On Time Duality for Markov Chains

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Abstract

For an irreducible continuous time Markov chain, we derive the distribution of the first passage time from a given state i to another given state j and the reversed passage time from j to i, each under the condition of no return to the starting point. When these two distributions are identical, we say that i and j are in *time duality*. We introduce a new condition called *permuted balance* that generalizes the concept of reversibility and provides sufficient criteria, based on the structure of the transition graph of the Markov chain. Illustrative examples are provided.

Keywords: Markov Chain, Time duality, First passage time, Reversibility, Permuted balance, detailed balance
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1. Introduction

In living cells transport molecules and molecular motors play a crucial role to support the survival and proper function of the organism. By exploiting an out of equilibrium condition of a chemical compound, like ATP, these molecules are able to change their conformation and to perform mechanical work. Justified by experiments and physical properties, continuous time Markov chains with discrete state space provide a very successful framework for the study of the dynamics of such molecules, see e.g. [DRJ$^+$10, LL07, Sei12, KlV13].

In this framework each state of the Markov chain represents a certain conformation of the molecule. For molecular motors involved in transport (e.g. kinesin) some of the transitions are also related to a directed change of position along a support structure by a thermodynamically driven conformation change, see [SSSB93, LLV09].

Recent studies [LW07, VLL08] have emphasized that certain first passage times in relatively complex models of kinesin's steps have the same distribution. More precisely, a passage without return from one state to another has been shown to take the same amount of time in distribution as the reversed passage.

In the simpler framework of birth and death processes, "time duality" is a consequence of the inherent reversibility of these processes since every path can be identified with its reversed path without changing its statistical properties. As there is only one possible passage way from any state i to another state j, any path from i to j has a unique counterpart, the reversed path, with the same distributional properties.

There are some generalizations made to processes with mirror symmetry and loop-free transition graphs, see e.g. [Pol01, Kij88]. In more complicated situations, however, reversibility is a property that seldom holds. Therefore, in this article, we depart from the simple linear structure of birth and death processes and investigate the properties of arbitrary (finite state) Markov chains to gain some criteria for time duality. We note that time duality, as we define it in the following, must not be confused with the duality notion known in the literature, see for example the above mentioned article by Pollett. We introduce it here merely in the sense of equality in distribution of certain absorption times. The main tool is here the calculus of phase type distributions that allows to derive simple conditions that involve submatrices of the original infinitesimal generator.

The article is organized as follows. In section 2 we formalize time duality, characterize the distribution of the first passage times without return and derive a sufficient criterion for time duality by comparing certain conditional moment generating functions. In section 3 we introduce *permuted balance* as a new generalization of reversibility and show that under some simple conditions time duality is implied. In section 4 we show how additional bottlenecks can simplify the criterion for time duality and treat the general case by relaxing the previously introduced conditions.

2. Time duality

Let $X := (X_t)_{t\geq 0}$ be a continuous time Markov chain on a finite state space E with cardinality $m+2$. We assume that its infinitesimal generator $Q := (q_{kl})_{k,l\in E}$ is irreducible. Therefore each state is recurrent and there exists a unique stationary distribution $\pi = (\pi_k)_{k\in E}$ solution of

$$\pi Q = 0, \qquad \pi \mathbf{1}^\top = 1\,, \tag{1}$$

where $\mathbf{1} := (1,1,1,\ldots,1)$ is a vector of length $m+2$.

2.1. Pure passage time

Fix two arbitrary states $i \neq j \in E$. The stopping time

$$\tau_{ij} := \inf\left\{t \geq 0 : X_t = j \mid X_0 \;=\; i\right\}$$

is the usual *first passage time* from i to j. We now define another meaningful random time,

$$\rho_{ij} := \sup\left\{t < \tau_{ij} : X_t = i\right\},$$

the time of the last departure from i before reaching j.

Definition 2.1. We call the difference

$$\tau^*_{ij} \;:=\; \tau_{ij} \;-\; \rho_{ij}$$

the *pure passage time* from i to j.

An illustration is provided in Figure 1.

Remark 2.2. When the transition rate q_{ij} is non-zero, the pure passage time τ^*_{ij} can take the value zero with positive probability since

$$\mathbb{P}(\tau^*_{ij} = 0) = \frac{q_{ij}}{\sum_{k\neq i} q_{ik}}.$$

In the case that $q_{ij}, q_{ji} > 0$, we therefore must assume $q_{ij} = q_{ji}$ as a necessary condition for time duality. Hereafter we assume for simplicity that

$$q_{ij} = q_{ji} = 0,$$

such that the distributions of τ^*_{ij} and τ^*_{ji} have no atom at zero.

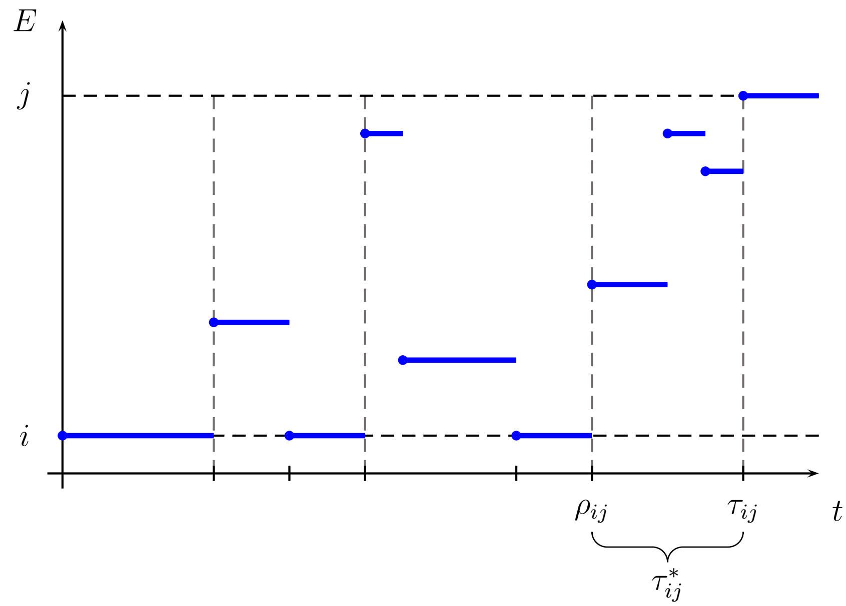

Figure 1: A path from i to j, which returns to i two times before reaching state j. The pure passage time is the time duration between the last departure from i and the arrival at state j.

