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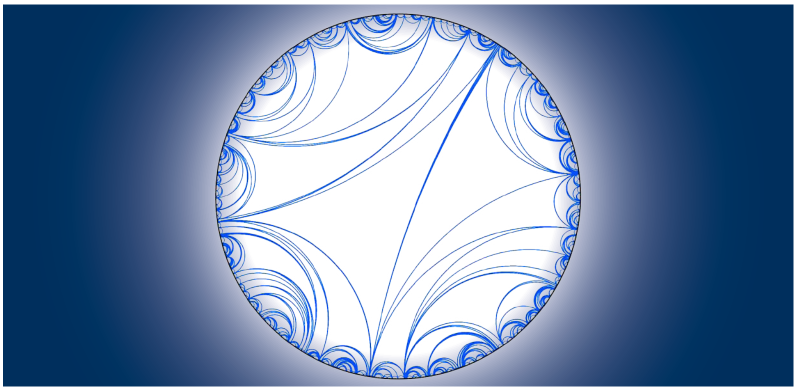

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ON TIME DUALITY FOR QUASI-BIRTH-AND-DEATH PROCESSES

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Abstract

We say that (weak/strong) *Time Duality* holds for continuous time quasi-birth-and-death-processes if, starting from a fixed level, the first hitting time of the next upper level and the first hitting time of the next lower level have the same distribution. We present here a criterion for Time Duality in the case that transitions from one level to another have to pass through a given single state, so called *bottleneck property.* We also prove that a weaker form of reversibility called *balanced under permutation* is sufficient for Time Duality to hold. We then discuss the general case.
Keywords: quasi-birth-and-death process, continuous time Markov Chain; hitting times; Time Duality; absorbing boundary

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Secondary 60J28; 60K40

1. Introduction

Hitting times play an important role in many applications of continuous time Markov Chains (CTMC). One example is provided by models that describe molecular motor proteins e.g. kinesin. In living eukaryotic cells, kinesin "walks" over long, relatively rigid strings called microtubules thereby transporting a cargo from one side of the cell

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to another. Due to the periodic molecular structure of the microtubules, the steps of the kinesin have all the same length equal to 8 nanometers. Under normal conditions present in living cells, this motor performs a random walk in one dimension with a drift on the microtubule. Experimental studies have led to rather detailed and successful models of the chemical processes in kinesin which control the movement of the motor. These chemical processes are characterized by a network of internal chemical states, see e.g. [8].

The analysis of kinesin and similar motor proteins is made by means of continuous time Markov Chains, as the transitions between chemical states are usually interpreted as transitions of a Markov Chain. The Markov Chain is linear periodic in the sense that copies of the same finite state continuous time Markov Chain are connected in a linear fashion. Such models are known in the literature as Quasi-Birth-and-Death Processes (QBD, see e.g. [6]) or as $M \setminus PH \setminus 1$-Queues (see e.g. [10]).

One relevant topic in the analysis of such models is the comparison between the first hitting time of the $(n+1)$-th level and the first hitting time of the $(n-1)$-th level, starting from level n, see fig. 1. If they are equal in law we say that *Time Duality* holds. Lindén and Wallin remarked in [7] through statistical analysis of experiments that, under the - very restrictive - reversibility assumption of the continuous time QBD , Time Duality holds. The first mathematical rigorous proof can be found in [5], and also in the recent paper [12]. However new models of motor proteins like the one introduced in [11] show that the property of Time Duality appears also for continuous time QBD's that are not reversible. The aim of this paper is to understand under which kind of weak assumptions Time Duality is satisfied by continuous time QBD's.

We first treat in Section 3 the so called *bottleneck case*, assuming that neighboring levels communicate only via given single states. For such models we prove in Section 4 that a weak form of reversibility, namely *balance under permutation*, is sufficient for Time Duality to hold. We then show in Section 5 that the methods used in the bottleneck case can be generalized to the case where neighboring levels communicate via several possible states. In this general framework the initial distributions play an important role, which leads to distinguish between *weak* Time Duality and *strong* Time Duality, new notions introduced in Definitions 2 and 3.

2. The framework

In this section we first define the class of Quasi-Birth-and-Death Processes we consider. We then introduce the concept of Time Duality and useful notations.

Let us define for $m \in \mathbb{N}^*$ a set of phases

$$M := \{1, \ldots, m\}$$

and the state space $\bar{E} := \mathbb{Z} \times M$. For any fixed n, the subset

$$l(n) := \{(n, i), i \in M\} \subset \bar{E}$$

is called n-th level and is supposed to form a single communication class.

