

# Stopping rule reversal for finite Markov chains

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## Abstract

Consider a finite irreducible Markov chain with transition matrix  $M = (p_{ij})$ . Fixing a target distribution  $\tau$ , we study a family of optimal stopping rules from the singleton distributions to  $\tau$ . We show that this family of rules is dual to a family of (not necessarily optimal) rules on the reverse chain from the singleton distributions to a related distribution  $\hat{\alpha}$  called the  $\tau$ -contrast distribution. This duality can be expressed using matrices of exit frequencies. Furthermore, we identify a third distribution  $\beta$  called the  $\tau$ -core such that  $\hat{\alpha}$  and  $\beta$  are entirely dual to one another: a family of optimal rules to  $\hat{\alpha}$  on the reverse chain are dual to a family of optimal rules to  $\beta$  on the forward chain.

Using this duality, we provide new proofs of some exact mixing measure results of Lovász and Winkler [11] concerning the *mixing time*, the *reset time* and the *forget time*. In addition, we show that the time between independent samples of  $\hat{\alpha}$  on the reverse chain is equal to the time between independent samples of  $\beta$  on the forward chain.

Finally, we study the properties of matrices of exit frequencies for optimal families of stopping rules. We show that the inverse of an exit frequency matrix can be obtained via an alteration of the singular matrix  $I - M$ . Our observations lead to new proofs of two spectral results for mixing measures.

## 1 Introduction

Consider a finite, irreducible, discrete time Markov chain on the state space  $S$  where  $|S| = n$  with transition matrix  $M = (p_{ij})$  and stationary distribution  $\pi$ . Reversing time results in the dual Markov chain, called the reverse chain, with transition matrix  $\hat{M} = (\hat{p}_{ij})$  where  $\hat{p}_{ij} = \pi_j p_{ji} / \pi_i$  and with the same stationary distribution as the original chain. In what follows, hatted symbols always refer to the reverse chain. Note that

$$\hat{M} = RM^\top R^{-1} \tag{1}$$

where  $R$  is the diagonal matrix of return times,  $R_{ii} = \text{Ret}(i) = 1/\pi_i$ .

In [11], Lovász and Winkler consider the relationship between time reversal and exact mixing measures defined via stopping rules. Given a starting distribution  $\sigma$  and a target distribution  $\tau$ , a stopping rule halts the Markov chain whose initial state is drawn from  $\sigma$  so that the final state is governed by  $\tau$  (see the next section for details). An *optimal* stopping rule from  $\sigma$  to  $\tau$  minimizes the expected time before the rule halts. The *access time* is the expected length of such an optimal stopping rule, which we denote by  $H(\sigma, \tau)$ . We may think of the access time as a generalization of the state-to-state hitting time  $H(i, j)$ .

Considering a target distribution that captures an aspect of mixing leads to a number of parameterless mixing measures. Three of the most important measures are the mixing time  $T_{\text{mix}} = \max_i H(i, \pi)$ , the reset time  $T_{\text{reset}} = \sum_j \pi_j H(j, \pi)$  and the forget time  $T_{\text{forget}} = \min_\tau \max_i H(i, \tau)$ . We interpret  $T_{\text{mix}}$  as the pessimal mixing time and  $T_{\text{reset}}$  as the average mixing time. The forget time  $T_{\text{forget}}$  is the minimum expected time to achieve some distribution regardless of our initial state (thus “forgetting” our starting point). Lovász and Winkler [11] prove the following two results.

**Theorem 1 (Lovász and Winkler)** *For every finite Markov chain,  $T_{\text{mix}} = \hat{T}_{\text{mix}}$ .*

**Theorem 2 (Lovász and Winkler)** *For every finite Markov chain,  $T_{\text{forget}} = \hat{T}_{\text{reset}}$  and  $T_{\text{reset}} = \hat{T}_{\text{forget}}$ . Moreover,  $T_{\text{forget}}$  is achieved uniquely by the target distribution  $\mu$  given by*

$$\mu_i = \pi_i \left( 1 + \sum_j \hat{p}_{ij} \hat{H}(j, \pi) - \hat{H}(i, \pi) \right) \quad (2)$$

and  $\hat{T}_{\text{forget}}$  is achieved uniquely by the target distribution  $\hat{\mu}$  given by

$$\hat{\mu}_i = \pi_i \left( 1 + \sum_j p_{ij} H(j, \pi) - H(i, \pi) \right). \quad (3)$$

Their proof of theorem 2 relies on a complicated linear programming duality argument. We provide a simple probabilistic proof of theorem 2 using Markov chain duality along with a new proof of theorem 1. The key to these proofs is the observation that a family of optimal stopping rules from the singleton distributions to  $\pi$  on the forward chain are dual to a family of (not necessarily optimal) rules from the singleton distributions to  $\hat{\mu}$  on the reverse chain.

We interpret  $\hat{\mu}_i$  as the scaled difference between two rules from  $i$  to  $\pi$  on the forward chain.  $H(i, \pi)$  is the expected length of an optimal rule from  $i$  to  $\pi$ , while the quantity  $1 + \sum_j p_{ij} H(j, \pi)$  is the expected length of the rule “make one transition according to  $M$

and then follow an optimal rule from this state to  $\pi$ .” Thus the quantity  $\hat{\mu}_i/\pi_i$  measures the distance from optimality of the latter rule. We think of  $\mu_i$  as contrasting the expected length of an optimal rule with the expected length of a second (and possibly non-optimal) rule from  $i$  to  $\pi$ .

The duality underlying theorem 2 holds for any target distribution. For ease of exposition, we introduce the following two functions between distributions on  $S$ .

**Definition.** Given a distribution  $\tau$ , the *forward contrast map* is the function  $c(\tau) = \hat{\alpha}$  where

$$\hat{\alpha}_i = \pi_i \left( 1 + \sum_j p_{ij} H(j, \tau) - H(i, \tau) \right). \quad (4)$$

We call  $\hat{\alpha}$  the *forward contrast distribution* of  $\tau$  or the *forward  $\tau$ -contrast*. The *reverse contrast map* is the function  $\hat{c}(\tau) = \alpha$  where

$$\alpha_i = \pi_i \left( 1 + \sum_j \hat{p}_{ij} \hat{H}(j, \tau) - \hat{H}(i, \tau) \right). \quad (5)$$

We call  $\alpha$  the *reverse contrast distribution* of  $\tau$  or the *reverse  $\tau$ -contrast*.

Singletons are the simplest examples of contrasted distributions:  $c(i) = \hat{c}(i) = i$  for any singleton distribution  $i$ . In general, for a non-reversible chain  $\alpha \neq \hat{\alpha}$ . We show that some hitting time identities that do not hold for general access times can be extended for contrasted distributions.

The family of optimal forward rules to  $\tau$  are dual to a family of (not necessarily optimal) reverse rules to  $\hat{\alpha}$ . Analogously, an optimal family of reverse rules to  $\tau$  are dual to a family of (not necessarily optimal) forward rules to  $\alpha$ . Since our designation “forward” and “reverse” is arbitrary, most discussion hereafter will focus on forward walks to  $\tau$  with the analogous statements concerning reverse walks to  $\tau$  also holding. Theorem 2 is an example of this duality for  $\tau = \pi$  and  $c(\tau) = \hat{\mu}$ . In general, the duality between  $\tau$  and  $\hat{\alpha}$  is most explicitly revealed via *exit frequencies*.