Note that $q_{ij} = q_{ji} = 0$ is a feasible assumption that is met in the application to reaction pathways we originally had in mind. In this framework, the states between carefully chosen i, j of the Markov Chain represent intermediate, non-skippable steps of a complicated multi-step reaction. For an example of the complexity of these reactions, we refer to [LL07].

□

2.2. Pure passage time as phase type distribution

Hereinafter it will be useful to rearrange the states of E in the sequence $i, E \setminus \{i,j\}, j$ in such a way that the infinitesimal generator Q decomposes into the following block matrices:

$$Q := \begin{pmatrix} q_{ii} & * & * \\ R_i^\top & S & R_j^\top \\ * & * & q_{jj} \end{pmatrix}, \tag{2}$$

where S is a $m \times m$-matrix containing all transition rates between the m states in $E \setminus \{i,j\}$ while R_i and R_j are vectors of length m that contain the transition rates from $E \setminus \{i, j\}$ to i and j, respectively ($*$ replaces expressions that are not relevant for us).

To compute the distribution of the pure passage time of X from i to j, we first slightly modify X to transform the states i and j into absorbing states. Then, the modified Markov chain, say $\tilde{X}$, admits as infinitesimal generator $\tilde{Q}$ a matrix which decomposes into

$$\tilde{Q} := \begin{pmatrix} 0 & 0 & 0 \\ R_i^\top & S & R_j^\top \\ 0 & 0 & 0 \end{pmatrix}. \tag{3}$$

Now, the paths of $\tilde{X}$ which are of interest for us are those which reach j without return to i, starting from the direct neighbours of i. We then describe below the dynamics of the process $\tilde{X}$ conditioned to be absorbed in j in terms of its unconditioned version via a Doob h-transform. It is an adaptation of an idea that appeared for discrete time Markov chains in [KS76].

Proposition 2.3. Define the Markov chain $\bar{X}$ on $E \setminus \{i\}$ by

$$\mathbb{P}(\bar{X}_t \in \cdot | \bar{X}_0 = l) := \mathbb{P}(\tilde{X}_t \in \cdot | \tilde{X}_0 = l, \tilde{X}_\infty = j).$$

Then its transition probabilities are given by

$$\mathbb{P}(\bar{X}_t = k | \bar{X}_0 = l) = \frac{h_j(k)}{h_j(l)} \, \mathbb{P}(\tilde{X}_t = k | \tilde{X}_0 = l), \; k, l \in E \setminus \{i\}, t > 0, \tag{4}$$

where $h_j(k) = -e_k \; S^{-1} R_j^\top$ is the probability for $\tilde{X}$ to be absorbed in j starting from $k \in E \setminus \{i\}$.
Thus $\bar{X}$ admits as infinitesimal generator the following $(m+1) \times (m+1)$-matrix $\bar{Q}$ (the last row and column concern the state j):

$$\bar{Q} := \begin{pmatrix} H_j^{-1} S H_j & H_j^{-1} R_j^\top \\ 0 & 0 \end{pmatrix} \text{ where } H_j := -diag(S^{-1} R_j^\top). \tag{5}$$

For a vector V, $diag(V)$ denotes the square matrix whose diagonal entries are the entries of V and which vanishes elsewhere.

Proof: The Markov property of $\tilde{X}$ yields

$$\begin{aligned}
\mathbb{P}(\tilde{X}_t = k|\tilde{X}_0 = l, \tilde{X}_\infty = j) &= \mathbb{P}(\tilde{X}_t = k|\tilde{X}_0 = l, \exists s \geq 0 : \tilde{X}_{t+s} = j) \\
&= \frac{\mathbb{P}(\exists s \geq 0 : \tilde{X}_{t+s} = j|\tilde{X}_t = k)}{\mathbb{P}(\exists s \geq 0 : \tilde{X}_{t+s} = j|\tilde{X}_0 = l)} \mathbb{P}(\tilde{X}_t = k|\tilde{X}_0 = l) \\
&= \frac{\mathbb{P}(\exists s \geq 0 : \tilde{X}_s = j|\tilde{X}_0 = k)}{\mathbb{P}(\exists s' \geq 0 : \tilde{X}_{s'} = j|\tilde{X}_0 = l)} \mathbb{P}(\tilde{X}_t = k|\tilde{X}_0 = l).
\end{aligned}$$

Furthermore

$$\begin{aligned}
h_j(k) := \mathbb{P}(\exists s \geq 0 : \tilde{X}_s = j|\tilde{X}_0 = k) &= e_k \int_0^\infty \exp(St)dt\, R_j^\top \\
&= -e_k S^{-1} R_j^\top.
\end{aligned}$$

■

Now, the pure passage time for X from i to j can be interpreted as the absorption time for $\bar{X}$ starting from the direct neighbours of i and is therefore a phase type distribution in the framework introduced by Neuts in [Neu94].

At this point the phase-type calculus allows to compute the moment generating function of the absorption time of $\bar{X}$ in j. Since the proof is classical (see [Neu94, Ch. 2]), we refer to the given reference for details. Recall that τ_{ij}^* does not have any atom in 0, see Remark 2.1, and therefore, as phase-type distribution, is absolutely continuous with respect to Lebesgue-measure.

