

SIEGMUND DUALITY FOR MARKOV CHAINS ON PARTIALLY ORDERED STATE SPACES

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For a Markov chain on a finite partially ordered state space, we show that its Siegmund dual exists if and only if the chain is Möbius monotone. This is an extension of Siegmund's result for totally ordered state spaces, in which case the existence of the dual is equivalent to the usual stochastic monotonicity. Exploiting the relation between the stationary distribution of an ergodic chain and the absorption probabilities of its Siegmund dual, we present three applications: calculating the absorption probabilities of a chain with two absorbing states knowing the stationary distribution of the other chain; calculating the stationary distribution of an ergodic chain knowing the absorption probabilities of the other chain; and providing a stable simulation scheme for the stationary distribution of a chain provided we can simulate its Siegmund dual. These are accompanied by concrete examples: the gambler's ruin problem with arbitrary winning/losing probabilities; a non-symmetric game; an extension of a birth and death chain; a chain corresponding to the Fisher–Wright model; a non-standard tandem network of two servers, and the Ising model on a circle. We also show that one can construct a strong stationary dual chain by taking the appropriate Doob transform of the Siegmund dual of the time-reversed chain.

Keywords: Doob h -transform, gambler's ruin problem, Markov chains, Möbius monotonicity, partial ordering, Siegmund duality, strong stationary duality

1. INTRODUCTION

Siegmund [27] introduced a notion of duality (today called *Siegmund duality*) for discrete time Markov chains with a general state space with a total ordering. This duality is intended to relate the stationary distribution of the process with the absorption probability of its dual. In the case of a total ordering, Siegmund showed that the dual chain exists if and only if the original chain is stochastically monotone (w.r.t. the total ordering). The aim of this note is to generalize this result to state spaces, which are only partially ordered. Liggett in his famous book [16] (Chapter II, Section 3, page 87) writes (about Siegmund's result for the total ordering):

“This result depends heavily on the fact that the state space of the processes is totally ordered. In the particle system context, the state spaces are only partially ordered, and unfortunately the analogous result fails. [...] having a (reasonable) dual is a much more special property than being monotone, when the state space is not totally ordered.”

As our main result, we show that the existence of the Siegmund dual is equivalent to the Möbius monotonicity of the chain (a concept introduced in Lorek and Szekli [21]) w.r.t. a fixed partial ordering. In this case, we give the transitions of the dual.

It turns out that the usual stochastic monotonicity of a chain does not imply the existence of the Siegmund dual for general partial orderings (it does for linear orderings, since then stochastic monotonicity is equivalent to Möbius monotonicity). In general, the required Möbius monotonicity is not stronger, but different than stochastic monotonicity (examples are provided in Section 7).

There is a one-to-one correspondence (the relation is given in (2.4)) between the stationary distribution of an ergodic chain and the absorption probabilities of its Siegmund dual. We will present three potential applications of this relation. The first application is that given a chain with two absorbing states (gambler's ruin-like), we can find an ergodic chain for which the original one is the Siegmund dual. Then finding the stationary distribution of this chain determines the absorption probabilities. We present two examples for this application: (a) we recover the ruin/winning probabilities in the gambler's ruin problem with arbitrary winning/losing probabilities; (b) we present a non-symmetric game which turns out to be the Siegmund dual of the non-symmetric random walk on the cube considered in Lorek and Szekli [21]. Second application: given an ergodic chain, the task is to find its stationary distribution. We can calculate its Siegmund dual, and finding the absorption probabilities of the dual recovers the stationary distribution of the ergodic chain. Two examples of this application are provided: (a) the chain for which the Siegmund dual corresponds to the *gambler's ruin with catastrophes* considered in Hunter et al. [14], for which the absorption probabilities are calculated therein explicitly; (b) the chain for which the Siegmund dual turns out to be the so-called Fisher–Wright model. In the latter case, we also give the eigenvalues of the corresponding transition matrix. Third application: this is similar to the second one; we are given an ergodic chain, and the task is again to find its stationary distribution. Calculating the Siegmund dual can be relatively easy, but finding the absorption probabilities is often a challenging task. However, if we are able to simulate the dual, then we can have a *stable simulation scheme* for the stationary distribution of the ergodic chain via simply estimating the absorption probabilities. In contrast to most Monte Carlo Markov chains (MCMC) methods, we do not require a priori any knowledge about the rate of convergence, the mean absorption time, etc. Besides, MCMC are designed to provide a sample from the stationary distribution, whereas a stable simulation scheme lets us estimate the stationary distribution at a specific state. As examples, we present the Ising model on a circle and a tandem network of two servers. The latter example is a modification of the standard tandem (for which the stationary distribution is known): when one of the servers is empty, the rates of the other are changed. It turns out that then the stationary distribution is not known. Foley and McDonald [10] considered a similar modified tandem (if the server is idle it helps the other) showing large deviations and rough asymptotics for the stationary distribution. In particular, they showed that such changes on the borders imply dramatic changes in the stationary distribution.

Siegmund dualities appear in various contexts. The original paper of Siegmund [27] deals with stochastically monotone chains w.r.t the total ordering. Many authors have focused on birth and death chains, for example, Cox and Rösler [3], Diaconis and Fill [5] (where connections to strong stationary duality are also given), Dette et al. [4] (where Siegmund duality is related to Wall duality), and Huillet [12] (where a specific birth and death chain, the Moran model, was considered). The observation that such duality holds for some random walks on $\{0, 1, \dots\}$ goes back to Lindley [17]. The duality was also studied in an insurance context, where the probability that the steady-state queue length exceeds a level k equals the probability that a dual-risk process starting at level k is ruined in a finite time. There

have been some approaches to extend this to non-linear state spaces. Błaszczyszyn and Sigman [2] considered R^d -valued Markov processes (their Siegmund dual was set-valued). Recently, Huillet and Martínez [13] considered dualities related to the Möbius matrix for other non-linear state spaces, namely for Markov chains on partitions and sets. In Lorek and Szekli [21], we consider general partial orderings and show that the Möbius monotonicity of a time-reversed chain implies the existence of a strong stationary dual (SSD) chain on the same state space (more details in Section 5).

Recently, in Fill and Lyzinski [9] and in Miclo [23], dualities for one-dimensional diffusions were studied. Further research includes studying the existence of a Siegmund dual in d -dimensional diffusions, for example, the ones studied in Harrison and Williams [11], as well as developing the theory for Möbius monotone processes for continuous time and general state space chains.

The rest of this note is organized as follows. In Section 2, we describe Siegmund duality and the relations between the stationary distribution of a chain and the absorption probabilities of its dual. In Section 3, we recall the notion of Möbius monotonicity. In Section 4, we present our main result (Theorem 4.1) on the equivalence of Möbius monotonicity with the existence of the Siegmund dual chain for general partial orderings. Section 5 gives a connection to strong stationary duality. In Section 6, we give three applications: in Section 6.1, we recover the ruin probabilities for the gambler’s ruin problem with arbitrary losing/winning probabilities and provide a similar result in a different game; in Section 6.2, we give the stationary distributions of two chains exploiting existing results on ruin probabilities; in Section 6.3, we present stable simulation schemes for some non-standard tandem queueing system and for the Ising model on a circle. Finally in Section 7, we provide examples of chains showing relations between Möbius monotonicity and stochastic monotonicity. In particular, we show that Möbius monotonicity does not imply stochastic monotonicity.

2. SIEGMUND DUALITY

Let $X \sim (\nu, \mathbf{P}_X)$ be a discrete-time Markov chain with the initial distribution ν , transition matrix \mathbf{P}_X , and finite state space $\mathbb{E} = \{\mathbf{e}_1, \dots, \mathbf{e}_M\}$ partially ordered by \preceq . Throughout this paper, we assume that it is ergodic with stationary distribution π . We assume that there exists a unique minimal state, say \mathbf{e}_1 , and a unique maximal state, say \mathbf{e}_M . For $A \subseteq \mathbb{E}$, define $\mathbf{P}_X(\mathbf{e}, A) := \sum_{\mathbf{e}' \in A} \mathbf{P}_X(\mathbf{e}, \mathbf{e}')$ and similarly $\pi(A) := \sum_{\mathbf{e} \in A} \pi(\mathbf{e})$. Define also $\{\mathbf{e}\}^\uparrow := \{\mathbf{e}' \in \mathbb{E} : \mathbf{e} \preceq \mathbf{e}'\}$, $\{\mathbf{e}\}^\downarrow := \{\mathbf{e}' \in \mathbb{E} : \mathbf{e}' \preceq \mathbf{e}\}$ and $\delta(\mathbf{e}, \mathbf{e}') = \mathbf{1}(\mathbf{e}, \mathbf{e}')$. Recall that the chain X is *stochastically monotone* if

$$\forall(\mathbf{e} \preceq \mathbf{e}') \forall(\mathcal{U} - \text{up-set}) \quad \mathbf{P}_X(\mathbf{e}, \mathcal{U}) \leq \mathbf{P}_X(\mathbf{e}', \mathcal{U}), \tag{2.1}$$

where \mathcal{U} is an up-set if $(\mathbf{e}_a \preceq \mathbf{e}_b, \mathbf{e}_a \in \mathcal{U})$ implies $\mathbf{e}_b \in \mathcal{U}$. We say that a Markov chain Z with transition matrix \mathbf{P}_Z is the **Siegmund dual** of X if

$$\forall(\mathbf{e}_i, \mathbf{e}_j \in \mathbb{E}) \forall(n \geq 0) \quad \mathbf{P}_X^n(\mathbf{e}_i, \{\mathbf{e}_j\}^\downarrow) = \mathbf{P}_Z^n(\mathbf{e}_j, \{\mathbf{e}_i\}^\uparrow). \tag{2.2}$$

Siegmund [27] showed that for a total ordering (let us then denote the elements of \mathbb{E} by the numbers $\{1, 2, \dots, M\}$) such a dual exists if and only if X is stochastically monotone. The main thing then is to show that (2.2) holds for the one-step transitions. Since the main part of the proof is one line long, we include it here. We want to have $\mathbf{P}_X(i, \{j\}^\downarrow) = \mathbf{P}_Z(j, \{i\}^\uparrow)$.

We can calculate

$$\mathbf{P}_Z(j, i) = \mathbf{P}_Z(j, \{i\}^\uparrow) - \mathbf{P}_Z(j, \{i + 1\}^\uparrow) = \mathbf{P}_X(i, \{j\}^\downarrow) - \mathbf{P}_X(i + 1, \{j\}^\downarrow). \tag{2.3}$$

The latter is non-negative if and only if X is stochastically monotone. Note that (2.3) does not have to define the transition matrix, since we may have $\sum_i \mathbf{P}_Z(j, i) < 1$. Siegmund [27] adds then one extra absorbing state, call it 0, and defines $\mathbf{P}_Z(j, 0) = 1 - \sum_{i=1}^M \mathbf{P}_Z(j, i)$. In a similar way, for a general partial ordering, if we are able to find a subprobability kernel fulfilling (2.2) for all $\mathbf{e}_i, \mathbf{e}_j \in \mathbb{E}$, we may be forced to add one extra absorbing state, call it \mathbf{e}_0 . Note that (2.2) implies that \mathbf{e}_M is an absorbing state, thus Z has two absorbing states. Taking the limits as $n \rightarrow \infty$ on both sides of (2.2), we have

$$\pi(\{\mathbf{e}_j\}^\downarrow) = \lim_{n \rightarrow \infty} \mathbf{P}_Z^n(\mathbf{e}_j, \{\mathbf{e}_i\}^\uparrow) = P(Z \text{ is absorbed in } \mathbf{e}_M | Z_0 = \mathbf{e}_j). \tag{2.4}$$

The stationary distribution of X is related in this way to the absorption of its Siegmund dual Z .