Given a stopping rule  $\Gamma$  from  $\sigma$  to  $\tau$ , its  $i$ th exit frequency  $x_i(\Gamma)$  is the expected number of times the rule  $\Gamma$  exits state  $i$ . Exit frequencies are key to virtually all stopping rule results. In particular, we can characterize an optimal rule from  $\sigma$  to  $\tau$  by its exit frequencies. Lovász and Winkler [10] prove that a stopping rule is optimal if and only if there is a so-called halting state  $k$  such that  $x_k(\Gamma) = 0$ . Moreover, each optimal stopping rule from  $\sigma$  to  $\tau$  has the same exit frequencies, denoted by  $x_k(\sigma, \tau)$ .

A forward  $\tau$ -family  $\{\Gamma(i, \tau)\}$  is a family of rules to  $\tau$ , one from each singleton. An optimal forward  $\tau$ -family is such a family where each rule is optimal. We define the forward optimal exit frequency matrix of  $\tau$ , denoted  $X_\tau$  to be the square matrix whose  $ij$ th entry is  $x_j(i, \tau)$ . The  $i$ th row of  $X_\tau$  contains the exit frequencies for an optimal rule from  $i$  to  $\tau$ . Note that each row must contain at least one zero entry, corresponding to a halting state for this optimal rule. Our main duality result is as follows.

**Theorem 3** *Consider a distribution  $\tau$  on the state space  $S$  and let  $\hat{\alpha} = c(\tau)$  and  $\alpha = \hat{c}(\tau)$  be the forward contrast distribution for  $\tau$ .*

- (a) *Let  $X_\tau$  be the exit frequency matrix for an optimal forward  $\tau$ -family. Then the matrix  $RX_\tau^\top R^{-1}$  is the exit frequency matrix for a (not necessarily optimal) reverse  $\hat{\alpha}$ -family.*
- (b) *The optimal exit frequency matrices for the contrast distributions of  $\tau$  are given by*

$$\hat{X}_{\hat{\alpha}} = R(X_\tau^\top - \mathbf{b}^\top \mathbf{1})R^{-1} \quad \text{where} \quad b_k = \min_i x_k(i, \tau).$$

Recall that equation (1) shows that we obtain the reverse transition matrix  $\hat{M}$  by taking the scaled transpose of the forward transition matrix. Analogously, theorem 3 states that  $RX_\tau^\top R^{-1}$  is nearly equal to the optimal reverse exit frequency matrix for  $\hat{\alpha}$ . (The rules may not be optimal as there may be columns of  $X_\tau$  which do not contain any zeros, giving rows of  $RX_\tau^\top R^{-1}$  without halting states.) We find  $\hat{X}_{\hat{\alpha}}$  by subtracting the smallest entry in each row of  $X_\tau^\top$  from all the entries in that row before scaling, guaranteeing that there is a zero in every row and every column of  $\hat{X}_{\hat{\alpha}}$ .

Let  $\beta = \hat{c}(\hat{\alpha}) = \hat{c}(c(\tau))$ . If every column of  $X_\tau$  contains a zero entry then we have equality  $\hat{X}_{\hat{\alpha}} = RX_\tau^\top R^{-1}$  and therefore  $\beta = \tau$ . Otherwise,  $\hat{c}(\hat{\alpha}) = \beta \neq \tau$ . The following corollary shows that the distribution  $\beta$  is fully dual to  $\alpha$  as well as being related to  $\tau$ .

**Definition.** Given a distribution  $\tau$ , the *forward  $\tau$ -core* distribution is given by  $\beta = \hat{c}(\hat{\alpha}) = \hat{c}(c(\tau))$  and the *reverse  $\tau$ -core* distribution is given by  $\hat{\beta} = c(\alpha) = c(\hat{c}(\tau))$ .

**Corollary 4** *If  $\hat{\alpha} = c(\tau)$  and  $\beta = \hat{c}(\hat{\alpha})$  then  $X_\beta = R\hat{X}_{\hat{\alpha}}^\top R^{-1}$  and therefore  $c(\hat{c}(\hat{\alpha})) = c(\beta) = \hat{\alpha}$ . If  $W_\tau = \{\sigma : \forall i, H(i, \sigma) + H(\sigma, \tau) = H(i, \tau)\}$ , then  $\beta \in W_\tau$ . Furthermore,  $\beta$  is the unique reverse contrasted distribution in  $W_\tau$  and  $H(\beta, \tau) = \max_{\sigma \in W_\tau} H(\sigma, \tau)$ .*

The forward  $\tau$ -contrast  $\hat{\alpha}$  and the forward  $\tau$ -core  $\beta$  are balanced in the sense that every state is a halting state for some other state. Moreover, if  $i$  is a reverse  $\hat{\alpha}$ -halting state for

$j$  then  $j$  is a forward  $\beta$ -halting state for  $i$ . We call  $\beta$  the forward  $\tau$ -core since it is the first distribution “on the way” to  $\tau$  in the sense that rule “walk from  $i$  to  $\beta$  and then from  $\beta$  to  $\tau$ ” is optimal for every singleton  $i$ . In other words, you may choose to obtain a sample from the  $\tau$ -core  $\beta$  on your way to obtaining a sample from  $\tau$  optimally.

The duality of the  $\tau$ -contrast  $\hat{\alpha}$  and the  $\tau$ -core  $\beta$  manifests itself in many ways. For example, generalizing the notion of state-to-state commute time  $\kappa(i, j) = H(i, j) + H(j, i)$  to distributions  $\kappa(\sigma, \tau) = H(\sigma, \tau) + H(\tau, \sigma)$ , we have the following extension for the known identity  $\kappa(i, j) = \hat{\kappa}(i, j)$  for all  $i, j$ .

**Corollary 5** *For a contrasting pair  $\hat{\alpha}, \beta$  and any state  $i$ ,  $\hat{\kappa}(i, \hat{\alpha}) = \kappa(i, \beta)$ .*

In addition, the average access times to these distributions are equal.

**Corollary 6** *The contrasting pair  $\hat{\alpha}$  and  $\beta$  satisfy*

$$\sum_k \pi_k \hat{H}(k, \hat{\alpha}) = \sum_k \pi_k H(k, \beta) \leq \sum_k \pi_k H(k, \tau).$$

Another duality result between the reverse  $\tau$ -contrast  $\hat{\alpha}$  and the forward  $\tau$ -core  $\beta$  concerns the regeneration time, which was studied in [5]. The regeneration time of a distribution  $\rho$  is the expected time between independent samples:  $T_{\text{regen}} = \sum_i \rho_i H(i, \rho)$ .

**Theorem 7** *For a distribution  $\tau$  with forward contrasting pair  $\hat{\alpha} = c(\tau)$  and  $\beta = \hat{c}(\hat{\alpha})$ ,*

$$\hat{T}_{\text{regen}}(\hat{\alpha}) = T_{\text{regen}}(\beta) \leq T_{\text{regen}}(\tau).$$

We are particularly interested in the case  $\tau = \pi$ . We have  $\hat{\mu} = c(\pi)$  and we introduce the notation  $\nu = \hat{c}(\hat{\mu}) = \hat{c}(c(\pi))$  for the  $\pi$ -core distribution. These three distributions will be used to prove the mixing results of theorems 1 and 2.