Proposition 2.4. Let X be a continuous time Markov chain on E with infinitesimal generator given by (2). The pure passage time τ_{ij}^* from a given state i to another state j admits as moment generating function

$$M(u) := \mathbb{E}(\exp(u\ \tau_{ij}^*)) = -\nu_i H_j^{-1}(uId + S)^{-1} R_j^\top,\ u \leq 0,$$

where the matrices S, R_j and H_j are defined in (2) resp. in (5). The probability distribution ν_i on $E \setminus \{i, j\}$ is given by

$$\nu_i(l) := \frac{1}{Z} q_{il} \text{ with } Z := \sum_{l \in E \setminus \{i,j\}} q_{il}.$$

Note that the l-th entry of the initial distribution ν_i is non-zero only if l can be reached in a single transition from i.

2.3. Time duality

We now define time duality between two states of E with respect to a given Markov chain as a binary relation, by comparing the two pure passage times between them.

Definition 2.5. Let $i, j \in E$. We say that i and j are in *time duality* with respect to X, if

$$\tau^*_{ij} \overset{(d)}{=} \tau^*_{ji}. \tag{6}$$

We denote this property with $i \overset{TD}{\leftrightarrow} j$.

We note that time duality between two disjoint sets of states can be defined in a completely analogous way. We treat here only the case of time duality between single states as the computations are the same for the more general case, except for very minor changes demanding to lump temporarily each set into a single (absorbing) state.

2.4. An algebraic condition for time duality

Due to Proposition 2.4, a reformulation of the equality (6) characterizing time duality is the following:

$$\forall u \leq 0, \quad \nu_i H_j^{-1}(uId + S)^{-1} R_j^\top = \nu_j H_i^{-1}(uId + S)^{-1} R_i^\top. \tag{7}$$

Let us now describe a particular situation.

Definition 2.6. We say that the state i has a *simple neighbourhood* if there is a unique state $n_i \in E \setminus \{i, j\}$ which is reachable from i in a single transition and the only state in $E \setminus \{i, j\}$ from which i can be reached.

The case in which both i and j have *simple neighbourhoods* is illustrated in Figure 2.

In this particular situation, two simplifications occur in the identity (7). First, the vectors ν_i and ν_j, introduced in Proposition 2.4, are in fact m-dimensional unit vectors, which we denote with e_{n_i} and e_{n_j}, with zero entries everywhere except at n_i and n_j, respectively. Secondly, the vectors R_i and R_j reduce to $R_i = q_{n_i i}\ e_{n_i}$ and $R_j = q_{n_j j}\ e_{n_j}$. Therefore the identity (7) becomes

$$\begin{aligned} \forall u \leq 0, \quad & \frac{e_{n_i}(uId + S)^{-1} e_{n_j}^\top}{e_{n_i} S^{-1} e_{n_j}^\top} = \frac{e_{n_j}(uId + S)^{-1} e_{n_i}^\top}{e_{n_j} S^{-1} e_{n_i}^\top} \\ \iff \forall u \leq 0, \quad & \frac{e_{n_i}(uId + S)^{-1} e_{n_j}^\top}{e_{n_j}(uId + S)^{-1} e_{n_i}^\top} = \frac{e_{n_i} S^{-1} e_{n_j}^\top}{e_{n_j} S^{-1} e_{n_i}^\top}. \end{aligned} \tag{8}$$

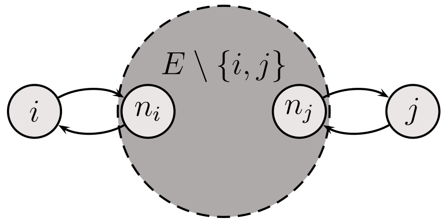

Figure 2: The states i and j have *simple neighbourhoods*: each passage between i and j is forced to pass through n_i as well as n_j.

Note that the exact value of the transition rates $q_{n_i i}$ and $q_{n_j j}$ does not appear in the different terms of (8). This property will be important also for the general case of non-simple neighbourhoods. Also note that the rhs of (8) does not need to be equal to one.

Remark 2.7. All the previous computations can be carried out for discrete time Markov chains, with only small changes. The non-conservative infinitesimal generator S is replaced by a sub-stochastic matrix S' and $(Id - S')^{-1}$ plays the same role as $(-S)^{-1}$ in the continuous case, see [DS67, DS65] for details. We only mention the distribution of the discrete pure passage time denoted by $\tau^*_{ij,d}$:

$$\forall k \geq 1,\ \mathbb{P}(\tau^*_{ij,d} = k) = \nu_i H_j^{-1} (S')^{k-1} R_j^\top \\ \text{with } H_j := diag((Id - S')^{-1} R_j^\top) \tag{9}$$

In this discrete time framework, time duality has to be interpreted as *path length equality*.

□

3. Permuted Balance

It is well known that the *detailed balance equations* are a local characterization of the reversibility of a Markov chain: X is reversible if there exists a distribution π such that

$$\forall k, l \in E, \quad \pi_k\ q_{kl} = \pi_l\ q_{lk}.$$

In that case, π is stationary. One can reformulate the above condition as the matrix equation

$$\Pi Q = Q^\top \Pi \tag{10}$$

where $\Pi := diag(\pi)$ is the diagonal matrix built on π.

As we mentioned in the introduction, under some assumptions, reversibility is sufficient to guarantee time duality. Indeed, we will show in Theorem 3.5 that even a weaker form of reversibility is enough to guarantee time duality. Let us introduce this new property in its local formulation.

Definition 3.1. Let X be an irreducible continuous time Markov chain on E and let σ be a permutation of the elements of E. The process X is in *permuted balance* for σ if there exists a probability distribution π which is invariant under σ, i.e. $\pi_{\sigma(k)} = \pi_k, k \in E$, and such that

$$\forall k, l \in E,\ \pi_k\ q_{kl} = \pi_{\sigma(l)}\ q_{\sigma(l)\sigma(k)}\ . \tag{11}$$

Obviously, if the permutation σ is the identity, one recovers the detailed balance equations.