3. MÖBIUS MONOTONICITY

Let $\mathbf{C}(\mathbf{e}_i, \mathbf{e}_j) = \mathbf{1}(\mathbf{e}_i \preceq \mathbf{e}_j)$. We can always rearrange the states so that $\mathbf{e}_i \preceq \mathbf{e}_j$ implies $i \leq j$. Then the matrix \mathbf{C} is 0–1 valued, upper triangular, and thus invertible. The inverse \mathbf{C}^{-1} is often denoted by μ and is called *the Möbius function*. Let $f, \bar{F} : \mathbb{E} \rightarrow \mathbb{R}$. The famous *Möbius inversion formula* (see, e.g., Rota [26]) states:

$$\text{Let } \bar{F}(\mathbf{e}) = \sum_{\mathbf{e}' \succeq \mathbf{e}} f(\mathbf{e}'), \text{ then } f(\mathbf{e}) = \sum_{\mathbf{e}' \succeq \mathbf{e}} \mu(\mathbf{e}, \mathbf{e}') \bar{F}(\mathbf{e}'). \tag{3.1}$$

We say that the function $\bar{F} : \mathbb{E} \rightarrow \mathbb{R}$ is Möbius monotone if $\sum_{\mathbf{e}' \succeq \mathbf{e}} \mu(\mathbf{e}, \mathbf{e}') \bar{F}(\mathbf{e}') \geq 0$ for all $\mathbf{e} \in \mathbb{E}$. This can be equivalently stated in matrix form: Let $\bar{\mathbf{F}} = (\bar{F}(\mathbf{e}_1), \dots, \bar{F}(\mathbf{e}_M))$. The Möbius monotonicity of \bar{F} means that $\mathbf{C}^{-1} \bar{\mathbf{F}} \geq 0$ (each entry is non-negative).

For each state $\mathbf{e}_2 \in \mathbb{E}$ write $\bar{F}_{\mathbf{e}_2}(\mathbf{e}') = \mathbf{P}_X(\mathbf{e}', \{\mathbf{e}_2\}^\downarrow)$. We say that the chain X is Möbius monotone if $\bar{F}_{\mathbf{e}_2}$ are Möbius monotone for all $\mathbf{e}_2 \in \mathbb{E}$. Equivalently, the definition can be stated in matrix form:

DEFINITION 3.1: *The Markov chain X with transition matrix \mathbf{P}_X is Möbius monotone w.r.t. the partial order \preceq if $\mathbf{C}^{-1} \mathbf{P}_X \mathbf{C} \geq 0$ (i.e., each entry is non-negative). In terms of the transition probabilities, this means that*

$$\forall (\mathbf{e}_i, \mathbf{e}_j \in \mathbb{E}) \quad \sum_{\mathbf{e} \succeq \mathbf{e}_i} \mu(\mathbf{e}_i, \mathbf{e}) \mathbf{P}_X(\mathbf{e}, \{\mathbf{e}_j\}^\downarrow) \geq 0.$$

Remark 3.2: In a similar way to (3.1), we have the following version of the Möbius inversion formula:

$$\text{Let } F(\mathbf{e}) = \sum_{\mathbf{e}' \preceq \mathbf{e}} f(\mathbf{e}'), \text{ then } f(\mathbf{e}) = \sum_{\mathbf{e}' \preceq \mathbf{e}} \mu(\mathbf{e}', \mathbf{e}) F(\mathbf{e}').$$

This way, once $\pi(\{\mathbf{e}_j\}^\downarrow)$ is calculated for all $\mathbf{e}_j \in \mathbb{E}$ in (2.4), we can calculate $\pi(\mathbf{e}_j) = \sum_{\mathbf{e} \preceq \mathbf{e}_j} \mu(\mathbf{e}, \mathbf{e}_j) \pi(\{\mathbf{e}\}^\downarrow)$.

For more details on Möbius monotonicity, see Lorek and Szekli [21].

4. MAIN RESULT

In this section, we will show the existence of the Siegmund dual on the state space $\mathbb{E}^* = \{\mathbf{e}_0\} \cup \mathbb{E}$, where we have added one extra absorbing state, \mathbf{e}_0 . At each step, the process can be possibly *killed*, that is, absorbed in this state.

THEOREM 4.1: *Let $X \sim (\nu, \mathbf{P}_X)$ be a Markov chain on $\mathbb{E} = \{\mathbf{e}_1, \dots, \mathbf{e}_M\}$ with partial ordering \preceq . Assume that \mathbf{e}_1 is the unique minimal state and \mathbf{e}_M is the unique maximal state. Then there exists a Siegmund dual Z of X on $\mathbb{E}^* = \{\mathbf{e}_0\} \cup \mathbb{E}$ if and only if X is Möbius monotone. The transitions of the dual are as follows:*

$$\begin{aligned}
 \mathbf{P}_Z(\mathbf{e}_j, \mathbf{e}_i) &= \sum_{\mathbf{e}' \succeq \mathbf{e}_i} \mu(\mathbf{e}_i, \mathbf{e}') \mathbf{P}_X(\mathbf{e}', \{\mathbf{e}_j\}^\downarrow), & \mathbf{e}_i, \mathbf{e}_j \in \mathbb{E}, \\
 \mathbf{P}_Z(\mathbf{e}_0, \mathbf{e}_j) &= \delta(\mathbf{e}_0, \mathbf{e}_j), & \mathbf{e}_j \in \mathbb{E}^*, \\
 \mathbf{P}_Z(\mathbf{e}_k, \mathbf{e}_0) &= 1 - \sum_{\mathbf{e} \in \mathbb{E}} \mathbf{P}_Z(\mathbf{e}_k, \mathbf{e}), & \mathbf{e}_k \in \mathbb{E}.
 \end{aligned}
 \tag{4.1}$$

PROOF: Note that the state space of the dual is enriched with one extra absorbing state, called \mathbf{e}_0 . We need Eq. (2.2) to hold for all states from \mathbb{E} . One can think that \mathbf{e}_0 is incomparable to all the other states in \mathbb{E}^* , which we assume, since it simplifies some of the notation.

First, we show that (2.2) holds for $n = 1$, which can be rewritten as

$$\mathbf{P}_X(\mathbf{e}_i, \{\mathbf{e}_j\}^\downarrow) = \sum_{\mathbf{e} \succeq \mathbf{e}_i} \mathbf{P}_Z(\mathbf{e}_j, \mathbf{e}).$$

Using the Möbius inversion formula (3.1), we have

$$\mathbf{P}_Z(\mathbf{e}_j, \mathbf{e}_i) = \sum_{\mathbf{e} \succeq \mathbf{e}_i} \mu(\mathbf{e}_i, \mathbf{e}) \mathbf{P}_X(\mathbf{e}, \{\mathbf{e}_j\}^\downarrow),
 \tag{4.2}$$

which is non-negative if and only if X is Möbius monotone. For a partial order with a unique minimal element \mathbf{e}_1 , the Möbius function satisfies $\sum_{\mathbf{e}_i \in \mathbb{E}} \mu(\mathbf{e}_i, \mathbf{e}) = \mathbf{1}(\mathbf{e} = \mathbf{e}_1)$ (to see this, consider the first row of \mathbf{C}^{-1} after applying the first elementary row operation of Gauss–Jordan elimination). This implies that the right-hand side of (4.2) is not greater than 1, since

$$\begin{aligned}
 \sum_{\mathbf{e}_i \in \mathbb{E}} \mathbf{P}_Z(\mathbf{e}_j, \mathbf{e}_i) &= \sum_{\mathbf{e}_i \in \mathbb{E}} \sum_{\mathbf{e} \succeq \mathbf{e}_i} \mu(\mathbf{e}_i, \mathbf{e}) \mathbf{P}_X(\mathbf{e}, \{\mathbf{e}_j\}^\downarrow) \\
 &\stackrel{(*)}{=} \sum_{\mathbf{e}_i \in \mathbb{E}} \sum_{\mathbf{e}} \mu(\mathbf{e}_i, \mathbf{e}) \mathbf{P}_X(\mathbf{e}, \{\mathbf{e}_j\}^\downarrow) \\
 &= \sum_{\mathbf{e}} \mathbf{P}_X(\mathbf{e}, \{\mathbf{e}_j\}^\downarrow) \sum_{\mathbf{e}_i \in \mathbb{E}} \mu(\mathbf{e}_i, \mathbf{e}) = \mathbf{P}_X(\mathbf{e}_1, \{\mathbf{e}_j\}^\downarrow) \leq 1,
 \end{aligned}$$

where in (*) we used the fact that $\mu(\mathbf{e}_i, \mathbf{e}) = 0$ for $\mathbf{e}_i \not\preceq \mathbf{e}$ (see, e.g., the proof of Proposition 1 in Rota [26]).

Note that the submatrix \mathbf{P}_Z with the column and row corresponding to state \mathbf{e}_0 excluded can be written as $(\mathbf{C}^{-1} \mathbf{P}_X \mathbf{C})^T$, that is, we have $\mathbf{P}_Z(\mathbf{e}_j, \mathbf{e}_i) = (\mathbf{C}^{-1} \mathbf{P}_X \mathbf{C})^T(\mathbf{e}_j, \mathbf{e}_i)$

for $\mathbf{e}_j, \mathbf{e}_i \in \mathbb{E}$. The Chapman–Kolmogorov equations allow extending the transition probabilities to $\mathbf{P}_Z^n(\mathbf{e}_j, \mathbf{e}_i)$ for all $\mathbf{e}_j, \mathbf{e}_i \in \mathbb{E}^*$ and $n \geq 0$. Then the dual chain is defined. To see that (2.2) holds for $\mathbf{e}_j, \mathbf{e}_i \in \mathbb{E}$, note that since \mathbf{e}_0 is an absorbing state, we must have $\mathbf{P}_Z^n = (\mathbf{C}^{-1}\mathbf{P}_X^n\mathbf{C})^T$, that is,

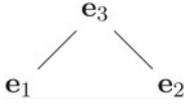
$$\mathbf{C}(\mathbf{P}_Z^n)^T = \mathbf{P}_X^n\mathbf{C}, \tag{4.3}$$

which is (2.2) written in matrix form. ■

Remark 4.2: Note that the Siegmund dual chain will have two absorbing states. Beside the extra state \mathbf{e}_0 , the state which is maximal w.r.t. \preceq is also absorbing. Indeed,

$$\begin{aligned} \mathbf{P}_Z(\mathbf{e}_M, \mathbf{e}_i) &= \sum_{\mathbf{e}' \succeq \mathbf{e}_i} \mu(\mathbf{e}_i, \mathbf{e}') \mathbf{P}_X(\mathbf{e}', \{\mathbf{e}_M\}^\downarrow) \\ &= \sum_{\mathbf{e}' \succeq \mathbf{e}_i} \mu(\mathbf{e}_i, \mathbf{e}') = \mathbf{1}(\mathbf{e}_i = \mathbf{e}_M). \end{aligned}$$

Remark 4.3: The assumption of the existence of the minimal state cannot be relaxed, as the following example shows (with the Hasse diagram of the ordering on the right-hand side):

$$\mathbf{P}_X = \begin{pmatrix} \frac{4}{6} & \frac{1}{6} & \frac{1}{6} \\ \frac{4}{6} & \frac{1}{6} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{6} & \frac{4}{6} \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix},$$


In other words, we have three states, say $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$. The state \mathbf{e}_3 is a maximal one and the states $\mathbf{e}_1, \mathbf{e}_2$ are incomparable. Then we can calculate

$$(\mathbf{C}^{-1}\mathbf{P}_X\mathbf{C})^T = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{6} \\ 0 & 0 & \frac{1}{6} \\ 0 & 0 & 1 \end{pmatrix}.$$

Thus, the \mathbf{P}_Z given in (4.2) does not define a subprobability kernel.

Remark 4.4: For given X we can distinguish two Siegmund dual chains. The one defined in (2.2) can be called the *Siegmund[↓] dual*, say Z^\downarrow . The other, say Z^\uparrow , called the *Siegmund[↑] dual*, is the one fulfilling

$$\forall(\mathbf{e}_i, \mathbf{e}_j \in \mathbb{E}) \forall(n \geq 0) \quad \mathbf{P}_X^n(\mathbf{e}_i, \{\mathbf{e}_j\}^\uparrow) = \mathbf{P}_Z^n(\mathbf{e}_j, \{\mathbf{e}_i\}^\downarrow).$$

The monotonicity defined in Lorek and Szekli [21] was actually called [↓]-Möbius monotonicity, whereas [↑]-Möbius monotonicity was defined as $(\mathbf{C}^T)^{-1}\mathbf{P}\mathbf{C}^T \geq 0$. In a similar way one can have a version of Theorem 4.1, showing that the Siegmund[↑] dual exists if and only if X is [↑]-Möbius monotone. We skip the details, noting that these monotonicities are not equivalent (see Lorek and Markowski [20] for details).