A continuous time QBD is a continuous time Markov Chain $\bar{X} := (\bar{X}_t)_{t \geq 0}$ with state space $\bar{E}$ such that the only possible transitions are between phases of neighboring levels or of the same level. Thus the infinitesimal generator of a continuous time QBD has the following special form

$$\bar{Q} := (\bar{q}_{ij})_{i,j \in \bar{E}} := \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ \ldots & \mathbf{A_2} & \mathbf{A_1} & \mathbf{A_0} & 0 & 0 & \ldots \\ \ldots & 0 & \mathbf{A_2} & \mathbf{A_1} & \mathbf{A_0} & 0 & \ldots \\ \ldots & 0 & 0 & \mathbf{A_2} & \mathbf{A_1} & \mathbf{A_0} & \ldots \\ & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

where $\mathbf{A_0}, \mathbf{A_1}, \mathbf{A_2}$ are $m \times m$-matrices, $\mathbf{A_0}, \mathbf{A_2}$ have non negative entries and $\mathbf{A_1}$ is an irreducible non conservative infinitesimal generator (these notations are consistent with those in [6] and [10]). To exclude trivial cases we assume that $\mathbf{A_2}$ and $\mathbf{A_0}$ contain at least one positive entry, such that communication between levels is ensured. For convenience we do not define any boundary.

Since $\bar{Q}$ is an infinitesimal generator, the following equality must hold

$$(\mathbf{A_0} + \mathbf{A_1} + \mathbf{A_2})\mathbf{1}^\top = \mathbf{0}.$$

Remark also that

$$\mathbf{A} := \mathbf{A_1} + \operatorname{diag}((\mathbf{A_0} + \mathbf{A_2})\mathbf{1}^\top) \tag{1}$$

is an irreducible infinitesimal generator on M, where, for a vector ν, $\operatorname{diag}(\nu)$ denotes the matrix whose diagonal entries are equal to the entries of ν and all other entries vanish.

A level n can be left to the next higher or lower level only through a specific set of states. We define the set of states leading to $l(n-1)$ by

$$\mathcal{N}^-(n) := \{n\} \times \left\{i \in M : q_{(n,i),(n-1,j)} > 0, j \in M\right\}$$

and the set of states leading to $l(n+1)$ by

$$\mathcal{N}^+(n) := \{n\} \times \left\{i \in M : q_{(n,i),(n+1,j)} > 0, j \in M\right\}.$$

Furthermore let

$$\mathcal{N}^{int}(n) := \{n\} \times M \setminus (\mathcal{N}^-(n) \cup \mathcal{N}^+(n))$$

is a non-empty set of states that are not connected to any other level but n, see fig. 1.

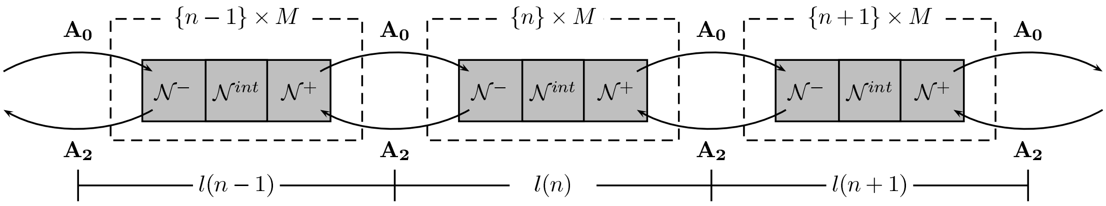

FIGURE 1: Schematic display of a continuous time QBD.

We define the first hitting time of $l(n+1)$ from $l(n)$ by

$$\bar{T}_+^n := \inf\left\{t \geq 0 : \forall s < t \ \bar{X}_s \in l(n) \text{ and } \bar{X}_t \in \mathcal{N}^-(n+1)\right\}$$

and the first hitting time of $l(n-1)$ from $l(n)$ by

$$\bar{T}_-^n := \inf\left\{t \geq 0 : \forall s < t \ \bar{X}_s \in l(n) \text{ and } \bar{X}_t \in \mathcal{N}^+(n-1), \right\}.$$

The first exit time of level n is clearly the minimum of $\bar{T}_-^n$ and $\bar{T}_+^n$. Its law does not depend on the chosen level n. To compute the distributions of $\bar{T}_-^n$ and $\bar{T}_+^n$ we consider a simpler process X, called *reduced model*, which is the restriction of the original continuous time QBD to only one arbitrarily chosen level in the following sense: $X := (X_t)_{t\geq 0}$ is a CTMC on the state space

$$E := \{a_-\} \cup M \cup \{a_+\}$$

defined by its infinitesimal generator

$$Q := \begin{pmatrix} 0 & 0 & 0 \\ \mathbf{A_2 1}^\top & \mathbf{A_1} & \mathbf{A_0 1}^\top \\ 0 & 0 & 0 \end{pmatrix}. \tag{2}$$

Here the states a_- and a_+ represent $\mathcal{N}^-(n+1)$ and $\mathcal{N}^+(n-1)$ and are thus absorbing and therefore all states in M are transient, see figure 2.