Finally, we consider the matrix properties of optimal exit frequency matrices. Not surprisingly, the exit frequency matrix  $X_\tau$  is closely related to  $I - M$ . The rank of  $I - M$  is  $n - 1$  ( $\pi$  is an eigenvector for eigenvalue 0). Depending on our target distribution, a slight alteration of  $I - M$  gives the inverse of  $X_\tau$ .

**Theorem 8** *Consider the (forward optimal) exit frequency matrix  $X_\tau$  for a distribution  $\tau$ .*

- (a) *If  $\tau$  is a singleton distribution on the state  $k$  then consider the  $(n - 1) \times (n - 1)$  matrix  $X'_k$  defined by deleting the  $k$ th row and the  $k$ th column of  $X_k$ . Let  $M'$  be defined similarly from the transition matrix  $M$ . Then  $X'_k$  is the inverse of  $(I - M')$ .*

(b) For any nonsingleton  $\tau$  with forward  $\tau$ -contrast  $\hat{\alpha}$ ,

$$X_\tau^{-1} = I - M + \frac{1}{T_{\text{regen}}(\tau)} \mathbf{a} \tau^\top \quad (6)$$

where  $\mathbf{a} = (a_1, a_2, \dots, a_n)$  is given by  $a_i = \hat{\alpha}_i / \pi_i$ .

Note that when our target is the singleton  $\tau = k$  then the  $k$ th row and the  $k$ th columns are all zero, hence  $n - 1$  is the largest possible rank for  $X_k$ . Part (b) shows that when  $\tau$  is any nonsingleton distribution,  $X_\tau$  has full rank and is obtained by adding the appropriate rank 1 matrix to the rank  $n - 1$  matrix  $I - M$ .

In general, the spectrum of  $X_\tau$  is difficult to describe. However, we can find the spectrum of  $X_\pi$  exactly.

**Theorem 9** *Denote the eigenvalues of  $M$  by  $\lambda_1 = 1 \geq \lambda_2 \geq \dots \geq \lambda_n$ . The largest eigenvalue for  $X_\pi$  is  $T_{\text{reset}}$  with corresponding left eigenvector  $\pi$ . The remaining eigenvalues are  $1/(1 - \lambda_k)$  for  $2 \leq k \leq n$ .*

It follows immediately that

$$\frac{1}{1 - \lambda_2} \leq T_{\text{reset}} \quad (7)$$

which was originally proven indirectly in [12].

The organization of this paper is the following: in Section 2 we recall some results concerning hitting times, access times and optimal stopping rules. Section 3 contains several examples to illustrate the duality of contrasted distributions. In Section 4, we prove our main duality result concerning contrasted distributions and derive some consequences. Section 5 contains the proofs of theorems 1 and 2. Finally, Section 6 contains some linear algebra and spectral results for exit frequency matrices.

## 2 Preliminaries

**Random Walks.** Let  $(w_0, w_1, \dots, w_t, \dots)$  be a finite irreducible Markov chain with state space  $S$  and transition probabilities  $p_{ij}$ . We define  $M = \{p_{ij}\}$  to be the matrix of transition probabilities. For two states  $i, j$ , the *hitting time*  $H(i, j)$  is the expected length of a walk from  $i$  to  $j$ . The expected number of steps before a walk started at  $i$  returns to  $i$  is

$$\text{Ret}(i) = \frac{1}{\pi_i}. \quad (8)$$

The sum  $\kappa(i, j) = H(i, j) + H(j, i)$  is the *commute time*. As a first example of the duality of the forward and reverse chains, we have

$$\kappa(i, j) = \hat{\kappa}(i, j). \quad (9)$$

More generally, the *cycle reversing identity* of [6] can be generalized (with a virtually identical proof) as

$$H(i, j) + H(j, k) + H(k, i) = \hat{H}(i, k) + \hat{H}(k, j) + \hat{H}(j, i) \quad (10)$$

for any states  $i, j$  and  $k$ . The analogous identity holds for more than three states. Another useful formula is the *random target identity* (see [2]) which states that

$$\sum_j \pi_j H(i, j) = T_{\text{hit}} \quad (11)$$

is independent of the starting state  $i$ . Multiplying (10) by  $\pi_k$ , summing over  $k$  and applying the random target identity gives

$$H(\pi, i) + H(i, j) = \hat{H}(\pi, j) + \hat{H}(j, i). \quad (12)$$

**Stopping Rules.** We briefly summarize some stopping rule results of Lovász and Winkler [10]. Let  $S^*$  be the space of finite walks on  $S$ , i.e. the set of finite strings  $w = (w_0, w_1, w_2, \dots, w_t)$ ,  $w_i \in V$  and  $p_{w_i, w_{i+1}} > 0$ . For a given initial distribution  $\sigma$ , the probability of  $w$  being the walk after  $t$  steps is

$$\Pr(w) = \sigma_{w_0} \prod_{i=0}^{t-1} p_{w_i, w_{i+1}}.$$

A *stopping rule*  $\Gamma$  is a map from  $S^*$  to  $[0, 1]$  such that  $\Gamma(w)$  is the probability of continuing given that  $w$  is the walk so far observed. We assume that with probability 1 the rule stops the walk in a finite number of steps.

Given another distribution  $\tau$  on  $V$ , we define the *access time*  $H(\sigma, \tau)$  to be the minimum expected length of a stopping rule  $\Gamma$  that produces  $\tau$  when started at  $\sigma$ . We say  $\Gamma$  is *optimal* if it achieves this minimum. Optimal stopping rules exist for any pair  $\sigma, \tau$  of distributions and the access time  $H(\sigma, \tau)$  has many useful algebraic properties. When  $\sigma$  and  $\tau$  are concentrated on states  $i$  and  $j$  respectively (we write  $\sigma = i, \tau = j$ ), the access time  $H(i, j)$  is the hitting time from  $i$  to  $j$ ; in this instance, the only optimal stopping rule is “walk until you hit  $j$ .” Whenever our target is a singleton, the analogous rule is optimal for any starting distribution:  $H(\sigma, j) = \sum_i \sigma_i H(i, j)$ . However, when our target is not a singleton the inequality  $H(\sigma, \tau) \leq \sum_i \sigma_i H(i, \tau)$  is usually strict.

Given a stopping rule  $\Gamma$  from  $\sigma$  to  $\tau$ , for each  $i \in S$  we define its *exit frequency*  $x_i(\Gamma)$  to be the expected number of times the walk leaves state  $i$  before halting. Exit frequencies are fundamental to virtually all access time results. A key observation, due to Pitman [13], is that exit frequencies satisfy

$$\sum_i p_{ij} x_i(\Gamma) - x_j(\Gamma) = \tau_j - \sigma_j. \quad (13)$$

It follows from this *conservation equation* that the exit frequencies for two rules from  $\sigma$  to  $\tau$  differ by  $K\pi_i$  where  $K$  is the difference between the expected lengths of these rules. Hence the distributions  $\sigma$  and  $\tau$  uniquely determine the exit frequencies for a mean optimal stopping rule between them. We denote these optimal exit frequencies by  $x_i(\sigma, \tau)$ . Moreover, a stopping rule  $\Gamma$  is mean-optimal if and only if there exists a *halting state*  $k$  such that  $x_k(\Gamma) = 0$ .

