reversible Markov chain with conductance Φ ,

$$\lambda_{max} \geq 1 - 2\Phi.$$

Combining Theorem 4.8 and Corollary 4.10 results in the following lower bound on the mixing time.

Theorem 4.11. For an irreducible and reversible Markov chain with conductance Φ ,

$$\tau(\varepsilon) \ge \frac{1 - 2\Phi}{2\Phi} \ln((2\varepsilon)^{-1}).$$

Therefore, to show that a Markov chain mixes slowly, it suffices to find a set S whose bottleneck ratio is very small.

4.2 The symmetric Markov chain of monotone paths in a strip.

Definition 4.12. (The symmetric Markov chain $M_{m,n}$ on monotone paths) Let $\Omega_{m,n}$ denote the set of monotone paths of length n in a strip of height m. For $t \ge 0$, if $X_t \in \Omega_{m,n}$ is the path at time t, we obtain the next path X_{t+1} as follows.

- 1. Choose any of the n + 1 vertices of the path uniformly at random, except the first one, so that each possibility has probability $\frac{1}{n}$.
- 2. (a) Suppose an interior vertex j is chosen. If X_t has a corner at vertex k, and the corner can be switched, switch that corner to get X_{t+1} . If it does not, let $X_{t+1} = X_t$.
 - (b) Suppose the last vertex is chosen. If the last step is N or S, flip it to E with probability $\frac{1}{2}$ and do nothing with probability $\frac{1}{2}$. If the last step is E, flip it to S with probability $\frac{1}{2}$ and to N with probability $\frac{1}{2}$.

Theorem 4.13. Let $m \geq 2$ be a fixed integer. The stationary distribution of the symmetric Markov chain $M_{m,n}$ is uniform. The mixing time of the chain $M_{m,n}$ grows exponentially with n; explicitly, there exists a constant C > 0 such that for n sufficiently large, the mixing time $\tau(\varepsilon)$ satisfies

$$\tau(\varepsilon) \ge C \cdot r_m^n \ln(\varepsilon^{-1})$$

where $r_m > 1$ is the Perron eigenvalue of A_m in Lemma 2.13.

Proof. To prove the first statement, we verify that our Markov chain $M_{m,n}$ on monotone paths has all the properties of Theorems 4.3 and 4.11. It is irreducible since there is a set of moves that allows us to go between any two arm configurations: one can start with the downset corresponding to the starting configuration, remove elements one at a time until we are at the empty downset, and then add elements back in to get to the final configuration. The chain is aperiodic since it contains states that are connected by one move to themselves. Finally, the chain is reversible with respect to the uniform distribution over monotone paths: for every pair of states x, y connected by a corner flip, $P(x,y) = P(y,x) = \frac{1}{n}$ while for a pair of states connected by flipping the end, $P(x,y) = P(y,x) = \frac{1}{2n}$. It follows that the stationary distribution is uniform.

To bound the mixing time, recall that in Lemma 3.19 we identified a small bottleneck of n+1 vertices in $S_{a \leftrightarrow b} := S(C_{m,n})_{a \leftrightarrow b}$ that separates the transition kernel $S = S(C_{m,n})$ of our Markov chain into two parts S_a and S_b that each contain roughly a constant fraction of the (exponentially many) vertices. This gives us that

$$\Phi \leq \frac{\sum\limits_{x \in \mathcal{S}_b, y \notin \mathcal{S}_b} \pi(x) P(x, y)}{\pi(\mathcal{S}_b)}$$
$$= \frac{\sum\limits_{x \in \mathcal{S}_b, y \in \mathcal{S}_a \nleftrightarrow b} P(x, y)}{|\mathcal{S}_b|}$$

since an edge xy that leaves S_b can only arrive in $S_{a \leftrightarrow b}$, and $\pi(x) = 1/c_m(n)$ for all x. Now, each $y \in S_{a \leftrightarrow b}$ is connected to at most one $x \in S_b$: if y corresponds to an order ideal I of the coral PIP $P_{m,n}$ that does not contain a or b, then x can only correspond to the order ideal $I \cup b$ that contains $b - \text{if } I \cup b$ is indeed an order ideal. It follows that

$$egin{array}{rcl} \Phi &\leq& \displaystylerac{|\mathcal{S}_{a \nleftrightarrow b}| \cdot rac{1}{n}}{|\mathcal{S}_b|} \ &\sim& \displaystylerac{1}{C_m q_m \cdot r_m^n} \end{array}$$

by Lemmas 3.17 and 3.19 and Corollary 2.14. The desired bound on the mixing time then follows from Theorem 4.11. $\hfill \Box$

4.3 The lazy simple Markov chain of monotone paths in a strip

The lazy simple Markov chain $N_{m,n}$ on monotone paths starts at an initial state Y_0 , and proceeds to state Y_{t+1} by uniformly at random performing one of the local moves that are available at Y_t . This Markov chain has period 2, because the parity of the number of vertical steps changes with every local move. To make it aperiodic, we apply the usual strategy: slow down the walk with probability 1 - p at each step.