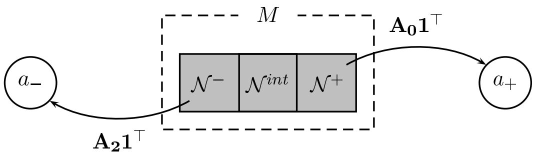

FIGURE 2: The reduced model.

The main interest of the reduced model is that its absorption time in a_+ (resp. . a_-) corresponds to the first hitting time of $l(n+1)$ (resp. $l(n-1)$) from $l(n)$ of the original continuous time QBD: Define

$$T_+ := \inf\{t \geq 0 : X_t = a_+\}, \quad T_- := \inf\{t \geq 0 : X_t = a_-\},$$

then

$$\bar{T}_+^n \overset{(d)}{=} T_+ \text{ and } \bar{T}_-^n \overset{(d)}{=} T_-.$$

Note that the absorption times T_+ and T_- can take the value $+\infty$.

Models often fulfill the special property that transitions between levels are done only through a single state (see [11] for examples). We call this *bottleneck property* and define it precisely as follows.

Definition 1. A continuous time QBD satisfies the *bottleneck property* if there exists two boundary states $b_-, b_+ \in M$ such that at each level n, $\mathcal{N}^-(n) = \{n\} \times \{b_-\}$ and $\mathcal{N}^+(n) = \{n\} \times \{b_+\}$.

Figure 3 illustrates what bottleneck means for the reduced model, where λ_+, λ_- are defined by

$$\mathbf{A_0 1}^\top = \lambda_+ e_{b_+}^\top, \qquad \mathbf{A_2 1}^\top = \lambda_- e_{b_-}^\top, \tag{3}$$

with e_{b_-} (resp. e_{b_+}) the m-dimensional unit vector with a unique non zero entry at the b_--th (resp. b_+-th) entry. Therefore the infinitesimal generator Q of the reduced

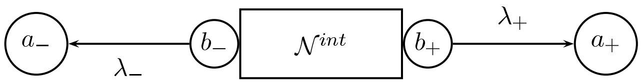

FIGURE 3: The reduced model derived from a continuous time QBD with bottleneck property.

model is given, in bottleneck case, by

$$Q = \begin{pmatrix} 0 & 0 & 0 \\ \lambda_- e_{b_-}^\top & \mathbf{A_1} & \lambda_+ e_{b_+}^\top \\ 0 & 0 & 0 \end{pmatrix}. \tag{4}$$

We consider now again the general reduced model generated by the matrix Q given in (2). To compute the distributions of T_+ and T_- we will condition the reduced model to be absorbed in either a_+ or a_-, which can be done through an *h-transform.* This standard technique is developed e.g. in [4] in the context of discrete Markov Chains. We present here the continuous time analogon. We treat only the case of absorption in a_+ since the method is identical for the absorption in a_-. To shorten notations let us write $\mathbb{P}_i(X_t = .)$ for $\mathbb{P}(X_t = .|X_0 = i)$.

Lemma 1. *The transition function of $(X_t)_{t\geq 0}$ conditioned to absorption in a_+ is given by*

$$\mathbb{P}_i(X_t = j|T_+ < T_-) = \frac{h_+(j)}{h_+(i)}\mathbb{P}_i(X_t = j),\ i, j \in M \tag{5}$$

where

$$h_+(i) := \mathbb{P}_i(T_+ < T_-) = -e_i \mathbf{A_1}^{-1}\mathbf{A_0}\mathbf{1}^\top. \tag{6}$$