The matrix form (4.3) implies the following corollary.

COROLLARY 4.5: *Denote the eigenvalues of \mathbf{P}_Z by $\lambda_0 = 1, \lambda_1, \dots, \lambda_M = 1$ (the eigenvalues λ_0 and λ_M correspond to two absorbing states). Then $\lambda_1, \dots, \lambda_M$ are the eigenvalues of \mathbf{P}_X .*

5. SIEGMUND DUALITY AND STRONG STATIONARY DUALITY

In this section, we point out a connection with strong stationary duality. Diaconis and Fill [5] show that their SSD chain can be constructed in three steps, where one step involves calculating the Siegmund dual w.r.t. the total ordering. It turns out that the SSD chain given in Lorek and Szekli [21] can be constructed in three similar steps, where one involves calculating the Siegmund dual w.r.t. a fixed partial ordering.

Recall that $X \sim (\nu, \mathbf{P})$ is an ergodic Markov chain on the finite state space $\mathbb{E} = \{\mathbf{e}_1, \dots, \mathbf{e}_M\}$ with the stationary distribution π . Let $\mathbb{E}^* = \{\mathbf{e}_1^*, \dots, \mathbf{e}_N^*\}$ be the, possibly different, state space of the absorbing Markov chain $X^* \sim (\nu^*, \mathbf{P}^*)$ whose unique absorbing state is denoted by \mathbf{e}_N^* . An $N \times M$ matrix Λ is called a *link* if it is a stochastic matrix satisfying $\Lambda(\mathbf{e}_N^*, \mathbf{e}) = \pi(\mathbf{e})$. We say that X^* is a SSD of X with link Λ if

$$\nu = \nu^* \Lambda \quad \text{and} \quad \Lambda \mathbf{P} = \mathbf{P}^* \Lambda.$$

Diaconis and Fill [5] prove that then the absorption time T^* of X^* is the so called *strong stationary time* for X . This is a random variable T such that X_T has distribution π and T is independent of X_T . The main application is to studying the rate of convergence of an ergodic chain to its stationary distribution, since for such a random variable we always have $d_{TV}(\nu \mathbf{P}^k, \pi) \leq \text{sep}(\nu, \mathbf{P}^k, \pi) \leq P(T > k)$, where d_{TV} stands for the *total variation distance*, and *sep* stands for the *separation “distance”*. For details, see Diaconis and Fill [5].

In general, there is no recipe on how to find an SSD, that is, a triple $\mathbb{E}^*, \mathbf{P}^*, \Lambda$. Diaconis and Fill [5] give a recipe for a dual on the same state space $\mathbb{E}^* = \mathbb{E}$ provided that the time-reversed chain \overleftarrow{X} is stochastically monotone with respect to the total ordering. For a given \mathbf{P} , let h be its harmonic function, that is, a non-negative function h such that $\mathbf{P}h = h$. By \mathbf{h} we denote the vector $\mathbf{h} = (h(\mathbf{e}_1), \dots, h(\mathbf{e}_M))$. Then \mathbf{P}_h , defined as $\mathbf{P}_h(\mathbf{e}, \mathbf{e}') = \mathbf{P}(\mathbf{e}, \mathbf{e}')h(\mathbf{e}')/h(\mathbf{e})$ on $\{\mathbf{e} : h(\mathbf{e}) > 0\}$, is a transition matrix and is often called the *Doob h-transform* of \mathbf{P} . The SSD, in the case when the time-reversed chain is stochastically monotone, is then given by the authors in three steps (Theorem 5.5 in Diaconis and Fill [5]):

- (i) Calculate the time reversal $\overleftarrow{\mathbf{P}}$ of \mathbf{P} .
- (ii) Calculate the Siegmund dual $(\overleftarrow{\mathbf{P}})_Z$ of $\overleftarrow{\mathbf{P}}$.
- (iii) Calculate the Doob \mathbf{H} -transform $\mathbf{P}^* = ((\overleftarrow{\mathbf{P}})_Z)_\mathbf{H}$ of $(\overleftarrow{\mathbf{P}})_Z$, where $\mathbf{H} = \pi \mathbf{C}$ with $\pi = (\pi(\mathbf{e}_1), \dots, \pi(\mathbf{e}_M))$.

In the above procedure, the Siegmund dual must be calculated w.r.t. a total ordering, and then we have $\mathbf{C}(\mathbf{e}, \mathbf{e}') = \mathbf{1}(\mathbf{e} \leq \mathbf{e}')$.

In Lorek and Szekli [21], we give a recipe for an SSD on the same state space $\mathbb{E}^* = \mathbb{E}$ for those chains whose time reversal is Möbius monotone with respect to a partial ordering expressed by the matrix $\mathbf{C}(\mathbf{e}, \mathbf{e}') = \mathbf{1}(\mathbf{e} \preceq \mathbf{e}')$. In matrix form, the transitions are given by

$$\mathbf{P}^* = \text{diag}(\mathbf{H})^{-1}(\mathbf{C}^{-1} \overleftarrow{\mathbf{P}} \mathbf{C})^T \text{diag}(\mathbf{H}),$$

where $\mathbf{H} = \pi \mathbf{C}$ (i.e., $\mathbf{H} = (H(\mathbf{e}_1), \dots, H(\mathbf{e}_M))$ with $H(\mathbf{e}) = \sum_{\mathbf{e}': \mathbf{e}' \preceq \mathbf{e}} \pi(\mathbf{e}')$) and $\text{diag}(\mathbf{H})$ denoting the diagonal matrix with the vector \mathbf{H} on the diagonal. Thus, \mathbf{P}^* is a Doob \mathbf{H} -transform of $(\mathbf{C}^{-1} \overleftarrow{\mathbf{P}} \mathbf{C})^T$, which is exactly the Siegmund dual of $\overleftarrow{\mathbf{P}}$ from Theorem 4.1. In other words, the SSD given in Lorek and Szekli [21] results from exactly the same steps (i)–(iii) as in Theorem 5.5 in Diaconis and Fill [5].

Remark 5.1: For a non-linear ordering, Möbius monotonicity and stochastic monotonicity are, in general, different. In particular, we can have a chain, which is not stochastically monotone, but for which we can construct both a Siegmund dual and a SSD, since it can be Möbius monotone (for an example, see Section 7.2). According to our knowledge, Falin [7] was the first who observed that these are two different notions of monotonicity (however, connections to dualities were not given there). In a subsequent paper, Lorek and Markowski [20], we gave more details on the relations between Möbius, realizable, weak, and the usual stochastic monotonicities in chains on partially ordered state spaces.

6. APPLICATIONS

Let us recall the relation between the stationary distribution of X and the absorption probabilities of its Siegmund dual Z (i.e., (2.4))

$$\pi(\{\mathbf{e}_j\}^\downarrow) = P(Z \text{ is absorbed in } \mathbf{e}_M | Z_0 = \mathbf{e}_j).$$

This relation can have three potential applications:

- (A1) Suppose we are given a Markov chain Z with two absorbing states (*winning* and *losing*). To calculate the probability of being absorbed in one of them, we can find an ergodic chain X for which Z is its Siegmund dual. Then the task reduces to calculating the stationary distribution of X .
- (A2) Suppose we are given an ergodic Markov chain X . The task is to find its stationary distribution. Then we can calculate its Siegmund dual Z and if we are able to determine the absorption probabilities, then we have found the stationary distribution of X .
- (A3) Similarly to (A2): We are given an ergodic chain X . Assume that the approach given in (A2) is infeasible: we can find the Siegmund dual, but we are unable to calculate its absorption probabilities, but we are nevertheless able to simulate it. Then we have a so-called *stable simulation scheme* for estimating the stationary distribution. To estimate $\pi(\{\mathbf{e}\}^\downarrow)$, we calculate the Siegmund dual Z of X and simulate it several times, always starting the chain at \mathbf{e} , and simply estimate the winning/losing probabilities. The value of $\pi(\mathbf{e})$ can be estimated by estimating $\pi(\{\mathbf{e}'\}^\downarrow)$ at several points \mathbf{e}' , see Remark 3.2.

In this section, we provide two examples for each type of application. In Section 6.1 (A1), we consider gambler's ruin problems: first we give a simple proof of the ruin probability in the gambler's ruin problem with arbitrary winning/losing probabilities, then we solve another version of the game. In Section 6.2 (A2), we exploit the results from the literature on the ruin probabilities in the Fisher–Wright population model and on the “gambler's ruin with catastrophes” problem to determine the stationary distribution of some chains. In the first one, we also determine its eigenvalues. Section 6.3 (A3) includes stable simulation schemes and numerical results for the Ising model (on a circle) and a non-standard tandem network of two stations. In both cases, an error analysis is provided.

Stable simulation schemes vs Markov chain Monte Carlo methods. Classical Markov chain Monte Carlo methods are mainly used to obtain a sample from the stationary distribution of given chain. They can however also be used to estimate $\pi(A)$ for some subset A of the state space. For example, a natural estimator of $\pi(A)$ is the sample proportion of visits to A , that is, $\hat{\pi}^{\text{MCMC}}(A) = (1/n) \sum_{i=1}^n \mathbf{1}_A(X_j)$, where $\mathbf{1}_A$ is the indicator of A .

However, the “quality” of the estimation depends strongly on the rate of convergence of X to its stationary distribution. Such an estimator was considered in Athreya and Majumdar [1]. Estimating the stationary distribution at one state was considered in Lee, Ozdaglar, and Shah [15]. In contrast, for a stable simulation scheme, we do not need any knowledge about, for example, the rate of convergence or the time to absorption, we simply run the Siegmund dual Z until it is absorbed. We thus actually estimate the mean of a Bernoulli random variable. This can be done by the Monte Carlo estimator, providing also a confidence interval (thus an error analysis can also be provided, which is done in Section 6.3).

6.1. Application A1: Explicit Formulas for the Probabilities of Winning and Losing

6.1.1. *Application A1: Recovering the ruin probability in the one-dimensional gambler’s ruin problem with arbitrary winning/losing probabilities.* Consider the chain Z on $\mathbb{E}^* = \{0, 1, \dots, M\}$ with the transitions

$$\mathbf{P}_Z(i, j) = \begin{cases} p_i & \text{if } j = i + 1, \\ q_i & \text{if } j = i - 1, \\ 1 - p_i - q_i & \text{if } j = i \end{cases} \tag{6.1}$$

with positive p_i, q_i such that $p_i + q_i \leq 1$ for $i = 1, \dots, M - 1$ and $p_0 = q_0 = 0, p_M = q_M = 0$. This is a birth and death chain with two absorbing states, 0 and M , which can be thought of as a generalized one-dimensional gambler’s ruin problem. We are interested in

$$\rho(i) = P(\tau_M < \tau_0 | Z_0 = i),$$

where $\tau_i = \inf\{n \geq 0 : Z_n = i\}$. The case $p_i = p > 0, q_i = q > 0$ for $i = 1, \dots, M$ is the classical gambler’s ruin problem. The formula for $\rho(i)$ goes back to Parzen [24] (Section 6-6, Eq. (6.27)). We will recover the result via Siegmund duality with an additional assumption. This example is intended to present a simple, yet powerful, application of (2.4) in the case of a total ordering.