If we associate a permutation matrix $P_\sigma = (\delta_{k\sigma(l)})_{k,l\in E}$ to the permutation σ, we can rewrite (11) as

$$P_\sigma \Pi Q = Q^\top P_\sigma \Pi. \tag{12}$$

In fact, the matrix P_σ acts by multiplication from the left as row permutation with respect to σ^{-1} and by multiplication from the right as column permutation with respect to σ.

To verify if permuted balance holds, is in general not straightforward and often computationally intense. But for graphs with a simple structure the verification is easy, as we now see.

Example 3.2. Let the Markov chain X be defined on $E := \{1, 2, 3, 4\}$ by its infinitesimal generator

$$Q := \begin{pmatrix} -\alpha & \alpha & 0 & 0 \\ 0 & -\beta & \beta & 0 \\ 0 & 0 & -\gamma & \gamma \\ \beta & 0 & 0 & -\beta \end{pmatrix}, \text{ with } \alpha, \beta, \gamma > 0.$$

The associated transition graph is given in Figure 3.
Permuted balance holds for the transposition $\sigma = (24)$. Indeed

$$\pi_1\ q_{12} = \pi_4\ q_{41} \text{ and } \pi_2\ q_{23} = \pi_3\ q_{34}$$

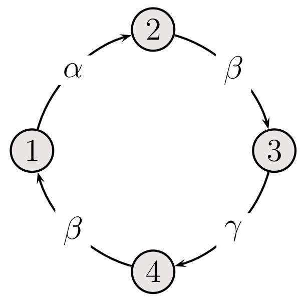

Figure 3: A Markov chain obeying permuted balance but not detailed balance.

where the (stationary) distribution π is given by

$$\pi = \frac{1}{2\alpha\gamma + (\alpha+\gamma)\beta}(\gamma\beta, \alpha\gamma, \alpha\beta, \alpha\gamma).$$

Remark that detailed balance can not hold since $q_{12} > 0$ but $q_{21} = 0$.

□

Let us analyse some meaningful properties satisfied by a Markov chain in permuted balance.

Proposition 3.3. Let X be an irreducible continuous time Markov chain on E in permuted balance for a permutation σ. Then

(i) the solution of (11) is its unique stationary distribution.

(ii) for all states $k \in E$

$$\sum_{l \in E\setminus\{k\}} \pi_k \; q_{kl} = \sum_{l \in E\setminus\{\sigma(k)\}} \pi_k \; q_{\sigma(k)l}$$

resp.

$$\sum_{l \in E\setminus\{k\}} \pi_l \; q_{lk} = \sum_{l \in E\setminus\{\sigma(k)\}} \pi_l \; q_{l\sigma(k)},$$

i.e. for each $k \in E$, k and $\sigma(k)$ are indistinguishable in terms of in and out going probability fluxes.

(iii) for every loop $(k_0, k_1, k_2, \ldots, k_n, k_0)$ $(n \geq 1)$ of the transition graph

$$q_{k_0k_1}q_{k_1k_2}\cdots q_{k_nk_0} = q_{\sigma(k_0)\sigma(k_n)}q_{\sigma(k_n)\sigma(k_{n-1})}\cdots q_{\sigma(k_1)\sigma(k_0)}, \tag{13}$$

i.e. the cumulated transition rate of each loop is equal to the cumulated transition rate of the image by σ of its reversed.

(iv) for every $T \geq 0$, $\quad (\sigma \circ X_{T-t})_{0\leq t\leq T} \overset{(d)}{=} (X_t)_{0\leq t\leq T}$,
the Markov chain has the same law as the image by σ of its reversed.

Proof:

(i) We have for arbitrary but fixed k:

$$\sum_{l\in E}\pi_l q_{lk} = \pi_k \sum_{l\in E} q_{\sigma(k)\sigma(l)} = 0$$

which implies the stationarity of π. The assumed irreducibility of X ensures the uniqueness of π.

(ii) Since π is stationary it satisfies the *global balance equations*

$$\sum_{l\in E\setminus\{k\}}\pi_k q_{kl} = \sum_{l\in E\setminus\{k\}}\pi_l q_{lk}. \tag{14}$$

We thus gain

$$\begin{aligned}\sum_{l\in E\setminus\{k\}}\pi_k q_{kl} &\overset{glob.\ bal.}{=} \sum_{l\in E\setminus\{k\}}\pi_l q_{lk} \overset{\pi\ stationary}{=} -\pi_k q_{kk} \\ &\overset{perm.\ bal.}{=} -\pi_{\sigma(k)}q_{\sigma(k)\sigma(k)} \overset{\pi\ stationary}{=} \sum_{l\in E\setminus\{\sigma(k)\}}\pi_{\sigma(k)}q_{\sigma(k)l} \\ &= \sum_{l\in E\setminus\{\sigma(k)\}}\pi_k q_{\sigma(k)l}.\end{aligned}$$

The second statement follows directly from these computations and the application of the global balance equation

$$\sum_{l\in E\setminus\{k\}}\pi_l q_{lk} \overset{gl.b.}{=} \sum_{l\in E\setminus\{k\}}\pi_k q_{kl} = \sum_{l\in E\setminus\{\sigma(k)\}}\pi_k q_{\sigma(k)l} \overset{gl.b.}{=} \sum_{l\in E\setminus\{\sigma(k)\}}\pi_l q_{l\sigma(k)}$$

(iii) Let π be in permuted balance. Then (11) implies that, for any two consecutive states in the loop $(k_0, k_1, \ldots, k_n, k_0)$,

$$\begin{aligned}
\pi_{k_0} q_{k_0 k_1} &= \pi_{k_1} q_{\sigma(k_1)\sigma(k_0)} \\
\pi_{k_1} q_{k_1 k_2} &= \pi_{k_2} q_{\sigma(k_2)\sigma(k_1)} \\
&\vdots \\
\pi_{k_n} q_{k_n k_0} &= \pi_{k_0} q_{\sigma(k_0)\sigma(k_n)}.
\end{aligned}$$

Multiplying all left hand sides and all right hand sides together and canceling the $\pi_i' s$ leads to (13).