Proof. Note that $\{T_+ < T_-\} = \{T_+ < +\infty\}$. We use the definition of conditional probability and the Markov property of X to derive

$$
\begin{aligned}
\mathbb{P}_i(X_t = j | T_+ < T_-) &= \mathbb{P}_i(X_t = j | \exists s \geq 0 : X_{t+s} = a_+) \\
&= \frac{\mathbb{P}_i(\exists s \geq 0 : X_{t+s} = a_+ | X_t = j)\mathbb{P}_i(X_t = j)}{\mathbb{P}_i(\exists s \geq 0 : X_{t+s} = a_+)} \\
&= \frac{\mathbb{P}_j(\exists s \geq 0 : X_s = a_+)}{\mathbb{P}_i(\exists s' \geq 0 : X_{s'} = a_+)}\mathbb{P}_i(X_t = j) \\
&= \frac{h_+(j)}{h_+(i)}\mathbb{P}_i(X_t = j).
\end{aligned}
$$

We now compute $h_+(i)$:

$$
\begin{aligned}
h_+(i) = \mathbb{P}_i(\exists s \geq 0 : X_s = a_+) &= e_i \int_0^\infty \exp(\mathbf{A_1} s) ds \, \mathbf{A_0} \mathbf{1}^\top \\
&= e_i(-\mathbf{A_1})^{-1}\mathbf{A_0}\mathbf{1}^\top, \quad i \in M.
\end{aligned}
$$

Clearly $h_+(a_+) = 1$ and $h_+(a_-) = 0$. The invertibility of $\mathbf{A_1}$ is justified in Lemma 2.2.1 of [10].

■

From Lemma 1 we directly derive the infinitesimal generator $Q_{|a_+}$ of the process conditioned on its absorption in a_+ knowing the infinitesimal generator Q of the unconditioned process given in (2). Fix

$$
\mathbf{H}_+ := \operatorname{diag}(h_+(1), h_+(2), \ldots, h_+(m)) \tag{7}
$$

then

$$
Q_{|a_+} = \begin{pmatrix} 0 & 0 & 0 \\ \mathbf{H}_+^{-1}\mathbf{A_2}\mathbf{1}^\top & \mathbf{H}_+^{-1}\mathbf{A_1}\mathbf{H}_+ & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{8}
$$

The law of absorption time for CTMC's with a single absorbing state is known as phase type distribution, see [10]. As the process X conditioned on absorption in a_+ is a CTMC with a single absorbing state, we get

Proposition 1. *The absorption time $T_-\mathbb{1}_{T_-<\infty}$ (resp. $T_+\mathbb{1}_{T_+<\infty}$) of the CTMC $(X_t)_{t\geq 0}$ with infinitesimal generator (2) and initial distribution μ concentrated on M is phase* *type distributed with representation* $PH(\mu, \mathbf{H}_{\text{-}}^{-1}\mathbf{A_1}\mathbf{H}_{\text{-}})$ *(resp.* $PH(\mu, \mathbf{H}_{+}^{-1}\mathbf{A_1}\mathbf{H}_{+})$*). Their Laplace transforms satisfy*

$$M_{-}^{\mu}(u) := \mathbb{E}(\exp(-uT_{-}\mathbb{1}_{T_{-}<\infty})) = -\mu\mathbf{H}_{\text{-}}^{-1}(\mathbf{A_1} - uId)^{-1}\mathbf{A_2}\mathbf{1}^{\top},\ u \geq 0,$$
$$M_{+}^{\mu}(u) := \mathbb{E}(\exp(-uT_{+}\mathbb{1}_{T_{+}<\infty})) = -\mu\mathbf{H}_{+}^{-1}(\mathbf{A_1} - uId)^{-1}\mathbf{A_0}\mathbf{1}^{\top},\ u \geq 0.$$

Proof. The result is a direct consequence of Lemma 1 and [10] (2.2.6).

■

Our aim is to study the conditions under which the equality in law of the absorption times T_{-} and T_{+} holds. These laws have a density with respect to Lebesgue Measure, but the computation of these densities contains a matrix exponential which is very difficult to treat, see e.g. [9] for an overview of the possible computation methods. So, we will compare the absorption times using their Laplace transform computed in Proposition 1, as the expressions appearing there only contain matrix inverses which are much more treatable than matrix exponentials.

Definition 2. Let $X = (X_t)_{t\geq 0}$ be the CTMC with infinitesimal generator (2) and let $\mu_{\text{-}}$ (resp. μ_{+}) be a probability distribution concentrated on $\mathcal{N}^{-}$ (resp. on $\mathcal{N}^{+}$). X is called $(\mu_{\text{-}}, \mu_{+})$-*time dual* or *weak time dual* if the law of $T_{-}\mathbb{1}_{T_{-}<\infty}$, when the initial distribution of X is $\mu_{\text{-}}$, is equal to the law of $T_{+}\mathbb{1}_{T_{+}<\infty}$, when the initial distribution of X is μ_{+}.