LEMMA 6.1: *Consider the above generalized one-dimensional gambler’s ruin problem. Assume that*

$$p_{i-1} + q_i \leq 1, i = 1, \dots, M. \tag{6.2}$$

Then we have

$$\rho(i) = \frac{\sum_{n=1}^i \prod_{r=1}^{n-1} (q_r/p_r)}{\sum_{n=1}^M \prod_{r=1}^{n-1} (q_r/p_r)}.$$

PROOF: Because of assumption (6.2), the matrix

$$\mathbf{P}_X(i, j) = \begin{cases} q_i & \text{if } j = i + 1, \\ p_{i-1} & \text{if } j = i - 1, \\ 1 - p_{i-1} - q_i & \text{if } j = i, \end{cases}$$

is the transition matrix of a chain X on $\mathbb{E} = \{1, \dots, M\}$. It turns out that Z is a Siegmund dual of X . Using (2.3), that is, $\mathbf{P}_Z(j, i) = \mathbf{P}_X(i, \{j\}^\downarrow) - \mathbf{P}_X(i + 1, \{j\}^\downarrow)$, we have

$$\begin{aligned} \mathbf{P}_Z(i, i - 1) &= \mathbf{P}_X(i - 1, \{i\}^\downarrow) - \mathbf{P}_X(i, \{i\}^\downarrow) = 1 - (1 - q_i) = q_i, & 1 < i \leq M, \\ \mathbf{P}_Z(i, i + 1) &= \mathbf{P}_X(i + 1, \{i\}^\downarrow) - \mathbf{P}_X(i + 2, \{i\}^\downarrow) = p_i, & 1 \leq i < M, \\ \mathbf{P}_Z(i, i) &= \mathbf{P}_X(i, \{i\}^\downarrow) - \mathbf{P}_X(i + 1, \{i\}^\downarrow) = 1 - q_i - p_i, & i \leq M, \\ \mathbf{P}_Z(i, j) &= 0, & |i - j| > 1. \end{aligned}$$

The first row is the only one which does not sum to 1 (it sums to $1 - q_1$). Thus, we add one extra absorbing state, “0” (i.e., $\mathbb{E}^* = \{0\} \cup \mathbb{E} = \{0, 1, \dots, M\}$) and transition $\mathbf{P}_Z(1, 0) = q_1$, obtaining the chain given in (6.1). Note that X is a birth and death chain on \mathbb{E} with birth rate q_i and death rate p_{i-1} (both given that we are at state i), thus its stationary distribution is

$$\pi(n) = \frac{\prod_{r=1}^{n-1} (q_r/p_r)}{\sum_{k=1}^M \prod_{r=1}^{k-1} (q_r/p_r)}.$$

Applying (2.4) completes the proof. ■

Remark 6.2: The assumption (6.2) is equivalent to the stochastic monotonicity of the chain (w.r.t. the total ordering, for which it is equivalent to Möbius monotonicity) and is not essentially needed for a duality-based proof, see Lorek [19] for details (where the more general, multidimensional gambler’s ruin problem is considered).

6.1.2. Application A1: A non-symmetric game: explicit formula for the probabilities of winning and losing. In this section, we consider another “gambler-ruin like” game. The states of the game are $(0, \text{WON}, \text{LOST})$. The state 0 means we have not yet either won or lost. The names of the other states speak for themselves. We start at state 0. At each step we can win with probability $p > 0$, lose with probability $q > 0$, or nothing can happen with probability $1 - (p + q)$. Of course, eventually we will end up in the *WON* or *LOST* state with probabilities $p/(p + q)$ and $q/(p + q)$, respectively.

Now consider the following generalization. We are given d games G_1, \dots, G_d and parameters $p_i, q_i, i = 1, \dots, d$ such that $\sum_{i=1}^d (p_i + q_i) \leq 1$. We win the whole game if we win all the games G_1, \dots, G_d and we lose the whole game if we lose at least one game $G_i, i \in \{1, \dots, d\}$. If we win game G_i , we will not play it anymore. The generic state is either $\mathbf{e}_L := \text{LOST}$ or $\mathbf{e} = (\mathbf{e}(1), \dots, \mathbf{e}(d)), \mathbf{e}(i) \in \{0, 1\}, i = 1, \dots, d$, where $\mathbf{e}(i) = 1$ means that we have already won game G_i . Write $\mathbf{e}_W := (1, \dots, 1)$. At each step we can win the new game G_i with probability p_i (provided we have not won it already) or lose it with probability q_i (in which case we automatically lose the whole game), or we can do nothing, with the remaining probability $1 - \sum_{i:\mathbf{e}(i)=0} (p_i + q_i)$. The described dynamics is a Markov chain, call it Z , on the state space $\mathbb{E}^* = \{0, 1\}^d \cup \{\mathbf{e}_L\}$, with the following transitions:

$$\mathbf{P}_Z(\mathbf{e}, \mathbf{e}') = \begin{cases} p_i & \text{if } \mathbf{e}' = \mathbf{e} + \mathbf{s}_i, \\ \sum_{i:\mathbf{e}(i)=0} q_i & \text{if } \mathbf{e}' = \mathbf{e}_L, \mathbf{e} \neq \mathbf{e}_L, \\ 1 - \sum_{i:\mathbf{e}(i)=0} (p_i + q_i) & \text{if } \mathbf{e}' = \mathbf{e} \neq \mathbf{e}_L, \\ 1 & \text{if } \mathbf{e}' = \mathbf{e} = \mathbf{e}_L, \end{cases} \tag{6.3}$$

where $\mathbf{s}_i = (0, \dots, 0, 1, 0, \dots, 0)$ with 1 at the i th coordinate. The chain has two absorbing states: \mathbf{e}_L and \mathbf{e}_W (we lose or we win). Eventually, the chain will be absorbed in one of them. A natural question arises: *What is the probability of winning the whole game starting with an arbitrary set of already won games $\mathbf{e}' \in \mathbb{E}$?* In other words, we want to calculate the following probabilities:

$$\rho(\mathbf{e}') = P(\tau_{\mathbf{e}_M} < \tau_{\mathbf{e}_L} \mid Z_0 = \mathbf{e}'),$$

where $\tau_{\mathbf{e}} := \inf\{n \geq 0 : Z_n = \mathbf{e}\}$. To answer the question, consider first another chain, the non-symmetric random walk X on $\mathbb{E} = \{0, 1\}^d$, defined for the same parameters $p_i, q_i, i = 1, \dots, d$, with the transitions

$$\mathbf{P}_X(\mathbf{e}, \mathbf{e}') = \begin{cases} q_i & \text{if } \mathbf{e}' = \mathbf{e} + \mathbf{s}_i, \\ p_i & \text{if } \mathbf{e}' = \mathbf{e} - \mathbf{s}_i, \\ 1 - \sum_{i:\mathbf{e}(i)=0} q_i - \sum_{i:\mathbf{e}(i)=1} p_i & \text{if } \mathbf{e}' = \mathbf{e}. \end{cases}$$

Under the mild assumption that at least for one state \mathbf{e} we have that $\mathbf{P}_X(\mathbf{e}, \mathbf{e}) > 0$, the chain is ergodic with the stationary distribution

$$\pi(\mathbf{e}) = \prod_{i:\mathbf{e}(i)=1} \frac{q_i}{p_i + q_i} \prod_{i:\mathbf{e}(i)=0} \frac{p_i}{p_i + q_i}.$$

Let $|\mathbf{e}| = \sum_{i=1}^d \mathbf{e}(i)$ (called a *level* of \mathbf{e}). We consider the coordinate-wise ordering, that is, $\mathbf{e} \preceq \mathbf{e}'$ if $\mathbf{e}(i) \leq \mathbf{e}'(i)$ for all $i = 1, \dots, d$. The state $\mathbf{e}_1 = (0, \dots, 0)$ is the unique minimal state and $\mathbf{e}_M = (1, \dots, 1)$ is the unique maximal one. Then (\mathbb{E}, \preceq) is a Boolean lattice with the following Möbius function:

$$\mu(\mathbf{e}, \mathbf{e}') = (-1)^{|\mathbf{e}'| - |\mathbf{e}|} \mathbf{1}(\mathbf{e} \preceq \mathbf{e}').$$

To calculate the Siegmund dual, we have to calculate

$$\mathbf{P}_Z(\mathbf{e}, \mathbf{e}') = \sum_{\mathbf{e}_2 \succeq \mathbf{e}'} \mu(\mathbf{e}', \mathbf{e}_2) \mathbf{P}_X(\mathbf{e}_2, \{\mathbf{e}\}^\downarrow). \tag{6.4}$$

Consider the case $\mathbf{e}' = \mathbf{e} + \mathbf{s}_i$. Then there is one state $\mathbf{e}_2 \succeq \mathbf{e} + \mathbf{s}_i$ in (6.4) for which $\mathbf{P}_X(\mathbf{e}_2, \{\mathbf{e}\}^\downarrow) > 0$, namely $\mathbf{e}_2 = \mathbf{e} + \mathbf{s}_i$. We have

$$\mathbf{P}_Z(\mathbf{e}, \mathbf{e} + \mathbf{s}_i) = \sum_{\mathbf{e}_2 \succeq \mathbf{e} + \mathbf{s}_i} \mu(\mathbf{e} + \mathbf{s}_i, \mathbf{e}_2) \mathbf{P}_X(\mathbf{e}_2, \{\mathbf{e}\}^\downarrow) = p_i.$$

In Lorek and Szekli [21], we calculated SSD of \mathbf{P}_X . Thus, according to Section 5, we have also calculated its Siegmund dual. That is why we skip the remaining calculations. It turns out that \mathbf{P}_Z given in (6.3) is the Siegmund dual of X . The chain X is thus Möbius monotone if and only if $\sum_{i=1}^d (p_i + q_i) \leq 1$. Note that for any $\mathbf{e} \in \mathbb{E}$, we have $\sum_{\mathbf{e}' \in \mathbb{E}} \mathbf{P}_Z(\mathbf{e}, \mathbf{e}') = 1 - \sum_{i:\mathbf{e}(i)=0} q_i$. We add one extra absorbing state, call it \mathbf{e}_L , and we end up exactly with the

transitions given in (6.3). Thus via (2.4), we have

$$\rho(\mathbf{e}') = \sum_{\mathbf{e} \leq \mathbf{e}'} \prod_{i:\mathbf{e}(i)=1} \frac{q_i}{p_i + q_i} \prod_{i:\mathbf{e}(i)=0} \frac{p_i}{p_i + q_i}.$$

For example, if $p_i = p$ and $q_i = q$ for all $i = 1, \dots, d$, then we have

$$\begin{aligned} \rho(\mathbf{e}') &= \frac{1}{(p + q)^d} \sum_{\mathbf{e} \leq \mathbf{e}'} q^{|\mathbf{e}'|} p^{d-|\mathbf{e}'|} \\ &= \frac{1}{(p + q)^d} \sum_{k=0}^{|\mathbf{e}'|} \binom{|\mathbf{e}'|}{k} q^k p^{d-k} = \left(\frac{p}{p + q}\right)^{d-|\mathbf{e}'|}. \end{aligned}$$

Note that then of course the probability $\rho(\mathbf{e}')$ depends only on the level $|\mathbf{e}'|$. In particular, for $p = q$ we have that $\rho(\mathbf{e}') = 2^{|\mathbf{e}'|-d}$.

Remark 6.3: The matrix \mathbf{P}_Z can be written as an upper triangular matrix, and thus we can read off the eigenvalues from the diagonal. Corollary 4.5 implies that $\lambda_A = 1 - \sum_{i \in A} (p_i + q_i)$, $A \subseteq \{1, \dots, d\}$ are the eigenvalues of \mathbf{P}_X .

6.2. Application A2: Explicit Formulas for the Stationary Distribution of Some Chains

6.2.1. Application A2: Finding the stationary distribution of an extension of the birth and death chain. Consider the classical birth and death chain on the state space $\mathbb{E} = \{1, 2, \dots, N\}$ with constant birth rate $q > 0$ and death rate $p > 0$. Assume that $p \neq q$ and $p + q < 1$. Let X be the following modification of this birth and death chain: in addition, there is an extra probability $1 - p - q$ of going from any state to the maximal state N . Formally, the transitions of X are given by

$$\mathbf{P}_X(i, j) = \begin{cases} q & \text{if } j = i + 1, i = 1, \dots, N - 2, \\ 1 - p & \text{if } (i = N - 1, j = N) \text{ or } (i = j = N), \\ p & \text{if } (j = i - 1, i = 2, \dots, N) \text{ or } (i = j = 1), \\ 1 - p - q & \text{if } i = 1, \dots, N - 2, j = N, \\ 0 & \text{otherwise.} \end{cases} \tag{6.5}$$

THEOREM 6.4: *Consider the Markov chain X on $\mathbb{E} = \{1, \dots, N\}$ with the transitions given in (6.5). Assume that $p \neq q$ and $p + q < 1$. Then the stationary distribution of the chain is given by*

$$\pi(k) = \frac{\left((1/2p) \sum_{j=0}^{\lfloor \frac{k-1}{2} \rfloor} \binom{k}{2j+1} \gamma^j - \sum_{j=0}^{\lfloor \frac{k}{2} \rfloor - 1} \binom{k-1}{2j+1} \gamma^j \right)}{\sum_{j=0}^{\lfloor N-1/2 \rfloor} \binom{N}{2j+1} \gamma^j} 2(2p)^{N-k+2}, \tag{6.6}$$

where $\gamma = (1 - 4pq)$.