Any three distributions  $\rho, \sigma$  and  $\tau$  satisfy the “triangle inequality”

$$H(\rho, \tau) \leq H(\rho, \sigma) + H(\sigma, \tau) \quad (14)$$

with equality holding if and only if there is a  $k$  that is a halting state from  $\rho$  to  $\sigma$  and also a halting state from  $\sigma$  to  $\tau$ . In particular,  $H(\sigma, j) \leq H(\sigma, \tau) + H(\tau, j)$  and equality holds if and only if  $j$  is a halting state for an optimal rule from  $\sigma$  to  $\tau$ . This gives

$$H(\sigma, \tau) = \max_j (H(\sigma, j) - H(\tau, j)). \quad (15)$$

In the case  $\sigma = i$  and  $\tau = \pi$ , the state  $j$  is halting for  $i$  if and only if  $\hat{H}(j, i) = \max_k \hat{H}(k, i)$ . Let  $i'$  be such an  *$i$ -pessimal* state. Combining equations (15) and (12) yields another formula for the access time from  $i$  to  $\pi$ :

$$H(i, \pi) = \hat{H}(i', i) - \hat{H}(\pi, i). \quad (16)$$

The exit frequencies for an optimal stopping rule from  $\sigma$  to  $\tau$  are given by

$$x_k(\sigma, \tau) = \pi_k (H(\sigma, \tau) + H(\tau, k) - H(\sigma, k)). \quad (17)$$

and sometimes it is more convenient to consider the *scaled exit frequencies*

$$y_i(\sigma, \tau) = \frac{1}{\pi_i} x_i(\sigma, \tau).$$

**Exit Frequency Matrix.** Fix the target distribution  $\tau$  and consider a family of optimal walks from all singleton distributions to  $\tau$ . We can naturally represent the exit frequencies for this family of rules in an  $n \times n$  matrix  $X_\tau$  whose  $ij$ th entry is  $x_j(i, \tau)$ . The  $i$ th row of  $X_\tau$

contains the exit frequencies for an optimal rule from  $i$  to  $\tau$ . We can rewrite the conservation equation (13) in matrix form:

$$X_\tau(I - M) = I - \mathbf{1}\tau^\top. \quad (18)$$

This matrix equation identifies connections between stopping rules on the forward and reverse chains.

**Lemma 10** *For any distribution  $\sigma$  on the forward chain  $M$  and any distribution  $\hat{\tau}$  on the reverse chain  $\hat{M}$ ,*

$$(I - \mathbf{1}\sigma^\top)R\hat{X}_{\hat{\tau}}^\top = X_\sigma R(I - \hat{\tau}\mathbf{1}^\top).$$

**Proof.** Transpose the matrix conservation equation (18) for the reverse walk to  $\hat{\tau}$  and substitute  $\hat{M}^\top = R^{-1}MR$  to yield  $R^{-1}(I - M)R\hat{X}_{\hat{\tau}}^\top = I - \hat{\tau}\mathbf{1}^\top$ . Multiplying on the left by  $X_\sigma R$  and using equation (18) for  $\sigma$  gives the result.  $\square$

The  $ij$ th entry gives a special case of lemma 1 of [11] which will be useful in later.

**Corollary 11**

$$\hat{y}_i(j, \hat{\tau}) - \sum_k \sigma_k \hat{y}_k(j, \hat{\tau}) = y_j(i, \sigma) - \sum_k \hat{\tau}_k y_k(i, \sigma).$$

$\square$

### 3 Examples

We illustrate contrast and core distributions with some examples on time reversible and general Markov chains. In particular, we will calculate the forget distribution  $\mu$  and the  $\pi$ -core  $\nu$  for these examples. When our Markov chain is time reversible, we use  $c$  to denote the unique contrast map and we denote the  $\tau$ -contrast and the  $\tau$ -core by  $\alpha$  and  $\beta$ , respectively.

**Complete Graph.** Let  $\alpha$  is a non-singleton contrasted distribution on the complete graph  $K_n$  ordered so that  $\alpha_1 \geq \alpha_2 \geq \dots \geq \alpha_n$ . Then  $\alpha$  is given by  $\alpha_1 \geq 1/n$  and  $\alpha_i = (1 - \alpha_1)/(n - 1)$  for  $2 \leq i \leq n$ . Indeed, let  $\tau$  be any distribution on  $K_n$  with nodes ordered so that  $\tau_1 \geq \tau_2 \geq \dots \geq \tau_n$ . By equation (15) and the fact that  $H(i, j) = n - 1$  for  $i \neq j$ , node 2 is  $\tau$ -halting for node 1 and node 1 is  $\tau$ -halting for  $i > 1$ . By theorem 3,  $RF_\alpha^\top R^{-1} = F_\tau - \mathbf{1}\mathbf{b}^\top$  where  $b_k = \min_i x_k(i, \tau)$ . By simply transposing  $F_\tau$  it is clear that every node  $i > 1$  is  $\alpha$ -halting for node 1, so  $\alpha_2 = \alpha_3 = \dots = \alpha_n$ . Moreover,  $x_1(1, \alpha) = x_1(1, \tau) = \frac{n-1}{n}(1 - \tau_1 + \tau_2)$ . Hence  $\alpha_1 = \frac{1}{n} + \frac{n-1}{n}(\tau_1 - \tau_2)$  and  $\alpha_k = \frac{1}{n}(1 - \tau_1 + \tau_2)$  for  $2 \leq k \leq n$ .

Note that every contrasted distribution on  $K_n$  is self-contrasting:  $c(\alpha) = \alpha$ , and therefore  $H(i, \alpha) + H(\alpha, \tau) = H(i, \tau)$  for all  $i$  by corollary 4. Turning our attention to the contrasting pair for  $\pi$ , we know that the mixing time is the same for all nodes, and hence  $\mu = \nu = \pi$ .

**Trees.** On a tree, a contrasted distribution must either be a singleton or concentrated on two adjacent nodes. Like the complete graph, each of these is self-contrasting. Assume that  $\tau$  is not a singleton. The contrast map compares the length of the rule “take one step and follow an optimal rule to  $\tau$ ” with the length of an optimal rule. In particular, if the node  $i$  and all of its neighbors share a common  $\tau$  halting state, then  $\alpha_i = 0$ . There can be at most two nodes for which this does not hold, and they must be adjacent.

We consider  $\tau = \pi$  for a path on  $n$  vertices and calculate  $\mu = \nu$ . In this case, the best choice to “forget” where we started is to walk to the center of the path. For a path of even length,  $\mu$  will be concentrated on the center of the path. For a path of odd length,  $\mu$  will be evenly divided between the two central nodes of the path. A general formula for  $\mu$  on a tree is given in [4].

**Winning Streak.** The winning streak chain (introduced in [11]) nicely illustrates how different mixing walks can be for the forward and reverse chain. The winning streak on  $n$  nodes  $\{0, 1, \dots, n-1\}$  has transition probabilities given by

$$p_{ij} = \begin{cases} 1/2 & j = i + 1 \\ 1/2 & j = 0 \text{ and } 0 \leq i \leq n-1 \\ 1/2 & i = j = n-1 \\ 0 & \text{otherwise.} \end{cases}$$

The stationary distribution is  $\pi = (1/2, 1/4, \dots, 2^{-n+1}, 2^{-n+1})$ . Both state 0 and  $n-1$  are mixing pessimal. For either one, the trivial rule “take  $n-1$  steps” is an optimal mixing rule.