(iv) It follows from successive iterations of the permuted balance equations that

$$\pi_{k_0} q_{k_1 k_2} \cdots q_{k_{n-1} k_n} = \pi_{k_n} q_{\sigma(k_n)\sigma(k_{n-1})} \cdots q_{\sigma(k_2)\sigma(k_1)}.$$

■

Remark 3.4. In [Kol36] Kolmogoroff shows how to characterize reversibility avoiding to use the explicit form of the stationary distribution. His now well known criterion (see for e.g. [Kel79, sec. 1.5, Th. 1.7] for a version for time continuous chains) states that reversibility holds if and only if for every loop $(i, i_1, i_2, \ldots, i_n, i)$ forward and backwards cumulated transition rates are identical, i.e.

$$q_{ii_1} q_{i_1 i_2} \cdots q_{i_n i} = q_{ii_n} q_{i_n i_{n-1}} \cdots q_{i_1 i}.$$

In Proposition 3.3 (iii) we have shown that permuted balance implies a modified loop criterion. However, the reverse assertion is no more true. We can only assure that the permuted loop criterion (13) together with a restrictive lumpability condition on the cycles of the permutation σ (for every $n \geq 1$ and $i, j \in E$, $q_{ij} = q_{i\sigma^n(j)}$ and $q_{ji} = q_{\sigma^n(j)i}$) implies permuted balance. In that case the lumped chain is even reversible.

□

We now prove that if permuted balance holds and two states i, j have simple neighbourhoods, $i \overset{TD}{\leftrightarrow} j$.

Theorem 3.5. Let i, j be two distinct states in E with simple neighbourhoods n_i resp. n_j. If the Markov chain X is in permuted balance for a permutation σ which leaves n_i and n_j invariant, then the states i and j are in time duality, i.e. $i \overset{TD}{\leftrightarrow} j$.

Proof: We use the matrix form (12) to characterize permuted balance. Then noting that P_σ and Π are always invertible, we get $S = (P_\sigma \Pi)^{-1} S^\top P_\sigma \Pi$ (after an obvious adaptation to the dimension of S). This leads to

$$\begin{aligned}
\frac{e_{n_i}(uId+S)^{-1}e_{n_j}^\top}{e_{n_j}(uId+S)^{-1}e_{n_i}^\top} &= \frac{e_{n_i}(uId+(P_\sigma\Pi)^{-1}S^\top(P_\sigma\Pi))^{-1}e_{n_j}^\top}{e_{n_j}(uId+S)^{-1}e_{n_i}^\top} \\
&= \frac{e_{n_i}(P_\sigma\Pi)^{-1}(uId+S^\top)^{-1}(P_\sigma\Pi)e_{n_j}^\top}{e_{n_j}(uId+S)^{-1}e_{n_i}^\top} \\
&= \frac{\pi_{n_j}}{\pi_{\sigma(n_i)}} \frac{e_{\sigma(n_i)}(uId+S^\top)^{-1}e_{\sigma^{-1}(n_j)}^\top}{e_{n_j}(uId+S)^{-1}e_{n_i}^\top} \\
&= \frac{\pi_{n_j}}{\pi_{n_i}} \frac{e_{n_i}(uId+S^\top)^{-1}e_{n_j}^\top}{e_{n_j}(uId+S)^{-1}e_{n_i}^\top} \overset{\text{numerator}}{\underset{\text{transposed}}{=}} \frac{\pi_{n_j}}{\pi_{n_i}}
\end{aligned}$$

which implies (8), as the last term is independent of u.

■

Example 3.6. Let X be the Markov chain defined on $E := \{0, 1, 2, 3, 4, 5\}$ by the infinitesimal generator

$$Q := \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & -\beta & \beta & 0 & 0 \\ 0 & 0 & 0 & -2 & 1 & 1 \\ 0 & \beta & 0 & 0 & -\beta & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 \end{pmatrix}.$$

The associated transition graph is drawn in Figure 4. It is an enlargement of Example 3 with $\alpha = \gamma = 1$. The stationary distribution is given by $\pi = \frac{1}{4\beta+2}(\beta, \beta, 1, \beta, 1, \beta)$. As in Example 3, permuted balance holds for the transposition $\sigma = (24)$. Therefore, by Theorem 3.5, the states 0 and 5 are in time duality.

A direct comparison of the pure passage times between $i = 0$ and $j = 5$ would have been more tedious. We should first identify

$$R_0^\top = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \ S = \begin{pmatrix} -2 & 1 & 0 & 0 \\ 0 & -\beta & \beta & 0 \\ 0 & 0 & -2 & 1 \\ \beta & 0 & 0 & -\beta \end{pmatrix}, \ R_5^\top = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix},$$

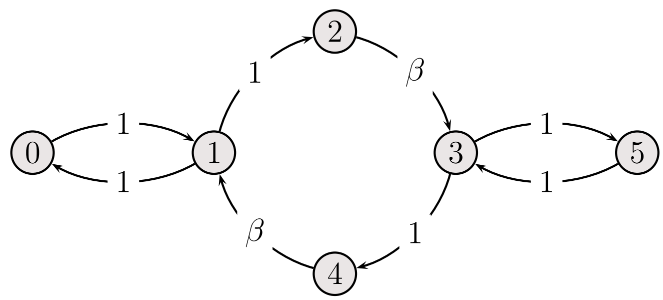

Figure 4: A Markov chain where 0 and 5 have simple neighbourhoods and are in time duality.

and compute the inverse matrix of $uId + S$. Then the left hand side of Equation (8) equals

$$\frac{(1,0,0,0)(uId+S)^{-1}(0,0,1,0)^\top}{(0,0,1,0)(uId+S)^{-1}(1,0,0,0)^\top} = \frac{\beta(u-\beta)}{\beta(u-\beta)} \equiv 1$$

for any $u \leq 0$, which indeed does not depend on u.