PROOF: First, we will calculate the Siegmund dual of X . Consider the linear ordering $\leq := \leq$ on \mathbb{E} . The transitions of the Siegmund dual are then calculated using (2.3), that is, $\mathbf{P}_Z(j, i) =$

$\mathbf{P}_X(i, \{j\}^\downarrow) - \mathbf{P}_X(i + 1, \{j\}^\downarrow)$. Considering all the cases, we have

$$\begin{aligned} \mathbf{P}_Z(j, j - 1) &= \mathbf{P}_X(j - 1, \{j\}^\downarrow) - \mathbf{P}_X(j, \{j\}^\downarrow) \\ &= q + p - p = q, \quad j = 2, \dots, N, \end{aligned}$$

$$\begin{aligned} \mathbf{P}_Z(j, j + 1) &= \mathbf{P}_X(j + 1, \{j\}^\downarrow) - \mathbf{P}_X(j + 2, \{j\}^\downarrow) \\ &= p - 0 = p, \quad j = 1, \dots, N - 1, \end{aligned}$$

$$\mathbf{P}_Z(N - 1, N) = \mathbf{P}_X(N, \{(N - 1)\}^\downarrow) = p,$$

$$\mathbf{P}_Z(N, N) = \mathbf{P}_X(N, \{N\}^\downarrow) = 1.$$

For every $j = 1, \dots, N - 1$ we have that $\sum_i \mathbf{P}_Z(j, i) < 1$, more precisely

$$\sum_{i=1}^N \mathbf{P}_Z(1, i) = p < 1,$$

$$\sum_{i=1}^N \mathbf{P}_Z(j, i) = p + q < 1, \quad j = 2, \dots, N - 1.$$

Thus we add one extra state, call it “0”, obtaining the transition matrix of the Siegmund dual Z on $\mathbb{E}^* = \{0, 1, \dots, N\}$:

$$\mathbf{P}_Z(i, j) = \begin{cases} p & \text{if } j = i + 1, i = 1, \dots, N - 1, \\ q & \text{if } j = i - 1, i = 2, \dots, N - 1, \\ 1 - p & \text{if } i = 2, j = 1, \\ 1 - p - q & \text{if } i = 2, \dots, N - 1, j = 0, \\ 1 & \text{if } (i = j = 0) \text{ or } (i = j = N), \\ 0 & \text{otherwise.} \end{cases} \tag{6.7}$$

These are exactly the transitions corresponding to the “gambler’s ruin with catastrophes” considered in Hunter [14]. The ruin probability is given therein in Eq. (2.6), the winning probability is (with $\rho(0) = 0$)

$$\rho(k) = \frac{\left(1 + \sqrt{1 - 4pq/2p}\right)^k - \left(1 - \sqrt{1 - 4pq/2p}\right)^k}{\left(1 + \sqrt{1 - 4pq/2p}\right)^N - \left(1 - \sqrt{1 - 4pq/2p}\right)^N}.$$

For a linear ordering, the relation (2.4) is $\pi(\{k\}^\downarrow) = \rho(k)$; thus

$$\pi(k) = \rho(k) - \rho(k - 1).$$

The above relation and some elementary calculations using the binomial expansion

$$(1 + \sqrt{x})^k - (1 - \sqrt{x})^k = 2\sqrt{x} \sum_{j=0}^{\lfloor k-1/2 \rfloor} \binom{k}{2j+1} x^j$$

yield (6.6), and thus complete the proof. ■

6.2.2. Application A2: Finding the stationary distribution, another example.

LEMMA 6.5: Let X be a Markov chain on $\mathbb{E} = \{1, \dots, 2N\}$ with the following transition matrix:

$$P_X(i, j) = \frac{1}{(2N)^{2N}} \sum_{r=i}^{2N} \binom{2N}{r} [j^r (2N - j)^{2N-r} - (j - 1)^r (2N - j + 1)^{2N-r}].$$

Then the chain has a uniform stationary distribution, it is not reversible, and the eigenvalues are

$$\lambda_k = \frac{k!}{(2N)^k} \binom{2N}{k}, \quad k = 1, \dots, N.$$

PROOF: We will calculate the transitions of the Siegmund dual Z of X with respect to the total ordering. To shorten the notation, let us write $P_X(2N + 1, j) = 0$ for any j . For any $i, s \in \mathbb{E}$, we have

$$\begin{aligned} P_X(i, s) - P_X(i + 1, s) &= \frac{1}{(2N)^{2N}} \binom{2N}{i} [s^i (2N - s)^{2N-i} - (s - 1)^i (2N - s + 1)^{2N-i}]. \end{aligned}$$

Using (2.3) we have

$$\begin{aligned} P_Z(j, i) &= P_X(i, \{j\}^\downarrow) - P_X(i + 1, \{j\}^\downarrow) = \sum_{s=1}^j (P_X(i, s) - P_X(i + 1, s)) \\ &= \frac{1}{(2N)^{2N}} \binom{2N}{i} j^i (2N - j)^{2N-i} = \binom{2N}{i} \left(\frac{j}{2N}\right)^i \left(1 - \frac{j}{2N}\right)^{2N-i}. \end{aligned}$$

For every $j < 2N$ we have $\sum_i P_Z(j, i) < 1$; thus we add one extra absorbing state, call it “0”, and set $P(j, 0) = 1 - \sum_{s=1}^{2N} P_Z(j, s)$. These are exactly the transitions of the so-called Fisher–Wright population model (see, e.g., Ewens [6]). The states 0 and $2N$ are absorbing. It is known that for this model $P(Z \text{ is absorbed in } 2N | Z_0 = i) = i/2N$, thus the relation (2.4) implies that $\pi(1) = \pi(\{1\}^\downarrow) = P(Z \text{ is absorbed in } 2N | Z_0 = 1) = 1/2N$ and for $i > 1$ we have $\pi(i) = \pi(\{i\}^\downarrow) - \pi(\{i - 1\}^\downarrow) = (i/2N) - ((i - 1)/2N)$. It is easy to verify that X is not reversible. The eigenvalues of the Fisher–Wright model are $\lambda_k = k!/(2N)^k \binom{2N}{k}$, $k = 0, \dots, N$, as shown in Feller [8]. Applying Corollary 4.5 completes the proof. ■

Remark 6.6: It is relatively easy to show directly that the uniform distribution is the stationary distribution of X . However, finding directly the eigenvalues seems to be a challenging task.

6.3. Application A3: Stable Simulation Schemes

We will present two examples: a non-standard two-node closed tandem network with an unknown stationary distribution, and the Ising model on a circle. In both cases, simulations for some concrete sets of parameters are provided. The procedure is the following:

- For an ergodic chain X on $\mathbb{E} = \{\mathbf{e}_1, \dots, \mathbf{e}_M\}$ (denote its stationary distribution by π), calculate its Siegmund dual Z with respect to a partial ordering \preceq on $\mathbb{E}^* = \{\mathbf{e}_0\} \cup \mathbb{E}$.

- For all \mathbf{e} , simulate n chains $Z^{(1)}, \dots, Z^{(n)}$ independently, each starting at \mathbf{e} .
- Estimate $\pi(\{\mathbf{e}\}^\downarrow)$ via (2.4) with the Monte Carlo estimator

$$\hat{\pi}(\{\mathbf{e}\}^\downarrow) = \frac{1}{n} \sum_{i=1}^n Y_j,$$

where $Y_j = \mathbf{1}(Z^{(j)} \text{ is absorbed in } \mathbf{e}_M | Z_0^{(j)} = \mathbf{e})$.

- Finally, approximate $\pi(\mathbf{e})$ by (see Remark 3.2)

$$\hat{\pi}(\mathbf{e}) = \sum_{\mathbf{e}' \preceq \mathbf{e}} \mu(\mathbf{e}', \mathbf{e}) \hat{\pi}(\{\mathbf{e}'\}^\downarrow),$$

where μ is the Möbius function of the partial ordering \preceq .

Remark 6.7: In practice, we usually deal with chains on a huge state space, and our goal is to approximate π at a given point \mathbf{e} . We then do not have to start the chains at every state (which is infeasible), but only for $\{\mathbf{e}' : \mu(\mathbf{e}', \mathbf{e}) \neq 0\}$.

In other words, we estimate the mean of the Bernoulli random variable Y with $\pi(\{\mathbf{e}\}^\downarrow)$ being its success probability (and thus the mean). From the Central Limit Theorem, we know that $\pi(\{\mathbf{e}\}^\downarrow)$ is in the interval $(\hat{Y}_n - z_{1-\alpha/2}(\sigma_Y/\sqrt{n}), \hat{Y}_n + z_{1-\alpha/2}(\sigma_Y/\sqrt{n}))$ with probability (approximately) $1 - \alpha$, where $\sigma_Y^2 = \pi(\{\mathbf{e}\}^\downarrow)(1 - \pi(\{\mathbf{e}\}^\downarrow))$ is the variance of Y and $z_{1-\alpha/2}$ is the α th quantile of the standard normal distribution. For a typical $\alpha = 0.05$ (then $z_{1-0.025} = 1.96$), we want to control the error $err = 1.96\sigma_Y/\sqrt{n}$. Since $\sigma_Y^2 \leq 1/4$, it is enough to run at least

$$n = \left(\frac{1.96}{2err} \right)^2 \tag{6.8}$$

simulations for any \mathbf{e} .

6.3.1. Application A3: A stable simulation scheme for a non-standard tandem network of two servers. In this section, we will present a two-node closed tandem network with an unknown stationary distribution. Studying the absorption probability in the resulting Siegmund dual chain is a rather complicated task. We will present a stable simulation scheme and will estimate the stationary distribution for some concrete parameters. It is also worth noting that the structure of the resulting Siegmund dual is interesting: for example, once it hits a barrier, it will not leave it; for details see below.

Consider a tandem network of two stations, each with a finite buffer of size N . Denote the chain by $X \equiv (X)_{n \geq 0}$ with state space $\mathbb{E} = \{0, \dots, N\}^2$, where (x, y) is the state in which there are x customers at server 1 and y customers at server 2.

When $x > 0$ and $y < N$, the system operates as the following classical tandem: with probability λ_1 there is an arrival at station 1 (if $x < N$); with probability λ_2 there is an arrival at station 2 (if $y < N$); with probability μ_1 customers traverse from server 1 to server 2; with probability μ_2 the customer from server 2 leaves the network (if $y > 0$); with the remaining probability nothing happens. Without loss of generality we may assume that $\lambda_1 + \mu_1 + \lambda_2 + \mu_2 = 1$. However, at the borders $x = 0$ and $y = N$, the system operates differently from the classical tandem: when $x = 0$, the probability of arrival at station 2 is $\lambda_2 + \mu_1$ (if $y < N$) and when $y = N$ there is a departure from server 1 with probability μ_1 (if $x > 0$). This can be seen as a modification of the standard Gordon-Newell network.