The transition probabilities for the reverse winning streak are

$$\hat{p}_{ij} = \begin{cases} 1 & j = i-1 \text{ and } 1 \leq i \leq n-2 \\ 2^{-j-1} & i = 0 \text{ and } 0 \leq i \leq n-2 \\ 2^{-n+1} & i = 0 \text{ and } j = n-1 \\ 1/2 & i = n-1 \text{ and } j = n-1 \text{ or } j = n-2 \\ 0 & \text{otherwise.} \end{cases}$$

For the reverse winning streak, state  $n-1$  is mixing pessimal and the rule “take  $n-1$  steps” is an optimal mixing rule from this state. However, state 0 is far from pessimal: the rule “take one step” takes us immediately from 0 to  $\pi$ .

We describe the forget distribution and  $\pi$ -core of both the forward and reverse winning streak chains, omitting the detailed calculations. The reverse forget distribution was calculated

in [11]:

$$\mu = \begin{cases} 1 - 2^{-n+1} & i = 0 \\ 2^{-n+1} & i = n - 1 \\ 0 & \text{otherwise.} \end{cases}$$

Moreover,  $H(i, \mu) = 2 - 2^{-n+2}$  for all  $i$  (walk until either state 0 is hit or  $n - 1$  steps have been made) and therefore  $\hat{\nu} = c(\mu) = \pi$ .

The contrasting pair  $\hat{\mu}$  and  $\nu$  are not as well behaved. A more complicated analysis of the mixing walks on forward chain shows that each state below roughly  $\log n$  has state  $n - 1$  as a  $\pi$ -halting state while each remaining state  $i$  has  $i - 1$  as a  $\pi$ -halting state. Let  $i_0$  be the unique node satisfying  $2^{i_0} + i_0 \leq n < 2^{i_0+1} + i_0 + 1$ . Some tedious calculations of access times gives

$$\hat{\mu} = \begin{cases} 0 & 0 \leq i < i_0 \\ \frac{\pi_{i_0}}{2}(2^{i_0+2} - n + i_0) & i = i_0 \\ \frac{\pi_{i_0}}{2}(2 + n - i) & i_0 < i \leq n - 2 \\ \pi_{n-1} & i = n - 1. \end{cases}$$

Finally, we may calculate  $\nu = \hat{c}(\hat{\mu})$  using theorem 3:

$$\nu = \begin{cases} \sum_{k=0}^{i_0} \pi_k & i = 0 \\ 0 & 1 \leq i \leq i_0 \\ \pi_i & i_0 < i \leq n - 1. \end{cases}$$

We note that  $\mu, \hat{\nu}, \hat{\mu},$  and  $\nu$  are all quite distinct from one another.

## 4 Contrasting Pairs

We examine the relationship between the exit frequencies for stopping rules concerning  $\tau$  and its forward contrast  $\hat{\alpha}$ . In this section, we assume that  $\hat{\alpha} = c(\tau)$  and  $\beta = \hat{c}(\hat{\alpha}) = \hat{c}(c(\tau))$ . We begin with a straightforward generalization of theorem 5 in [11].

**Proposition 12** *If  $\hat{\alpha} = c(\tau)$  then the scaled exit frequencies for the reverse walk from  $\pi$  to  $\hat{\alpha}$  and vice versa are given by*

$$\hat{y}_i(\pi, \hat{\alpha}) = H(i, \tau) - \min_k H(k, \tau)$$

and

$$\hat{y}_i(\hat{\alpha}, \pi) = \max_k H(k, \tau) - H(i, \tau).$$

**Proof.** Rewriting equation (4) gives

$$\sum_j \hat{p}_{ji} \pi_j H(i, \tau) - \pi_i H(i, \tau) = \hat{\alpha}_i - \pi_i.$$

By equation (13), the numbers  $\hat{y}_i = H(i, \tau)$  are the scaled exit frequencies of some (non-optimal) stopping rule for a walk from  $\pi$  to  $\hat{\alpha}$  on the reverse chain. Therefore  $H(i, \tau) - \min_k H(k, \tau)$  is the  $i$ th exit frequency for an optimal stopping rule. Taking the negative of both sides and following a similar argument gives the second statement of the theorem.  $\square$

**Corollary 13** *A state  $z$  is a halting state from  $\pi$  to  $\hat{\alpha}$  on the reverse chain if and only if it achieves  $\min_k H(k, \tau)$ . Moreover,*

$$\min_k H(k, \tau) = \sum_i \pi_i H(i, \tau) - \hat{H}(\pi, \hat{\alpha}).$$

$\square$

**Corollary 14** *A state  $z$  is a halting state from  $\hat{\alpha}$  to  $\pi$  on the reverse chain if and only if it achieves  $\max_k H(k, \tau)$ . Moreover,*

$$\max_k H(k, \tau) = \sum_i \pi_i H(i, \tau) + \hat{H}(\hat{\alpha}, \pi).$$

$\square$

We now focus on the central result of this paper: the relationship between forward rules from singletons to  $\tau$  and reverse rules from singletons to  $\hat{\alpha}$ . In particular, we show that the relationship between  $X_\tau$  and  $\hat{X}_{\hat{\alpha}}$  mirrors the relationship between  $M$  and  $\hat{M}$ . Recall that the transition matrix for the reverse chain is the scaled transpose of the transition matrix for the forward chain:  $\hat{M} = RM^\top R^{-1}$ . Analogously, theorem 3 shows that the reverse exit frequency matrix for  $\hat{\alpha}$  is derived from the scaled transpose of the exit frequency matrix for  $\tau$ .

**Proof of Theorem 3.** The  $ij$ th component of  $(I - M)X_\tau$  is

$$\begin{aligned} & x_j(i, \tau) - \sum_k p_{ik} x_j(k, \tau) \\ &= \pi_j \left( H(i, \tau) - \sum_k p_{ik} H(k, \tau) - H(i, j) + \sum_k p_{ik} H(k, j) \right) \\ &= i_j - \pi_j \hat{\alpha}_i / \pi_i \end{aligned}$$

since  $1/\pi_i = \text{Ret}(i) = 1 + \sum_k p_{ik} H(k, i)$ , and therefore  $(I - M)X_\tau = I - R\hat{\alpha}\mathbf{1}^\top R^{-1}$ . Rewriting the reverse conservation equation for  $\hat{\alpha}$  gives  $\hat{\alpha}\mathbf{1}^\top = I - (I - \hat{M}^\top)\hat{X}_{\hat{\alpha}}^\top$ . Substituting this value into the previous equation and using  $\hat{M}^\top = R^{-1}MR$  yields

$$(I - M)X_\tau = (I - M)R\hat{X}_{\hat{\alpha}}R^{-1}.$$

Hence  $R\hat{X}_\alpha^\top R^{-1} = X_\tau + L$  where  $(I - M)L = 0$ . The rank of  $I - M$  is  $n - 1$  and  $\mathbf{1}$  is a right eigenvector for 0, so  $L = \mathbf{1}\mathbf{b}^\top$  for some constant vector  $\mathbf{b}$ . Since every column of  $\hat{X}_\alpha$  must contain a zero element, we must have  $b_k = \min_i x_k(i, \tau)$  for  $1 \leq k \leq n$ .  $\square$

Theorem 3 states that for each  $i$ ,  $y_i(1, \tau), y_i(2, \tau), \dots, y_i(n, \tau)$  is a set of scaled exit frequencies for a (not necessarily optimal) stopping rule on the reverse chain from  $i$  to  $\hat{\alpha}$ . These exit frequencies correspond to an optimal rule if and only if there exists a  $k$  such that  $i$  is a halting state for the forward  $(k, \tau)$ -walk. On the other hand, for each  $i$  there exists some  $k$  such that  $y_k(i, \tau) = 0$  which means that for *every* state  $i$  there always exists a  $k$  such that  $\hat{y}_i(k, \hat{\alpha}) = 0$ .