□

4. Bottleneck and non-simple neighbourhood

4.1. Bottlenecks and transitivity of the time duality relation

Time duality is a binary relation, which is here automatically symmetric and reflexive, but it is not immediate whether this relation is also transitive or not. In fact, there is no answer in a general framework. However, if the state space is decomposable into two disjoint subsets E_1, E_2, and, in between, one *bottleneck* state y satisfying that every passage from E_1 to E_2 goes through y, then we obtain a representation of the pure passage time from any $i \in E_1$ to any $j \in E_2$ as a sum of two independent phase-type distributed random variables. We give here the proof only for the case where i, j and y have simple neighbourhoods, as the more general case with non-simple boundaries yields the same result. The situation of a bottleneck with simple neighbourhoods is depicted in figure 5.

Note that the notion of simple neighbourhood for the bottleneck y means in fact that it has only two direct neighbours, n_{y1} in E_1 and n_{y2} in E_2.

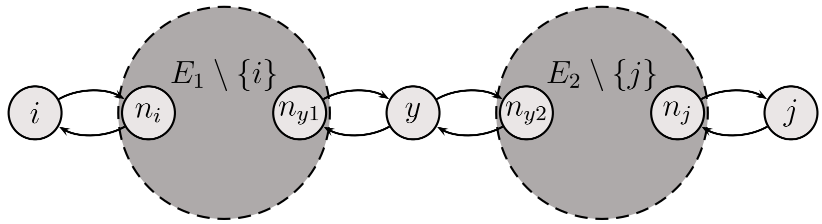

Figure 5: The structure of the graph forces any path from i to j through the state y and vice versa.

Theorem 4.1. Let $E = E_1 \sqcup \{y\} \sqcup E_2$ where y is a bottleneck and $i \in E_1$, $j \in E_2$ have simple neighbourhoods. Assume the transition graph has the form drawn in Figure 5. Then,

$$i \overset{TD}{\leftrightarrow} y \text{ and } y \overset{TD}{\leftrightarrow} j \quad \Longrightarrow \quad i \overset{TD}{\leftrightarrow} j.$$

Proof: We further decompose the matrix S introduced in (2). Assuming that the states are ordered in the sequence $y, E_1 \setminus \{i\}, E_2 \setminus \{j\}$ we obtain

$$S = \begin{pmatrix} q_{yy} & q_{yn_{y1}} e_{n_{y1}} & q_{yn_{y2}} e_{n_{y2}} \\ q_{n_{y1}y} e_{n_{y1}}^\top & S_1 & 0 \\ q_{n_{y2}y} e_{n_{y2}}^\top & 0 & S_2. \end{pmatrix} \tag{15}$$

As the states i and j have simple neighbourhoods, it is enough to check if (8) is satisfied. To compute the relevant entries of the inverse of S we use the Banachiewicz inversion formula for block matrices, see e.g. [Gan86],(86)-(89):

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}^{-1} = \begin{pmatrix} K^{-1} & -K^{-1} M_{12} M_{22}^{-1} \\ -M_{22}^{-1} M_{21} K^{-1} & M_{22}^{-1} + M_{22}^{-1} M_{21} K^{-1} M_{12} M_{22}^{-1} \end{pmatrix} \tag{16}$$

$$= \begin{pmatrix} M_{11}^{-1} + M_{11}^{-1} M_{12} L^{-1} M_{21} M_{11}^{-1} & -M_{11}^{-1} M_{12} L^{-1} \\ -L^{-1} M_{21} M_{11}^{-1} & L^{-1} \end{pmatrix} \tag{17}$$

$$\text{with} \quad L := M_{22} - M_{21} M_{11}^{-1} M_{12}, \qquad K := M_{11} - M_{12} M_{22}^{-1} M_{21}.$$

The matrices L and K, called *Schur complements*, see e.g. [Zha05], have a probabilistic interpretation, see [LR99, sec. 5.3]. To simplify the notations we write $A_u := uId + A$ for any square matrix A (if the matrix has an index we add the small u after a comma). We apply (16) for $M_{11} = q_{yy} + u$. The quantity K is in this case a real number, thus

$$(S_u)^{-1} = \begin{pmatrix} * & * \\ * & T^{-1} + \frac{1}{K} T^{-1} \begin{pmatrix} q_{n_{y1}y} e_{n_{y1}}^\top \\ q_{n_{y2}y} e_{n_{y2}}^\top \end{pmatrix} (q_{yn_{y1}} e_{n_{y1}}, q_{yn_{y2}} e_{n_{y2}}) T^{-1} \end{pmatrix}$$

where

$$T = \begin{pmatrix} S_{1,u} & 0 \\ 0 & S_{2,u} \end{pmatrix}.$$

The $*$ replace expressions that are not relevant for us.

We now compute the lhs of (8):

$$\begin{aligned} \frac{e_{n_i} S_u^{-1} e_{n_j}^\top}{e_{n_j} S_u^{-1} e_{n_i}^\top} &= \frac{q_{n_{y1}y} e_{n_i} S_{1,u}^{-1} e_{n_{y1}}^\top q_{yn_{y2}} e_{n_{y2}} S_{2,u}^{-1} e_{n_j}^\top}{q_{n_{y2}y} e_{n_j} S_{2,u}^{-1} e_{n_{y2}}^\top q_{yn_{y1}} e_{n_{y1}} S_{1,u}^{-1} e_{n_i}^\top} \\ &= \frac{q_{n_{y1}y} e_{n_i} S_{1,u}^{-1} e_{n_{y1}}^\top}{q_{yn_{y1}} e_{n_{y1}} S_{1,u}^{-1} e_{n_i}^\top} \cdot \frac{q_{yn_{y2}} e_{n_{y2}} S_{2,u}^{-1} e_{n_j}^\top}{q_{n_{y2}y} e_{n_j} S_{2,u}^{-1} e_{n_{y2}}^\top} \end{aligned}$$

and conclude that the moment generating function of the pure passage time τ_{ij}^* is indeed the product of two moment generating functions.