A similar modification (of the Jackson network, that is, with a countable state space) was considered in Foley and McDonald [10], where the rough asymptotics (and large deviations) were derived, showing that a relatively slight modification (only at the borders) changes the stationary distribution dramatically. The transitions of the chain are as follows:

$$\mathbf{P}_X((x, y), (x', y')) = \begin{cases} \lambda_1 & \text{if } (x' = x + 1, y' = y) \\ & \text{or } (x = x' = N, 0 < y' = y < N), \\ \lambda_2 & \text{if } (y' = y + 1, x' = x > 0) \\ & \text{or } (0 < x' = x < N, y' = y = N), \\ \mu_1 & \text{if } (x' = x - 1, y' = y + 1) \\ & \text{or } (x' = x - 1, y' = y = N), \\ \mu_2 & \text{if } (y' = y - 1, x' = x) \\ & \text{or } (x' = x < N, y' = y = 0), \\ \mu_1 + \lambda_2 & \text{if } (y' = y + 1, x' = x = 0) \\ & \text{or } (x' = x = 0, y' = y = N), \\ \mu_2 + \lambda_1 & \text{if } x' = x = N, y' = y = 0, \\ \lambda_1 + \lambda_2 & \text{if } x' = x = y' = y = N. \end{cases} \tag{6.9}$$

Consider the coordinate-wise ordering, that is, $(x, y) \preceq (x', y') \iff x \leq x'$ and $y \leq y'$. Then the Möbius function is

$$\mu((x, y), (x', y')) = \begin{cases} 1 & \text{if } (x' = x \text{ and } y' = y) \text{ or} \\ & (x' = x + 1 \text{ and } y' = y + 1), \\ -1 & \text{if } (x' = x + 1 \text{ and } y' = y) \text{ or} \\ & (x' = x \text{ and } y' = y + 1), \\ 0 & \text{otherwise.} \end{cases} \tag{6.10}$$

We will calculate the transition matrix \mathbf{P}_Z of the Siegmund dual Z directly from Theorem 4.1:

$$\mathbf{P}_Z((x_1, y_1), (x_2, y_2)) = \sum_{(x, y) \succeq (x_2, y_2)} \mu((x_2, y_2), (x, y)) \mathbf{P}_Y((x, y), (x_1, y_1)^\downarrow),$$

where $\mathbf{P}_Y((x, y), (x_1, y_1)^\downarrow) := \sum_{(x', y') \preceq (x_1, y_1)} \mathbf{P}_Y((x, y), (x', y'))$. With our Möbius function μ we have

$$\begin{aligned} \mathbf{P}_Z((x_1, y_1), (x_2, y_2)) &= \mathbf{P}_Y((x_2, y_2), (x_1, y_1)^\downarrow) - \mathbf{P}_Y((x_2 + 1, y_2), (x_1, y_1)^\downarrow) \\ &\quad - \mathbf{P}_Y((x_2, y_2 + 1), (x_1, y_1)^\downarrow) + \mathbf{P}_Y((x_2 + 1, y_2 + 1), (x_1, y_1)^\downarrow), \end{aligned} \tag{6.11}$$

where we should understand that, for example, for $y_2 = N$ the corresponding terms, in this case $\mathbf{P}_Y((x_2, y_2 + 1), (x_1, y_1)^\downarrow)$ and $\mathbf{P}_Y((x_2 + 1, y_2 + 1), (x_1, y_1)^\downarrow)$, are equal to 0. Let us

start with the case $x_1, x_2, y_1, y_2 > 1$ and $x_1, x_2, y_1, y_2 < N$. Then using (6.11) we have, for example,

$$\begin{aligned} \mathbf{P}_Z((x_1, y_1), (x_1 - 1, y_1)) &= \mathbf{P}_Y((x_1 - 1, y_1), (x_1, y_1)^\downarrow) - \mathbf{P}_Y((x_1, y_1), (x_1, y_1)^\downarrow) \\ &\quad - \mathbf{P}_Y((x_1 - 1, y_1 + 1), (x_1, y_1)^\downarrow) + \mathbf{P}_Y((x_1, y_1 + 1), (x_1, y_1)^\downarrow) \\ &= \lambda_1 + \mu_2 - \mu_2 - \mu_2 + \mu_2 = \lambda_1. \end{aligned}$$

We also have $\mathbf{P}_Z((x_1, y_1), (x_1 - k, y_1)) = 0$ for $k = 1, \dots, x_1 - 1$. Considering some possible transitions to the border of the state space:

$$\begin{aligned} \mathbf{P}_Z((x_1, y_1), (0, y_1 - 1)) &= \mathbf{P}_X((0, y_1 - 1), (x_1, y_1)^\downarrow) - \mathbf{P}_X((1, y_1 - 1), (x_1, y_1)^\downarrow) \\ &\quad - \mathbf{P}_X((0, y_1), (x_1, y_1)^\downarrow) + \mathbf{P}_X((1, y_1), (x_1, y_1)^\downarrow) \\ &= 1 - 1 - (\lambda_1 + \mu_2) + (\mu_2 + \lambda_1) = 0. \end{aligned}$$

We will skip the rest of the (lengthy) calculations, but considering it on a case-by-case basis, X turns out to be Möbius monotone. We add one extra state, let us name it $(+\infty, +\infty)$. The transitions of the Siegmund dual are as follows:

$$\mathbf{P}_Z((x, y), (x', y')) = \begin{cases} \lambda_1 & \text{if } (N - 1 > x' = x - 1, y' = y) \\ & \text{or } (x' = x = N, y' = y < N) \\ & \text{or } (x = 0, y > 0, x' = +\infty, y' = +\infty), \\ \lambda_2 & \text{if } N - 1 > y' = y - 1, x' = x < N, \\ \mu_1 & \text{if } x' = x + 1, N - 1 > y' = y - 1 \\ & \text{or } x' = x + 1, y' = y = N, \\ \mu_2 & \text{if } x' = x, y' = y + 1, \\ \mu_1 + \lambda_2 & \text{if } (N - 1 > y' = y - 1, x' = x = N) \\ & \text{or } (x > 0, y = 0, x' = +\infty, y' = +\infty), \\ \mu_2 + \lambda_2 & \text{if } x' = x < N, y' = y = N \\ \lambda_1 + \lambda_2 + \mu_1 & \text{if } x = 0, y = 0, x' = +\infty, y' = +\infty, \\ 1 & \text{if } (x' = x = y' = y = N) \\ & \text{or } (x' = x = y' = y = +\infty). \end{cases} \tag{6.12}$$

Note that outside the borders, the transitions look like a *reversed* network (however, note that this is not the usual time reversal). The behavior on the borders is different. First, the chain can go to $(+\infty, +\infty)$ only from states of the form $(0, y)$ or $(x, 0)$. Second, once the process is on the “upper” $((x, N))$ or the “right” $((N, y))$ border, it behaves like the usual, absorbing birth and death chain with probabilities of being killed only possible on $(0, N)$ and $(N, 0)$, respectively. On the upper border, the birth rate is μ_1 and the death rate is λ_1 , whereas on the right border, the birth rate is μ_2 and the death rate is $\mu_1 + \lambda_2$.

One can also notice a similar behavior (i.e., not leaving the borders) in the SSD for the two-node network representing two independent servers, see Lorek and Szekli [22] for details.

Stable simulation scheme. We will estimate the stationary distribution of the tandem for $N = 5$ (thus the state space is $\mathbb{E} = \{0, \dots, 5\}^2$ with $|\mathbb{E}| = 36$) with parameters $\lambda_1 = 3/16, \lambda_2 = 1/16, \mu_1 = \mu_2 = 6/16$. The simulations were performed in **The Julia Language**. We consider two levels of accuracy: $err_1 = 0.005$ and $err_2 = 0.0005$. Using (6.8) we calculate a sufficient number of simulations:

$$err_1 = 0.005 : \left(\frac{1.96}{0.01}\right)^2 = 3.8416 \times 10^4 \leq 4 \times 10^4 =: n_1,$$

$$err_2 = 0.0005 : \left(\frac{1.96}{0.001}\right)^2 = 3.8416 \times 10^6 \leq 4 \times 10^6 =: n_2.$$

Once we estimate $\pi(\{x, y\}^\downarrow)$ by $\hat{\pi}(\{x, y\}^\downarrow)$, we estimate $\pi(x, y)$ by (see Remark 3.2)

$$\begin{aligned} \hat{\pi}(x, y) &= \sum_{(x', y') \preceq (x, y)} \mu((x', y'), (x, y)) \hat{\pi}(\{x', y'\}^\downarrow) \\ &= \hat{\pi}(\{(x, y)\}^\downarrow) - \hat{\pi}(\{(x - 1, y)\}^\downarrow) \\ &\quad - \hat{\pi}(\{(x, y - 1)\}^\downarrow) + \hat{\pi}(\{(x - 1, y - 1)\}^\downarrow), \end{aligned} \tag{6.13}$$

(where we should understand that $\hat{\pi}(\{(x, y)\}^\downarrow) = 0$ if some coordinate is negative). The results of the simulations are presented in Table 1. Besides estimating the stationary distribution, we also estimate the mean ($\hat{\tau}$) and the standard deviation ($\hat{\sigma}^2$) of time till absorption.

Although it is not included in Table 1, repeating the simulations for $n_2 = 4 \times 10^6$ several times yields estimators of π which always agree to the first three decimal places. The total variation distance between two such estimations was always ≤ 0.0071 .

6.3.2. Application A3: Stable simulation scheme for the Ising model on a circle. Let $G = (V, E)$ be a finite graph. Let $\mathbb{E} = \{-1, 1\}^V$ (set of so-called configurations). The Ising model on graph G with parameter $\beta \geq 0$ is the probability measure on \mathbb{E} given by

$$\pi(\mathbf{e}) = \frac{1}{C_\beta} \exp \left(\beta \sum_{\{x, y\} \in E} \mathbf{e}(x) \mathbf{e}(y) \right),$$

where sum is over all edges of the graph and C_β is a normalizing constant (hard to compute in general). We shall consider G being a circle, that is, $V = \{0, \dots, N - 1\}$ and $E = \{(i, (i + 1) \bmod N) : i = 0, \dots, N - 1\}$. The distribution is then of form

$$\pi(\mathbf{e}) = \frac{1}{Z} \exp \left(\beta \sum_{i=0}^{N-1} \mathbf{e}(i) \mathbf{e}(i + 1) \right), \tag{6.14}$$

TABLE 1. Results of $n_1 = 4 \times 10^4$ and $n_2 = 4 \times 10^6$ simulations for the non-standard tandem queue system with $N = 5, \lambda_1 = 3/16, \lambda_2 = 1/16, \mu_1 = \mu_2 = 6/16$. Together with the estimator $\hat{\pi} \equiv \hat{\pi}(x, y), x, y \in \{0, \dots, N\}$ the estimators of the expected time to absorption ($\hat{\tau}$) and its variance ($\hat{\sigma}^2$) are presented. The total variation distance between the estimated stationary distribution after n_1 and n_2 simulations was ≤ 0.056 .