The forward exit frequencies to  $\tau$  become (not necessarily optimal) reverse exit frequencies to  $\hat{\alpha}$ , however the reverse statement need not hold. Instead, the scaled transpose of  $\hat{X}_\alpha$  gives a set of optimal exit frequencies to the  $\tau$ -core  $\beta = \hat{c}(\hat{\alpha}) = \hat{c}(c(\tau))$ .

**Proof of Corollary 4.** By the theorem,  $RX_\beta^\top R^{-1} = \hat{X}_\alpha - \mathbf{1}\mathbf{b}^\top$  where  $b_i = \min_k \hat{x}_k(i, \hat{\alpha})$ . Each column of  $\hat{X}_\alpha$  contains at least one zero entry, and therefore  $\mathbf{b} = 0$ . In addition, each row of  $\hat{X}_\alpha$  contains at least one zero, and therefore  $c(\beta) = \hat{\alpha}$ .

Since  $x_k(i, \beta) \leq x_k(i, \tau)$  for all  $i, k$ , we have  $H(i, \tau) = H(i, \beta) + H(\beta, \tau)$  as the rule “walk from  $i$  to  $\beta$  and then from  $\beta$  to  $\tau$ ” has a halting state. If  $\sigma$  is any distribution such that  $H(i, \tau) = H(i, \sigma) + H(\sigma, \tau)$  for all  $i$ , we have  $x_k(i, \sigma) + x_k(\sigma, \tau) = x_k(i, \tau)$ . Since  $x_k(\sigma, \tau)$  is independent of  $i$  and all exit frequencies must be nonnegative,  $x_k(i, \sigma) \geq x_k(i, \tau) - \min_j x_k(j, \tau) = x_k(i, \beta)$  for all  $i, k$ . So  $H(i, \sigma) \geq H(i, \beta)$  for all  $i$  and  $H(\sigma, \tau) \leq H(\beta, \tau)$ . Clearly  $\beta$  is the unique reverse contrasted distribution among all  $\sigma$  such that  $H(i, \tau) = H(i, \beta) + H(\beta, \tau)$  for all  $i$ .  $\square$

The relationship described in corollary 4 is summarized via a formula using scaled exit frequencies:

$$\hat{y}_i(j, \hat{\alpha}) = y_j(i, \beta) \text{ for all } i, j. \quad (19)$$

The  $\tau$ -contrast  $\hat{\alpha}$  has a natural association with the reverse chain, and it captures the differences between walks from neighboring states to  $\tau$ . On the other hand, the  $\tau$ -core  $\beta$  has a natural association with the forward chain, and complementary to  $\hat{\alpha}$ ,  $\beta$  captures the maximum commonality among all walks from singletons to  $\tau$ . It is also important to note that both  $\hat{\alpha}$  and  $\beta$  are “balanced” in the sense that every state is a halting state for at least one other state. Furthermore,  $j$  is a halting state for the reverse  $(i, \hat{\alpha})$ -walk if and only if  $i$  is a halting state for the forward  $(j, \beta)$ -walk.

We spend the remainder of this section developing the duality of the contrasting pair  $\hat{\alpha}$  and  $\beta$ . First, we prove that the the contrasting pair have the same commute times to singletons

and that the average access times to each of the contrasting pair are equal.

**Proof of Corollary 5.** Since  $y_i(i, \beta) = \hat{y}_i(i, \hat{\alpha})$ ,  $H(i, \beta) + H(\beta, i) = \hat{H}(i, \hat{\alpha}) + \hat{H}(\hat{\alpha}, i)$ .  $\square$

**Proof of Corollary 6.** Taking the trace of both  $\hat{X}_{\hat{\alpha}}$  and  $RX_{\beta}^{\top}R^{-1}$ ,

$$\sum_k \pi_k (\hat{H}(k, \hat{\alpha}) + \hat{H}(\hat{\alpha}, k)) = \sum_k \pi_k (H(k, \beta) + H(\beta, k))$$

therefore  $\sum_k \pi_k \hat{H}(k, \hat{\alpha}) = \sum_k \pi_k H(k, \beta)$  by the random target identity (11). Since  $H(k, \beta) \leq H(k, \tau)$  for all  $k$ , we have  $\sum_k \pi_k H(k, \beta) \leq \sum_k \pi_k H(k, \tau)$ .  $\square$

The next two results follow immediately from the theorem and corollaries 13 and 14.

**Corollary 15** *A state  $z$  is a halting state from  $\pi$  to  $\hat{\alpha}$  on the reverse chain if and only if it achieves  $\min_k H(k, \beta)$ . Moreover,*

$$\min_k H(k, \beta) = \sum_i \pi_i \hat{H}(i, \hat{\alpha}) - \hat{H}(\pi, \hat{\alpha}).$$

$\square$

**Corollary 16** *A state  $z$  is a halting state from  $\hat{\alpha}$  to  $\pi$  on the reverse chain if and only if it achieves  $\max_k H(k, \beta)$ . Moreover,*

$$\max_k H(k, \beta) = \sum_i \pi_i \hat{H}(i, \hat{\alpha}) + \hat{H}(\hat{\alpha}, \pi).$$

$\square$

In addition to the equality of the average access times for the contrasting pair, we also have  $\hat{T}_{\text{regen}}(\hat{\alpha}) = T_{\text{regen}}(\beta) \leq T_{\text{regen}}(\tau)$ .

**Proof of Theorem 7.** Taking  $i = j$  in corollary 11, consider equation (19) with  $\sigma = \beta$ ,  $\hat{\tau} = \hat{\alpha}$ . Choosing  $i, j$  such that  $y_j(i, \sigma) = \hat{y}_i(j, \hat{\tau}) = 0$ ,

$$\begin{aligned} \sum_k \beta_k \hat{y}_k(i, \hat{\alpha}) &= \sum_k \hat{\alpha}_k y_k(j, \beta) \\ \sum_k \beta_k y_i(k, \beta) &= \sum_k \hat{\alpha}_k \hat{y}_j(k, \hat{\alpha}) \\ \sum_k \beta_k (H(k, \beta) + H(\beta, i) - H(k, i)) &= \sum_k \hat{\alpha}_k (\hat{H}(k, \hat{\alpha}) + \hat{H}(\hat{\alpha}, j) - \hat{H}(k, j)) \\ \sum_k \beta_k H(k, \beta) &= \sum_k \hat{\alpha}_k \hat{H}(k, \hat{\alpha}). \end{aligned}$$

The inequality  $\hat{T}_{\text{regen}}(\hat{\alpha}) \leq T_{\text{regen}}(\tau)$  follows similarly, using  $y_k(i, \tau) \geq \hat{y}_i(k, \hat{\alpha})$  for all  $i, k$ .  $\square$

We extend the cycle reversing identity (10) for contrasting pairs.