■

4.2. The case of non-simple neighbourhoods

Simple neighbourhoods simplify the comparison of paths connecting i and j, but this assumption is quite restrictive. One can circumvent the difficulties arising when the neighbourhoods are not simple by introducing new states to mimic the simple neighbourhood case as we will discuss now. Note that this extension does not necessarily leave permuted or detailed balance invariant, see Remark 4.3 for an explanation.

Define an enlargement of the state space E by $E' := \{i'\} \cup E \cup \{j'\}$ and construct on it the following modification and extension of Q:

$$Q' = \begin{pmatrix} -1 & e_i & 0 \\ e_i^\top & S' & e_j^\top \\ 0 & e_j & -1 \end{pmatrix} \text{ with } S' := \begin{pmatrix} q'_{ii} & R_{iS} & 0 \\ R_i^\top & S & R_j^\top \\ 0 & R_{jS} & q'_{jj} \end{pmatrix}. \tag{18}$$

The matrix S' is equal to Q except for a modification of the input vectors from i to $E \setminus \{i,j\}$ resp. from j to $E \setminus \{i,j\}$. They are now called R_{iS} and R_{jS} and are given by

$$R_{iS} := \nu_i H_j^{-1}, \quad R_{jS} := \nu_j H_i^{-1}$$

with the same notations as in Proposition 2.4. (The (i,i) and (j,j) entries of Q are also modified in order to lead to a proper infinitesimal generator Q' on E'. They become q'_{ii} and q'_{jj}.) The associated extended transition graph is represented in Figure 6.

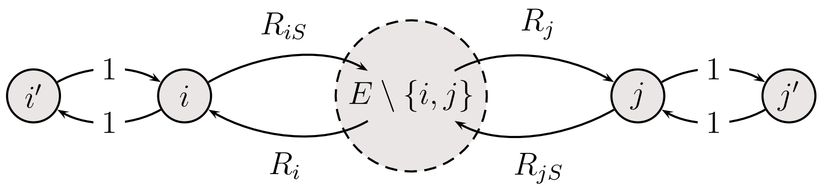

Figure 6: Non-simple neighbourhoods of i and j in E reformulated in the flavour of simple ones by enlargement of the state space.

Theorem 4.2. Suppose that X is a continuous time Markov chain on E with irreducible infinitesimal generator and consider i and j, two states of E with non-simple neighbourhoods. After enlarging the state space by i' and j' as indicated in Figure 6, the following holds:

$$i' \overset{TD}{\leftrightarrow} j' \quad \Longrightarrow \quad i \overset{TD}{\leftrightarrow} j.$$

Proof: The states i' and j' have simple neighbourhoods. Thus, since time duality holds between them, by (8)

$$\forall u \leq 0, \quad \frac{e_i(uId + S')^{-1}e_j^\top}{e_j(uId + S')^{-1}e_i^\top} = \frac{e_i(S')^{-1}e_j^\top}{e_j(S')^{-1}e_i^\top}. \tag{19}$$

Again, we use the notation $A_u = uId + A$ for a square matrix A. We now compute the upper right (i,j)-th entry of $(S'_u)^{-1}$ using (16) and then by (17) we obtain:

$$
\begin{aligned}
-\frac{1}{K}(R_{iS}, q_{ij}) \begin{pmatrix} S_u & R_j^\top \\ R_{jS} & s \end{pmatrix}^{-1} \\
&= -\frac{1}{LK}(R_{iS}, 0) \begin{pmatrix} S_u^{-1} + S_u^{-1} R_j^\top R_{jS} S_u^{-1} & -S_u^{-1} R_j^\top \\ R_{jS} S_u^{-1} & 1 \end{pmatrix} \\
&= \frac{1}{LK}(*, R_{iS} S_u^{-1} R_j^\top)
\end{aligned}
$$

with the scalar coefficients

$$
K = q'_{ii} + u - (R_{iS}, q_{ij}) \begin{pmatrix} S_u & R_j^\top \\ R_{jS} & u \end{pmatrix}^{-1} \begin{pmatrix} R_i^\top \\ q_{ji} \end{pmatrix} \text{ and } L = u - R_{jS} S_u^{-1} R_j^\top .
$$

Now the (i, j)-th entry of $(S'_u)^{-1}$ is $\frac{1}{LK} R_{iS} S_u^{-1} R_j^\top$. In a similar way, the (j, i)-th entry is equal to $\frac{1}{LK} R_{jS} S_u^{-1} R_i^\top$.

Thus the identity (19) now reads (the scalar numbers L and K cancel out):

$$
\frac{R_{iS}(uId + S)^{-1} R_j^\top}{R_{jS}(uId + S)^{-1} R_i^\top} = \frac{R_{iS} S^{-1} R_j^\top}{R_{jS} S^{-1} R_i^\top} = \frac{\nu_i H_j^{-1} H_j \mathbf{1}^\top}{\nu_j H_i^{-1} H_i \mathbf{1}^\top} = 1, \tag{20}
$$

which implies $R_{iS}(uId + S)^{-1} R_j^\top = R_{jS}(uId + S)^{-1} R_i^\top$. This is equivalent to (7). Therefore time duality holds between i and j.