$y \backslash x$		0	1	2	3	4	5
0	$\hat{\pi}$	0.030349	0.051093	0.064	0.089953	0.115488	0.152256
	$\hat{\tau}$	3.432581	6.516953	8.838628	10.490814	11.159698	10.898512
	$\hat{\sigma}^2$	37.126458	71.878733	92.804187	107.71656	110.579045	107.214705
1	$\hat{\pi}$	0.027628	0.029558	0.046256	0.04214	0.053326	0.061907
	$\hat{\tau}$	5.174186	9.379605	12.625	14.243023	14.688047	13.80893
	$\hat{\sigma}^2$	59.11922	89.951922	104.240892	102.786725	99.409276	96.261684
2	$\hat{\pi}$	0.02193	0.023814	0.018767	0.026605	0.01507	0.019116
	$\hat{\tau}$	5.92793	10.416093	13.449814	14.923465	14.533163	12.371256
	$\hat{\sigma}^2$	68.774475	94.621951	97.120298	91.983189	90.545936	84.547763
3	$\hat{\pi}$	0.014721	0.011116	0.01714	4.7e-5	0.014814	0.004
	$\hat{\tau}$	6.109372	10.44014	13.141	13.863535	12.545814	9.115233
	$\hat{\sigma}^2$	70.331045	92.117536	88.790347	84.163846	83.647753	72.533966
4	$\hat{\pi}$	0.00893	0.008651	0.00093	0.010442	0.005093	0.001233
	$\hat{\tau}$	5.829372	9.947884	12.078233	12.073163	9.741093	4.85114
	$\hat{\sigma}^2$	62.136261	80.03354	81.073393	77.194024	74.588772	44.553598
5	$\hat{\pi}$	0.009233	0.001465	0.000953	0.006791	0.000651	0.001326
	$\hat{\tau}$	5.579488	9.188023	10.855837	10.235651	6.744186	0.0
	$\hat{\sigma}^2$	55.045706	70.475751	71.311736	73.753556	66.707552	0.0
$n_1 = 4 \times 10^4$ ($err_1 = 0.005$)							
$y \backslash x$		0	1	2	3	4	5
0	$\hat{\pi}$	0.029462	0.049277	0.067276	0.087678	0.115476	0.158547
	$\hat{\tau}$	3.42784	6.48493	8.857538	10.419037	11.117143	10.907459
	$\hat{\sigma}^2$	35.946223	70.050356	93.86759	107.100301	111.100368	105.813727
1	$\hat{\pi}$	0.029505	0.033735	0.041213	0.046289	0.052367	0.051459
	$\hat{\tau}$	5.186866	9.447477	12.550259	14.317646	14.701667	13.70708
	$\hat{\sigma}^2$	59.127635	91.033304	102.503483	102.602434	99.065673	94.155181
2	$\hat{\pi}$	0.02127	0.021866	0.020932	0.023654	0.021371	0.017472
	$\hat{\tau}$	5.892092	10.463687	13.501422	14.889388	14.544947	12.450019
	$\hat{\sigma}^2$	68.901012	95.30462	97.564506	92.816501	89.189174	85.646968
3	$\hat{\pi}$	0.014304	0.012097	0.011997	0.009563	0.009726	0.00579
	$\hat{\tau}$	6.029211	10.440957	13.09187	13.842725	12.557437	9.142111
	$\hat{\sigma}^2$	69.044913	90.025534	89.396487	84.83922	82.871419	72.118169
4	$\hat{\pi}$	0.008411	0.007586	0.005305	0.004613	0.003635	0.002299
	$\hat{\tau}$	5.846186	9.8955	12.065144	12.108027	9.742326	4.82419
	$\hat{\sigma}^2$	63.076118	79.801387	79.770588	78.464214	74.763627	43.825968
5	$\hat{\pi}$	0.006554	0.003745	0.002153	0.001752	0.000802	0.000818
	$\hat{\tau}$	5.476035	9.225108	10.904013	10.212549	6.723262	0.0
	$\hat{\sigma}^2$	53.437619	70.099047	72.300547	74.038874	65.987165	0.0
$n_2 = 4 \times 10^6$ ($err_2 = 0.0005$)							

where we always perform addition modulo N . Let X on \mathbb{E} be the classical Gibbs sampler for this model, it has the following dynamics. Given $X_k = \mathbf{e}$,

- Choose vertex $i \in V$ with probability $\frac{1}{N}$.
- Take U_{k+1} , uniform random variable $U(0, 1)$, independent of $U_j, j \leq k$. Update the value at vertex i :

$$X_{k+1}(i) = \begin{cases} +1 & \text{if } U_{k+1} < \frac{e^{2\beta(\mathbf{e}(i+1)+\mathbf{e}(i-1))}}{1 + e^{2\beta(\mathbf{e}(i+1)+\mathbf{e}(i-1))}}, \\ -1 & \text{otherwise.} \end{cases}$$

Denote the transition matrix of X by \mathbf{P} . Let \preceq denote coordinate-wise partial ordering of \mathbb{E} , that is, $\mathbf{e} \preceq \mathbf{e}'$ if $\mathbf{e}(i) \leq \mathbf{e}'(i)$ for $i = 0, \dots, N - 1$. We will start with:

Numerical results. Let X be the Gibbs sampler for the Ising model on a circle with 3 points ($N = 2$). Let us enumerate the states in the following way: $\mathbf{e}_1 = (-1, -1, -1)$, $\mathbf{e}_2 = (+1, -1, -1)$, $\mathbf{e}_3 = (-1, +1, -1)$, $\mathbf{e}_4 = (-1, -1, +1)$, $\mathbf{e}_5 = (+1, +1, -1)$, $\mathbf{e}_6 = (+1, -1, +1)$, $\mathbf{e}_7 = (-1, +1, +1)$, $\mathbf{e}_8 = (+1, +1, +1)$. The transition matrix of X is following:

$$\mathbf{P}_X = \begin{pmatrix} 1 - q & \frac{1}{3}q & \frac{1}{3}q & \frac{1}{3}q & 0 & 0 & 0 & 0 \\ \frac{1}{3} - \frac{1}{3}q & \frac{1}{3} + \frac{1}{3}q & 0 & 0 & \frac{1}{6} & \frac{1}{6} & 0 & 0 \\ \frac{1}{3} - \frac{1}{3}q & 0 & \frac{1}{3} + \frac{1}{3}q & 0 & \frac{1}{6} & 0 & \frac{1}{6} & 0 \\ \frac{1}{3} - \frac{1}{3}q & 0 & 0 & \frac{1}{3} + \frac{1}{3}q & 0 & \frac{1}{6} & \frac{1}{6} & 0 \\ 0 & \frac{1}{6} & \frac{1}{6} & 0 & \frac{2}{3} - \frac{1}{3}p & 0 & 0 & \frac{1}{3}p \\ 0 & \frac{1}{6} & 0 & \frac{1}{6} & 0 & \frac{2}{3} - \frac{1}{3}p & 0 & \frac{1}{3}p \\ 0 & 0 & \frac{1}{6} & \frac{1}{6} & 0 & 0 & \frac{2}{3} - \frac{1}{3}p & \frac{1}{3}p \\ 0 & 0 & 0 & 0 & \frac{1}{3} - \frac{1}{3}p & \frac{1}{3} - \frac{1}{3}p & \frac{1}{3} - \frac{1}{3}p & p \end{pmatrix},$$

where $p = e^{4\beta}/1 + e^{4\beta}$ and $q = e^{-4\beta}/1 + e^{-4\beta}$. The stationary distribution in this case is given by:

$$\pi(\mathbf{e}_1) = \pi(\mathbf{e}_8) = \frac{e^{3\beta}}{C_\beta}, \pi(\mathbf{e}_2) = \dots = \pi(\mathbf{e}_7) = \frac{e^{-\beta}}{C_\beta}, C_\beta = 2e^{3\beta} + 6e^{-\beta}.$$

Introducing coordinate-wise partial ordering, it is easy to calculate the Siegmund dual chain Z on $\mathbb{E}^* = \mathbb{E} \cup \{\mathbf{e}_0\}$. Its transition matrix \mathbf{P}_Z is following (with states enumerated:

$\mathbf{e}_0, \dots, \mathbf{e}_8$)

$$\mathbf{P}_Z = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 - p_1 & 0 & \frac{1}{3}p_1 & \frac{1}{3}p_1 & \frac{1}{3}p_1 & 0 & 0 & 0 & 0 \\ \frac{1}{3}(1 - p_2) & 0 & \frac{1}{3} & \frac{1}{6}p_2 & \frac{1}{6}p_2 & \frac{1}{6} & \frac{1}{6} & 0 & 0 \\ \frac{1}{3}(1 - p_2) & 0 & \frac{1}{6}p_2 & \frac{1}{3} & \frac{1}{6}p_2 & \frac{1}{6} & 0 & \frac{1}{6} & 0 \\ \frac{1}{3}(1 - p_2) & 0 & \frac{1}{6}p_2 & \frac{1}{6}p_2 & \frac{1}{3} & 0 & \frac{1}{6} & \frac{1}{6} & 0 \\ \frac{1}{3}(1 - (q_1 + q_2)) & 0 & 0 & 0 & 0 & \frac{2}{3} & \frac{1}{6}q_2 & \frac{1}{6}q_2 & \frac{1}{3}q_1 \\ \frac{1}{3}(1 - (q_1 + q_2)) & 0 & 0 & 0 & 0 & \frac{1}{6}q_2 & \frac{2}{3} & \frac{1}{6}q_2 & \frac{1}{3}q_1 \\ \frac{1}{3}(1 - (q_1 + q_2)) & 0 & 0 & 0 & 0 & \frac{1}{6}q_2 & \frac{1}{6}q_2 & \frac{2}{3} & \frac{1}{3}q_1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

where

$$p_1 = \frac{1}{1 + e^{-4\beta}}, \quad p_2 = \frac{1 - e^{-4\beta}}{1 + e^{-4\beta}}, \quad q_1 = \frac{1}{1 + e^{4\beta}}, \quad q_2 = \frac{e^{4\beta} - 1}{1 + e^{4\beta}}.$$

We consider two different values for β , $\beta_1 = 0.01$ and $\beta_2 = 0.1$, and two levels of accuracy $err_1 = 0.005$ and $err_2 = 0.0005$. These are the same accuracy levels as in Section 6.3.1, thus similarly we take $n_1 = 4 \times 10^4$ and $n_2 = 4 \times 10^6$. The results, together with mean and variance of absorption time (denoted by $\hat{\tau}$ and $\hat{\sigma}^2$) are given in Table 2.

For $N = 2$ of course the stationary distribution can be calculated, thus we can compare it with simulations' results. From Table 2 we can read that estimating π using $n_1 = 4 \times 10^4$ simulations was more accurate for $\beta = 0.1$ than for $\beta = 0.01$ (total variation distance between the estimated and the real stationary distribution being 0.003 and 0.01 respectively). However, after $n_2 = 4 \times 10^6$ simulations no significant differences can be observed. Note also that each simulation took on average around 0.7 steps longer for $\beta = 0.1$ than for $\beta = 0.01$.

Remark 6.8: In estimating the mean value of Bernoulli random variable one may want err to be a fraction of variance σ_Y^2 . The variance is unknown; however, it can be first estimated by running initially some number of simulations and calculating its sample variance. This should be done separately for each \mathbf{e} for which we want to estimate $\pi(\{\mathbf{e}\}^\downarrow)$.

General N . We presented an example with three vertices ($N = 2$). In this case, we can simply calculate $\mathbf{P}_Z = (\mathbf{C}^{-1}\mathbf{P}_X\mathbf{C})^T$ (and add an extra absorbing state). How should one proceed with the general number of vertices? This chain was considered in Lorek and Szekli [22] in the context of strong stationary duality (and studying the rate of convergence of the chain to its stationary distribution), where the form of this dual for general N was given in Conjecture 1. The conjecture translates into

Conjecture 6.9: Let X be the Gibbs sampler for the Ising model on a circle. Then it is Möbius monotone with respect to the coordinate-wise partial ordering. The transitions of

TABLE 2. Simulation results for two Ising models (with $\beta = 0.01$ and $\beta = 0.1$) on a circle with three vertices. We calculated: $\hat{\pi}(\mathbf{e}_i)$ – the estimator of the stationary distribution; $\hat{\tau}$, $\hat{\sigma}^2$ – estimators of expected number of steps till absorption and its variance. The actual stationary distribution is bolded. The total variation distance between the stationary distribution and its estimation is given in last row.