Definition 4.14. (The lazy simple Markov chain $N_{m,n}^p$ on monotone paths) Let $0 . Let <math>\Omega_{m,n}$ denote the set of monotone paths of length n in a strip of height m. For $t \ge 0$, if $Y_t \in \Omega_{m,n}$ is the position of the path at time t, we obtain Y_{t+1} as follows:

- 1. With probability (1-p), do nothing: let $Y_{t+1} = Y_t$.
- 2. With probability p obtain Y_{t+1} by uniformly at random performing one of the local moves that are available at Y_t .

Theorem 4.15. Let $m \ge 2$ be a fixed integer. Let $N_{m,n}^p$ be the lazy simple Markov chain on monotone paths of length n in a strip of height m. The stationary distribution of $N_{m,n}^p$ is given by

$$\pi(x) \propto \deg x$$

for each path x, where deg x is the number of different local moves available at x.

The mixing time of the chain $N_{m,n}^p$ grows exponentially with n; explicitly, there exists a constant C > 0 such that for n sufficiently large, the mixing time $\tau(\varepsilon)$ satisfies

$$\tau(\varepsilon) \ge C \cdot \frac{1}{n} r_m^n \ln(\varepsilon^{-1})$$

where $r_m > 1$ is the Perron eigenvalue of A_m in Lemma 2.13.

Proof. The chain $N_{m,n}$ is irreducible for the same reasons as the chain $M_{m,n}$. It is aperiodic by construction. It can be verified that the chain is reversible with respect to the distribution π since for each pair of states $x \neq y$, $P(x, y) = p/\deg(x)$. Hence, π is the unique stationary distribution of the chain.

For the mixing time, we modify the proof in Theorem 4.13. Following the same notation, we have

$$\Phi \leq \frac{\sum\limits_{x \in \mathcal{S}_{b}, y \notin \mathcal{S}_{b}} \pi(x) P(x, y)}{\pi(\mathcal{S}_{b})}$$

$$= \frac{\sum\limits_{x \in \mathcal{S}_{b}, y \in \mathcal{S}_{a \nleftrightarrow b}} \deg(x) P(x, y)}{\sum\limits_{x \in \mathcal{S}_{b}} \deg(x)}$$

$$= \frac{\sum\limits_{x \in \mathcal{S}_{b}, y \in \mathcal{S}_{a \nleftrightarrow b}, xy \in E(S_{m,n})} p}{\sum\limits_{x \in \mathcal{S}_{b}} \deg(x)}$$

since $P(x, y) = p(1/\deg(x))$ whenever x and y are adjacent in the graph $S_{m,n}$, by the definition of the Markov chain.

Again, there are exactly n + 1 vertices in $S_{a \leftrightarrow b}$; let Y_0, \ldots, Y_n be the corresponding order ideals of the coral PIP $C_{m,n}$, where Y_i is a chain of length *i*. Notice that Y_i has exactly one neighbor in S_b – namely $X_i = Y_i \cup \{b\}$ – for $i = 2, \ldots, n$, and none for i = 0, 1. Also deg $(x) \geq 1$ for all x. This implies

$$\Phi \leq \frac{p(n-1)}{|\mathcal{S}_b|} \\ \sim \frac{pn}{C_m q_m \cdot r_m^n}$$

by Lemma 3.19 and Corollary 2.14. The desired bound on the mixing time follows by Theorem 4.11. $\hfill \Box$

5 Further Directions

- For the first few values of m, the polynomial $a_m(x)$ factor into two polynomials of degree $\lfloor \frac{1}{2}(3m+1) \rfloor$ and $\lceil \frac{1}{2}(3m+1) \rceil$ that are irreducible over \mathbb{Z} . Is this always the case? Which factor contributes the largest real root r_m ? Is r_m always inexpressible in terms of radicals?
- The denominator $\det(I xA_m) = (-x)^{3m+1}a_m(-1/x)$ in Theorem 2.7 is essentially equal to the characteristic polynomial $a_m(x)$, for which we found an explicit formula in Proposition 2.5. Can we also find an explicit formula for the numerator?
- Can we generalize the results in this paper to monotone paths in wedges, as studied by Janse van Rensburg, Prellberg, and Rechnitzer[JVRPR08]?
- The authors of [ABCG17a], ask whether the configuration space of not necessarily monotone, but still self-avoiding paths in a strip of height m is still CAT(0). In our context, we can ask about the growth rate constants which have been computed for $m \leq 2$ by Dangovski and Lalov [DL17] and the mixing times of the corresponding Markov chains.
- Is there a natural set of moves that connects the monotone paths of length n in a strip of height m, for which the Markov chain mixes in polynomial time?

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