**Proposition 17** *The distributions  $\hat{\alpha}$  and  $\beta$  are a contrasting pair if and only if*

$$\hat{H}(i, \hat{\alpha}) + \hat{H}(\hat{\alpha}, j) + \hat{H}(j, i) = H(j, \beta) + H(\beta, i) + H(i, j).$$

**Proof.** The distributions are a contrasting pair if and only if  $\hat{y}_j(i, \hat{\alpha}) = y_i(j, \beta)$  for all  $i, j$ . By equation (9),  $\hat{y}_j(i, \hat{\alpha}) + \hat{\kappa}(i, j) = y_i(j, \beta) + \kappa(i, j)$  and expanding completes the proof.  $\square$

We say that a distribution  $\gamma$  is *self-contrasting* if  $c(\gamma) = \hat{c}(\gamma) = \gamma$ . Obviously, any singleton is self contrasting. It follows from the proposition that  $\gamma$  is self contrasting if and only if

$$\hat{H}(i, \gamma) + \hat{H}(\gamma, j) + \hat{H}(j, i) = H(j, \gamma) + H(\gamma, i) + H(i, j). \quad (20)$$

## 5 Mixing Measures

We provide new proofs of theorems 1 and 2 using the duality of contrasting pairs. For the equality  $\hat{T}_{\text{forget}} = T_{\text{reset}}$  of theorem 2, this proof offers new insight into the relationship between  $\pi$  and the reverse forget distribution  $\hat{\mu}$ . Recall that  $\nu = \hat{c}(\hat{\alpha}) = \hat{c}(c(\pi))$  and  $\hat{\nu} = c(\alpha) = c(\hat{c}(\pi))$  are the forward  $\pi$ -core and the reverse  $\pi$ -core, respectively.

**Proof of Theorem 2.** If  $\hat{\sigma}$  achieves  $\min_{\tau} \max_i \hat{H}(i, \tau)$  then  $\hat{\sigma}$  must be contrasted: we have  $\hat{x}_k(i, c(\hat{c}(\hat{\sigma}))) \leq \hat{x}_k(i, \hat{\sigma})$  by theorem 3, so  $\hat{H}(i, c(\hat{c}(\hat{\sigma}))) \leq \hat{H}(i, \hat{\sigma})$ . Thus we may assume that our minimum is achieved by  $\hat{\alpha}$  where  $\hat{\alpha} = c(\beta)$  and  $\beta = \hat{c}(\hat{\alpha})$  are a contrasting pair. Applying corollary 16 for the reverse chain (and switching the roles of  $\hat{\alpha}$  and  $\beta$ ),

$$\max_i \hat{H}(i, \hat{\alpha}) = \sum_j \pi_j (H(j, \beta) + H(\beta, \pi)) \geq \sum_j \pi_j H(j, \pi) = T_{\text{reset}}.$$

Using corollary 4 with  $\tau = \pi$ , we find that  $\hat{\alpha} = \hat{\mu}$  and  $\beta = \nu$  shows that  $H(j, \nu) + H(\nu, \pi) = H(j, \pi)$  for all  $j$  and therefore  $\hat{\mu}$  achieves this lower bound. The uniqueness of  $\hat{\mu}$  also follows from corollary 4.  $\square$

We now use theorem 2 to prove theorem 1, showing that  $T_{\text{mix}} = \hat{T}_{\text{mix}}$ .

**Proof of Theorem 1.** By corollary 14 with  $\tau = \pi$  and  $\hat{\alpha} = \hat{\mu}$ ,  $T_{\text{mix}} = \max_k H(k, \pi) = T_{\text{reset}} + \hat{H}(\hat{\mu}, \pi) = \hat{T}_{\text{forget}} + \hat{H}(\hat{\mu}, \pi) = \max_k (\hat{H}(k, \hat{\mu}) + \hat{H}(\mu, \pi)) \geq \max_k H(k, \pi) = \hat{T}_{\text{mix}}$ . Starting with the mixing time for the reverse chain, we similarly find that  $\hat{T}_{\text{mix}} \geq T_{\text{mix}}$  so equality must hold everywhere.  $\square$

**Corollary 18** *If  $z$  is  $\pi$ -pessimal on the forward chain then  $\hat{H}(z, \hat{\mu}) + \hat{H}(\hat{\mu}, \pi) = \hat{H}(z, \pi)$ .  $\square$*

**Proposition 19** *A state  $z$  is forget pessimal if and only if it is a halting state for some mixing walk on the reverse chain.*

**Proof.** Summing across the  $i$ th row of  $\hat{X}_{\hat{\mu}}$  gives

$$\hat{H}(i, \mu) = \sum_j \pi_j \hat{y}_j(i, \hat{\mu}) = \sum_j \pi_j y_i(j, \pi) - \min_k y_i(k, \pi) = \sum_j \pi_j H(j, \pi) - \min_k y_i(k, \pi)$$

which is maximized whenever  $\min_k y_i(k, \pi) = 0$ .  $\square$

This is an improvement over corollary 6 of [11] which only identifies the  $\pi$ -pessimal state as a pessimal state for the forget walk.

Finally, the following corollary is dual to theorem 4 of [11], which states that  $T_{\text{forget}} = \sum_j \pi_j (H(j', j) - H(\pi, j))$  where  $\hat{H}(j', j) = \max_k \hat{H}(k, j)$ .

**Corollary 20**  $\hat{T}_{\text{forget}} = \sum_j \mu_k (\hat{H}(j', j) - \hat{H}(\hat{\mu}, j))$  where  $\hat{H}(j', j) = \max_k \hat{H}(k, j)$ .

**Proof.** Since  $j'$  is a halting state for the mixing walk from  $j$ , proposition 19 implies that  $j$  is a halting state for the reverse walk from  $j'$  to  $\hat{\mu}$  and that  $\hat{H}(j', j) - \hat{H}(\hat{\mu}, j) = \hat{H}(j', \hat{\mu}) = \hat{T}_{\text{forget}}$  for all  $j$ .  $\square$

## 6 Exit Frequency Matrices

The matrix form of the conservation equation (18) shows that  $X_\tau$  is *almost* the inverse for the (singular) matrix  $I - M$ . We now prove Theorem 8, which explains how to alter the matrix  $I - M$  so that  $X_\tau$  is the inverse of the resulting matrix.

**Proof of Theorem 8(a).** Fix a target singleton distribution  $k$  and let  $X_k = (x_j(i, k))$  be the exit frequency matrix of an optimal family of rules from the singletons to  $k$ . Note that the  $k$ th row and  $k$ th column are both 0, and therefore the rank of  $X_k$  is at most  $n - 1$ . Let  $X'_k$  and  $M'$  be the matrices defined by deleting the  $k$ th row and column from  $X_k$  and  $M$ , respectively. Consider the  $ij$ th entry of  $F'_k(I - M')$  which is

$$x_j(i, k) - \sum_r p_{rj} x_r(i, k) = i_j$$

by the conservation equation (13). Hence  $F'_k(I - M') = I$ . Similarly, we see that the  $ij$ th entry of  $(I - M')F'_k$  satisfies

$$x_j(i, k) - \sum_r p_{ir} x_j(r, k) = i_j$$

by considering the optimal rule “take one step from  $i$  and follow an optimal rule to  $k$ .” Thus,  $X'_k$  is the inverse of  $I - M'$  and therefore has rank  $n - 1$ .  $\square$

In the case of a nonsingleton target distribution  $\tau$ , we find that  $X_\tau$  has full rank.