	$\beta = 0.01$						$\beta = 0.1$							
	π	$n_1 = 4 \times 10^4$ ($err_1 = 0.005$)			$n_2 = 4 \times 10^6$ ($err_2 = 0.0005$)			π	$n_1 = 4 \times 10^4$ ($err_1 = 0.005$)			$n = 4 \times 10^6$ ($err = 0.0005$)		
		$\hat{\pi}$	$\hat{\tau}$	$\hat{\sigma}^2$	$\hat{\pi}$	$\hat{\tau}$	$\hat{\sigma}^2$		$\hat{\pi}$	$\hat{\tau}$	$\hat{\sigma}^2$	$\hat{\pi}$	$\hat{\tau}$	$\hat{\sigma}^2$
\mathbf{e}_1	0.129	0.128	2.563	5.587	0.129	2.564	5.574	0.166	0.166	3.235	9.463	0.166	3.237	9.498
\mathbf{e}_2	0.124	0.123	3.050	6.263	0.124	3.063	6.310	0.111	0.111	3.731	10.224	0.111	3.736	10.209
\mathbf{e}_3	0.124	0.128	3.062	6.328	0.124	3.063	6.312	0.111	0.110	3.742	10.297	0.111	3.735	10.226
\mathbf{e}_4	0.124	0.124	3.059	6.284	0.124	3.063	6.322	0.111	0.112	3.733	10.164	0.111	3.742	10.268
\mathbf{e}_5	0.124	0.116	3.062	6.329	0.123	3.060	6.314	0.111	0.113	3.731	10.229	0.112	3.735	10.233
\mathbf{e}_6	0.124	0.128	3.054	6.251	0.124	3.061	6.315	0.111	0.109	3.742	10.246	0.112	3.738	10.236
\mathbf{e}_7	0.124	0.122	3.065	6.337	0.124	3.061	6.319	0.111	0.111	3.743	10.240	0.112	3.736	10.243
\mathbf{e}_8	0.129	0.131	–	–	0.128	–	–	0.166	0.168	–	–	0.165	–	–
$d(\pi, \hat{\pi})$	0.010	0.010			0.001			0.003	0.003			0.001		

its Siegmund dual Z on $\mathbb{E}^* = \{\mathbf{e}_0\} \cup \mathbb{E}$ are as follows:

$$\mathbf{P}_Z(\mathbf{e}, \mathbf{e}') \tag{6.15}$$

$$= \begin{cases} 0 & \text{if } \mathbf{e} \succ \mathbf{e}', \\ \frac{1}{N} S(\mathbf{e}) & \text{if } \mathbf{e} = \mathbf{e}', \\ \frac{1}{N} \left(1 - \frac{e^{2\beta(\mathbf{e}(i+1)+\mathbf{e}(i-1))}}{1 + e^{2\beta(\mathbf{e}(i+1)+\mathbf{e}(i-1))}} \right) & \text{if } \mathbf{e}' = \mathbf{e} + s_v, \mathbf{e}(v) = -1, \\ \frac{1}{N} \left(\frac{e^{2\beta(\mathbf{e}(i+1)+\mathbf{e}(i-1)+2)}}{1 + e^{2\beta(\mathbf{e}(i+1)+\mathbf{e}(i-1)+2)}} - \frac{e^{2\beta(\mathbf{e}(i+1)+\mathbf{e}(i-1))}}{1 + e^{2\beta(\mathbf{e}(i+1)+\mathbf{e}(i-1))}} \right) & \text{if } \mathbf{e}' = \mathbf{e}(i \leftrightarrow i + 1), \\ & \mathbf{e}(i)\mathbf{e}(i + 1) = -1, \\ 1 - \sum_{\mathbf{e}' \in \mathbb{E}} \mathbf{P}_Z(\mathbf{e}, \mathbf{e}') & \text{if } \mathbf{e}' = \mathbf{e}_0, \end{cases}$$

where $s_v = (0, \dots, 0, 2, 0, \dots, 0)$ (the 2 on the coordinate corresponding to vertex v), $S(\mathbf{e}) = \sum_{i=0}^{N-1} \mathbf{1}\{\mathbf{e}(v) = 1\}$ and $\mathbf{e}(i \leftrightarrow i + 1)$ denotes the state \mathbf{e} with spins at vertices i and $i + 1$ swapped.

Note that if the conjecture is true, then it is easy to simulate the Siegmund dual. The only non-zero transitions are: (i) the chain can stay at each state (except $\mathbf{e} = (0, \dots, 0)$); (ii) it can change some coordinate from -1 to $+1$; (iii) if $+1$ and -1 are neighbors, then they can be “swapped”; (iv) with the remaining probability the chain can be absorbed in \mathbf{e}_0 . Thus, it is easy to estimate $\pi(\{\mathbf{e}\}^\downarrow)$. However, estimating $\pi(\mathbf{e})$ for large N is not trivial. Remark 3.2 (with the Möbius function of the coordinate-wise ordering on $\{0, 1\}^N$) implies that we need to estimate $\pi(\{\mathbf{e}'\}^\downarrow)$ for $2^{S(\mathbf{e})}$ different states \mathbf{e}' . Note that in the *non-standard queue* example (Section 6.3.1), for each $\mathbf{e} = (x, y)$ we had to estimate π at at most four other states (cf. (6.13)).

Note that for the minimal state, we have $\{\mathbf{e}_1\}^\downarrow = \mathbf{e}_1$, thus to estimate $\pi(\mathbf{e}_1)$ we need only to run chains starting at this minimal state. For example, we can estimate then the normalizing constant C_β (often called a *partition function*) via $\hat{C}_\beta = e^{3\beta} / \hat{\pi}(\mathbf{e}_1)$. For the Ising model on a circle with N vertices it is known that $C_\beta = (2 \sinh(\beta))^N + (2 \cosh(\beta))^N$.

7. STOCHASTIC VS MÖBIUS MONOTONICITY

In Section 4, we showed that the Siegmund dual exists if and only if the chain is Möbius monotone. We also mentioned that this monotonicity and stochastic monotonicity are indeed different. In this section, we will present two chains: (a) a chain which is stochastically but not Möbius monotone, and (b) a chain which is Möbius but not stochastically monotone.

7.1. Example of a Chain that is Stochastically but not Möbius Monotone

Consider X on $\mathbb{E} = \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4\}$ with the following partial ordering (expressed by \mathbf{C} , its Hasse diagram is presented)

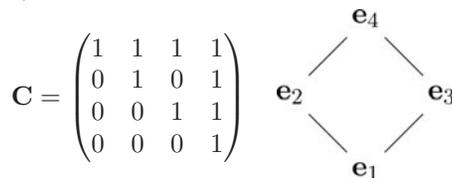


TABLE 3. Conditions for stochastic monotonicity of X .

\mathbf{e}	\preceq	\mathbf{e}'	\mathcal{U}	$\mathbf{P}(\mathbf{e}, \mathcal{U}) \leq \mathbf{P}(\mathbf{e}', \mathcal{U})$
\mathbf{e}_1	\preceq	\mathbf{e}_2	$\{\mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4\}$	$\alpha_1 + \alpha_2 + \beta_1 \leq 1$
\mathbf{e}_1	\preceq	\mathbf{e}_3	$\{\mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4\}$	$\alpha_1 + \alpha_2 + \beta_2 \leq 1$
\mathbf{e}_2	\preceq	\mathbf{e}_4	$\{\mathbf{e}_4\}$	$\alpha_2 + \beta_1 + \beta_2 \leq 1$
\mathbf{e}_3	\preceq	\mathbf{e}_4	$\{\mathbf{e}_4\}$	$\alpha_1 + \beta_1 + \beta_2 \leq 1$

Let $\alpha_1, \alpha_2, \beta_1, \beta_2$ be non-negative numbers such that

$$\max(\alpha_1 + \alpha_2, \beta_1 + \alpha_2, \beta_1 + \beta_2, \alpha_1 + \beta_2) \leq 1. \tag{7.1}$$

Define the transition matrix

$$\mathbf{P}_X = \begin{pmatrix} 1 - \alpha_1 - \alpha_2 & \alpha_1 & \alpha_2 & 0 \\ \beta_1 & 1 - \beta_1 - \alpha_2 & 0 & \alpha_2 \\ \beta_2 & 0 & 1 - \alpha_1 - \beta_2 & \alpha_1 \\ 0 & \beta_2 & \beta_1 & 1 - \beta_1 - \beta_2 \end{pmatrix}.$$

Simple computations yield

$$(\mathbf{C}^{-1} \mathbf{P}_X \mathbf{C})^T = \begin{pmatrix} 1 - \alpha_1 - \alpha_2 - \beta_1 - \beta_2 & \beta_1 & \beta_2 & 0 \\ 0 & 1 - \alpha_2 - \beta_2 & 0 & \beta_2 \\ 0 & 0 & 1 - \alpha_1 - \beta_2 & \beta_1 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Thus, the chain is Möbius monotone iff $\alpha_1 + \alpha_2 + \beta_1 + \beta_2 \leq 1$. As for stochastic monotonicity, condition (2.1) is calculated for some $\mathbf{e} \preceq \mathbf{e}'$ and some up-sets, the results are given in Table 3.

It can be checked that the conditions from Table 3 imply all other conditions for stochastic monotonicity. The chain is stochastically monotone iff

$$\max \left(\alpha_1 + \alpha_2 + \max_{i=1,2} \{\beta_i\}, \beta_1 + \beta_2 + \max_{i=1,2} \{\alpha_i\} \right) \leq 1.$$

Thus, in this example, Möbius monotonicity implies stochastic monotonicity but not vice versa. For example, for $\alpha_1 = \alpha_2 = \beta_1 = \beta_2 = \frac{1}{3}$ the chain is stochastically but not Möbius monotone.

7.2. Example of a Chain that is Möbius Monotone but not Stochastically Monotone

This example is taken from Lorek and Markowski [20] (the chain with the transition matrix \mathbf{P}_6). The detailed calculations were not given therein, which is why we include them here. The state space is $\mathbb{E} = \{\mathbf{e}_1, \dots, \mathbf{e}_6\}$ and the partial order (and its Hasse diagram)

is the following:

$$\mathbf{C} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

The transitions are

$$\mathbf{P}_X = \begin{pmatrix} 17/24 & 0 & 0 & 1/8 & 1/8 & 1/24 \\ 1/8 & 5/16 & 5/16 & 1/12 & 1/12 & 1/12 \\ 1/8 & 5/16 & 5/16 & 1/12 & 1/12 & 1/12 \\ 1/12 & 1/12 & 1/12 & 5/16 & 5/16 & 1/8 \\ 1/12 & 1/12 & 1/12 & 5/16 & 5/16 & 1/8 \\ 1/24 & 1/8 & 1/8 & 0 & 0 & 17/24 \end{pmatrix}.$$

Simple calculations yield

$$(\mathbf{C}^{-1}\mathbf{P}_X\mathbf{C})^T = \begin{pmatrix} 7/12 & 0 & 0 & 1/24 & 1/24 & 1/24 \\ 0 & 13/48 & 13/48 & 0 & 0 & 1/6 \\ 0 & 13/48 & 13/48 & 0 & 0 & 1/6 \\ 0 & 0 & 0 & 13/48 & 13/48 & 7/24 \\ 0 & 0 & 0 & 13/48 & 13/48 & 7/24 \end{pmatrix},$$

thus the chain is Möbius monotone. Consider the up-set $\mathcal{U} = \{e_4, e_5, e_6\}$. For $e_1 \preceq e_2$ we have

$$\mathbf{P}(e_1, \mathcal{U}) = \frac{7}{24} \not\leq \frac{1}{4} = \mathbf{P}(e_2, \mathcal{U}),$$

thus the chain is not stochastically monotone.

Remark 7.1: There are many chains where Möbius monotonicity implies stochastic monotonicity. For example, the non-standard queue system considered in Section 6.3.1 was both Möbius and stochastically monotone. If one considers a standard tandem (without changes at the border), it turns out to be stochastically but not Möbius monotone. The example from Section 7.1 is a special case of a nearest neighbor walk on the cube considered in Lorek and Szekli [21] (Chapter 4, Eq. (4.1)). Roughly speaking, this is the following chain on $\mathbb{E} = \{0, 1\}^d$. At any step, only at most one coordinate can be changed: a 0 on the i -th coordinate can be changed to 1 with probability α_i and a 1 on the i -th coordinate can be changed to 0 with probability β_i with proper sequences $\alpha_i, \beta_i, i = 1, \dots, d$ assuring aperiodicity. Considering the coordinate-wise ordering, the chain is Möbius monotone iff $\sum_{i=1}^d (\alpha_i + \beta_i) \leq 1$ (Theorem 3 in Lorek and Szekli [21]), whereas it is stochastically monotone iff

$$\max \left(\sum_{i=1}^d \alpha_i + \max_i \{\beta_i\}, \sum_{i=1}^d \beta_i + \max_i \{\alpha_i\} \right) \leq 1$$

as was determined in Lorek [18] (Lemma 5.4.1). It can also be checked that in this example Möbius monotonicity is equivalent to *realizable monotonicity* (required, e.g., for efficient perfect simulation via the coupling from the past algorithm Propp and Wilson [25]).

However, so far we do not have any “natural” example of a chain which is Möbius but not stochastically monotone. By natural, we mean, for example, a chain having some interpretation in terms of a random walk on some known structure, etc. (The example from Section 7.2 – and taken from Lorek and Markowski [20] – was found ad hoc). Note that such an example could potentially strongly benefit from the results of this paper.

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