■

Remark 4.3. One could think that the extension of the state space by i' and j' has no influence on an existing permuted balance with respect to a permutation since, by construction of the extension, there are no additional loops, except the trivial loops (i, i', i) and (j, j', j), that contain i' or j'. Nevertheless the necessary introduction of the new vectors R_{iS} and R_{jS} destroys this false intuition. Indeed, it is possible to construct an example of reversible chain without time duality as in Figure 7. In particular, the constructed extension is not reversible anymore, and even not permuted balanced.

□

We give an example to illustrate Theorem 4.2.

Example 4.4. Let $E := \{1, 2, 3, 4\}$ and X the Markov chain on E with

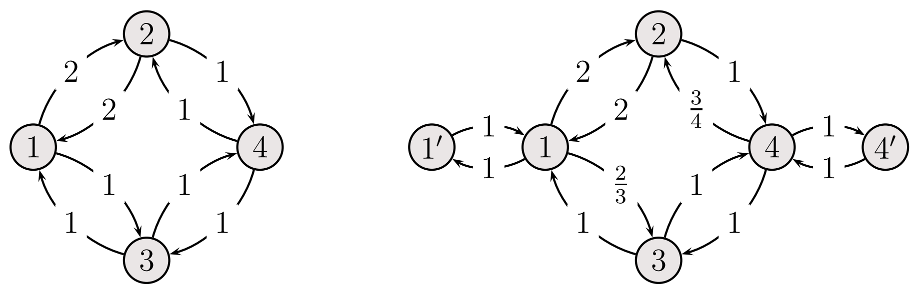

Figure 7: To check time duality between 1 and 4 in the left model, we extend the model according to Theorem 4.2. Although the initial model is reversible, the modification (right) is not.

infinitesimal generator

$$Q := \begin{pmatrix} -3 & 2 & 1 & 0 \\ 1 & -2 & 0 & 1 \\ 1 & 0 & -2 & 1 \\ 0 & 2 & 1 & -3 \end{pmatrix}$$

Its transition graph is given in the top of Figure 8. It contains a unique non trivial loop, with length 4, equal to (1,2,4,3,1). The cumulated transition rate of this loop is equal to $q_{12}q_{24}q_{43}q_{31} = 2$. The cumulated transition rate of its reversed $q_{13}q_{34}q_{42}q_{21}$ takes also the value 2. Therefore X satisfies Kolmogoroff's criterion and is reversible. However, we may not use Corollary 3.5 to conclude time duality between 1 and 4, since the neighbourhoods of 1 and 4 are *not* simple.

We therefore need to extend the state space E. Define $E' := \{1'\} \cup E \cup \{4'\}$ and construct on it an extended modified Markov chain as described above, see Figure 6. Here, we compute

$$R_{1S} = \nu_1 H_4^{-1} = \frac{1}{3}(2,1)\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} = \left(\frac{4}{3}, \frac{2}{3}\right) = R_{4S}$$

and thus

$$S' = \begin{pmatrix} * & 4/3 & 2/3 & 0 \\ 1 & -2 & 0 & 1 \\ 1 & 0 & -2 & 1 \\ 0 & 4/3 & 2/3 & * \end{pmatrix}.$$

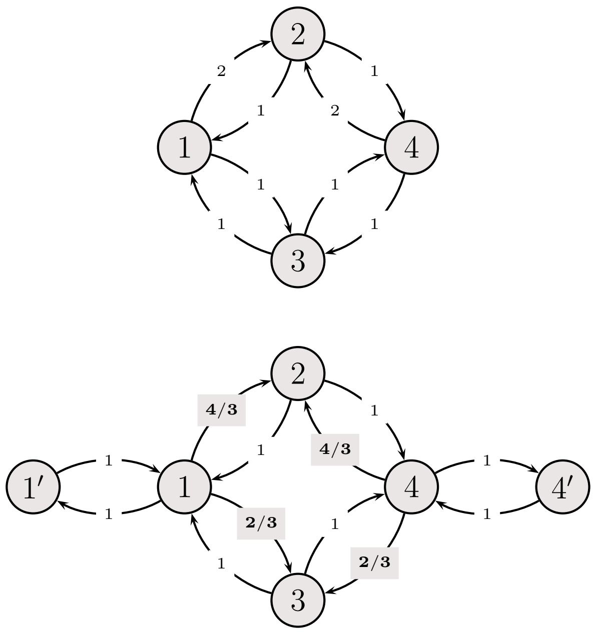

Figure 8: The transition graph of the example (top) and its extended version (bottom).

We get for the new Markov chain the transition graph drawn at the bottom of Figure 8. It is reversible too, but the cumulated transition rate of the loop $(1, 2, 4, 3, 1)$ is now equal to $8/9$. By Corollary 3.5, we conclude that time duality holds between $1'$ and $4'$. Finally, Theorem 4.2 implies time duality between the states 1 and 4.

□

5. Discussion

In this article we introduce the notion of time duality, which can be useful in several frameworks, e.g. to analyse dynamics of molecular motors, see [KlV13],[LW07],[VLL08]. We present an algebraic criterion that allows to check time duality between two arbitrary states of a finite state Markov chain. It is well adapted to be treated by computers as it contains only matrix multiplication and inversion, which can be done efficiently with any modern computer algebra system, even if the state space is large. We show in Theorem 3.5 that permuted and thus detailed balance implies time duality, if the neighbourhoods of the states are simple. For the more complex case of non-simple boundary we provide a simple construction to “reduce” the general case to the simple boundary case.

However, time duality is not completely exploited by permuted balance, as the application in [VLL08] shows. The model introduced there is neither in detailed nor in permuted balance, but still shows time duality. Following Proposition 3.3, iv, we can understand time duality under permuted balance and simple neighbourhood on the path level, since we assign to every path its unique time reversed and possibly permuted counterpart. But in the general case this no longer holds true. To fully clarify this issue is beyond the scope of this paper and is left for future research.

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