**Proof of Theorem 8(b).** If  $X_\tau^{-1}$  exists, then by equation (18) we must have

$$I - M = X_\tau^{-1} X_\tau (I - M) = X_\tau^{-1} (I - \mathbf{1} \tau^\top) = X_\tau^{-1} - \mathbf{c} \tau^\top$$

where  $c_i = \sum_k (X_\tau^{-1})_{ik}$ . Therefore if  $X_\tau^{-1}$  exists then it must be of the form  $X_\tau^{-1} = I - M + \mathbf{c} \tau^\top$  for some vector  $\mathbf{c}$ . For a nonsingleton  $\tau$ , we show that we can always find such a  $\mathbf{c}$  by solving

$$I = (I - M + \mathbf{c} \tau^\top) X_\tau. \quad (21)$$

The  $ij$ th entry of the right hand side of (21) is

$$\begin{aligned} & x_j(i, \tau) + \sum_k p_{ik} x_j(k, \tau) + c_i \sum_k \tau_k x_i(k, \tau). \\ &= \pi_j \left( H(i, \tau) - \sum_k p_{ik} H(k, \tau) - H(i, j) + \sum_k p_{ik} H(k, j) + c_i T_{\text{regen}}(\tau) \right) \end{aligned}$$

by equation (17). Considering the case  $i \neq j$ , we have  $H(i, j) - \sum_k p_{ik} H(k, j) = 1$  and the  $ij$ th entry of equation (21) is

$$\begin{aligned} 0 &= \pi_j \left( H(i, \tau) - \sum_k p_{ik} H(k, \tau) - 1 + c_i T_{\text{regen}}(\tau) \right) \\ &= \pi_j \left( -\frac{\hat{\alpha}_i}{\pi_i} + c_i T_{\text{regen}}(\tau) \right) \end{aligned}$$

by equation (4). Since  $\tau$  is not a singleton,  $T_{\text{regen}}(\tau) > 0$  and we may solve for  $\mathbf{c}$ :

$$c_i = \frac{1}{T_{\text{regen}}(\tau)} \frac{\hat{\alpha}_i}{\pi_i} \text{ for } 1 \leq i \leq n.$$

These values are consistent with the diagonal entries of equation (21). For  $i = j$ , the right hand side becomes

$$\begin{aligned} & \pi_i \left( H(i, \tau) - \sum_k p_{ik} H(k, \tau) + \sum_k p_{ik} H(k, i) + c_i T_{\text{regen}}(\tau) \right) \\ &= 1 - \hat{\alpha}_i + \pi_i c_i T_{\text{regen}}(\tau) = 1 \end{aligned}$$

since  $1 + \sum_k p_{ik}H(k, i) = \text{Ret}(i) = 1/\pi_i$  is the return time to  $i$ .  $\square$

In the important case where  $\tau = \pi$ , we rewrite this equation using our mixing measure notation

**Corollary 21** *The inverse of the mixing matrix  $X_\pi$  is*

$$F_\pi^{-1} = I - M + \frac{1}{T_{\text{reset}}}\mathbf{c}\pi^\top$$

where  $\mathbf{c}$  is given by  $c_i = \hat{\mu}_i/\pi_i$ .  $\square$

Turning to the spectrum of  $F_\pi$ , we can determine the largest eigenvalue and its left eigenvector. Theorem 9 states that the largest eigenvalue of  $F_\pi$  is  $T_{\text{reset}}$  and its other eigenvalues are derived from  $I - M$ .

**Proof of Theorem 9.** Using equation (17) with the  $i$ th component of  $\pi^\top F_\pi$  yields  $\sum_k \pi_k x_i(k, \pi) = \pi_i \sum_k \pi_k (H(k, \pi) + H(\pi, i) - H(k, i)) = \pi_i \sum_k \pi_k H(k, \pi) = \pi_i T_{\text{reset}}$  by the random target identity (11). Since all of the components of its left eigenvector are positive, the Frobenius-Perron theorem [8] proves that  $T_{\text{reset}}$  is the largest eigenvalue of  $X_\pi$ .

Denote the eigenvalues of  $M$  by  $\lambda_1 = 1, \lambda_2, \dots, \lambda_n$  where  $1 > |\lambda_k|$  for  $2 \leq k \leq n$ . Let  $\mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_n$  be the respective right eigenvectors of  $\lambda_2, \dots, \lambda_n$ . The vector  $\pi^\top$  is a left eigenvector of  $M$ , hence  $\pi$  is orthogonal to each of these vectors, so that

$$X_\pi^{-1}\mathbf{v}_k = \left( I - M + \frac{1}{T_{\text{reset}}}\mathbf{c}\pi^\top \right) \mathbf{v}_k = (I - M)\mathbf{v}_k = (1 - \lambda_k)\mathbf{v}_k \text{ for } 2 \leq k \leq n$$

and the theorem follows.  $\square$

In addition to equation (7), we can confirm another spectral result by taking the trace of  $X_\pi$ . The trace is equal to the sum of the eigenvalues and hence

$$T_{\text{reset}} + \sum_{k=2}^n \frac{1}{1 - \lambda_k} = \sum_k x_k(k, \pi) = T_{\text{reset}} + T_{\text{hit}},$$

recovering the identity  $T_{\text{hit}} = \sum_{k=2}^n 1/(1 - \lambda_k)$ .

We conclude this section by giving necessary and sufficient conditions for a matrix to be the exit frequency matrix for some distribution  $\tau$ .

**Proposition 22** *The matrix  $X$  contains the exit frequencies for a (possibly non-optimal)  $\tau$ -family on the Markov chain with transition matrix  $M$  if and only if the following two conditions hold:*

$$(a) (I - M)X(I - M) = (I - M)$$

$$(b) I - X(I - M) \geq 0$$

The matrix  $X$  is the optimal exit frequency matrix for  $\tau$  if and only if in addition to the above two conditions, we have

$$(c) \min_j X_{ij} = 0 \text{ for } 1 \leq i \leq n.$$

The matrix  $X$  is the optimal exit frequency matrix for a reverse contrasted distribution if and only if in addition to the above three conditions, we have

$$(d) \min_i X_{ij} = 0 \text{ for } 1 \leq j \leq n.$$

**Proof.** If  $X$  is an exit frequency matrix for some family of (possibly non-optimal) rules, then (a) and (b) follow from the conservation equation (13). Considering the reverse direction, assume that  $X$  satisfies both conditions. By (a),  $(I - M)(X(I - M) - I) = 0$  and therefore  $X(I - M) - I = -\tau \mathbf{1}^\top$  for some vector  $\tau$ , which verifies the conservation equation (18). Furthermore,  $\sum_k \tau_k = \tau \mathbf{1}^\top \mathbf{1} = (I - F(I - M))\mathbf{1} = 1$  and condition (b) ensures that  $\tau \geq 0$ , so  $\tau$  is a distribution.

$X$  is an optimal exit frequency if and only if each row contains a halting state, proving (c). Condition (d) follows similarly: the target distribution is reverse contrasted if and only if each column contains a zero entry.  $\square$

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