Therefore, X is $(\mu_{\text{-}}, \mu_{+})$-time dual if and only if $M_{-}^{\mu_{\text{-}}} \equiv M_{+}^{\mu_{+}}$.

Definition 3. If the CTMC $(X_t)_{t\geq 0}$ is weak time dual for every choice of probability distributions $(\mu_{\text{-}}, \mu_{+})$, we say that *strong Time Duality* holds.

3. A criterion for Time Duality in bottleneck case

We first investigate the simpler case with bottleneck, where each absorbing state can be reached only through a unique boundary state b_{-} or b_{+}, see figure 3. In this case, weak and strong Time Duality are clearly equivalent. Furthermore, the method presented in this section will become useful in Section 5, where we approach the more general case without bottleneck.

By Proposition 1 and using equations (3), Time Duality holds if and only if

$$\frac{e_{b_-}(\mathbf{A_1} - uId)^{-1} e_{b_+}^\top}{e_{b_-}(-\mathbf{A_1})^{-1} e_{b_+}^\top} = \frac{e_{b_+}(\mathbf{A_1} - uId)^{-1} e_{b_-}^\top}{e_{b_+}(-\mathbf{A_1})^{-1} e_{b_-}^\top}, \quad u \geq 0. \tag{9}$$

We partition $\mathbf{A_1}$ into a block matrix

$$\mathbf{A_1} = \begin{pmatrix} \mathfrak{b}_- & R_{b_-S} & \lambda_{b_-b_+} \\ R_{Sb_-}^\top & S & R_{Sb_+}^\top \\ \lambda_{b_+b_-} & R_{b_+S} & \mathfrak{b}_+ \end{pmatrix} \tag{10}$$

with $\mathfrak{b}_- := -(R_{b_-S}\mathbf{1}^\top + \lambda_{b_-b_+} + \lambda_+)$, $\mathfrak{b}_+ := -(R_{b_+S}\mathbf{1}^\top + \lambda_{b_+b_-} + \lambda_-)$ and $\lambda_{b_-b_+}$, $\lambda_{b_+b_-}$ the transition rates between b_- and b_+. This yields the following analytic characterization of Time Duality.

Theorem 1. *Let $(X_t)_{t\geq 0}$ be a CTMC on the state space $E := \{a_-, b_-\} \cup \mathcal{N}^{int} \cup \{b_+, a_+\}$ with infinitesimal generator (4). Then Time Duality holds if and only if*

$$\exists c \in \mathbb{R}^+ \forall u \geq 0 : \ \frac{R_{b_-b_+}(u) + \lambda_{b_-b_+}}{R_{b_+b_-}(u) + \lambda_{b_+b_-}} = c \tag{11}$$

where $R_{kl}(u) := -R_{kS}(S - uId)^{-1} R_{Sl}^\top$ and the different matrices are defined by (10). The constant c is then equal to $\frac{R_{b_-b_+}(0)+\lambda_{b_-b_+}}{R_{b_+b_-}(0)+\lambda_{b_+b_-}}$.

Proof. We already know that Time Duality is equivalent to (9). We proceed by unveiling the structure of $(\mathbf{A_1} - uId)^{-1}$ in terms of block matrices using the block partition introduced in (10). Define the following submatrix of $\mathbf{A_1} - uId$:

$$\bar{S}_u := \begin{pmatrix} S - uId & R_{Sb_+}^\top \\ R_{b_+S} & \mathfrak{b}_+ - u \end{pmatrix}.$$

The inverse of $\bar{S}_u$ can be derived according to [2], (86)-(89) via the identities

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

if M_{11} is invertible, resp.

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}^{-1} = \begin{pmatrix} K^{-1} & -K^{-1} M_{12} M_{22}^{-1} \\ -M_{22}^{-1} M_{21} K^{-1} & M_{22}^{-1} + M_{22}^{-1} M_{21} K^{-1} M_{12} M_{22}^{-1} \end{pmatrix} \tag{13}$$

if M_{22} is invertible where

$$H := M_{22} - M_{21}M_{11}^{-1}M_{12}, \qquad K := M_{11} - M_{12}M_{22}^{-1}M_{21}.$$

Therefore due to (12)

$$\begin{aligned}
&\bar{S}_u^{-1} \\
&= H^{-1}\begin{pmatrix} H(S-uId)^{-1} + (S-uId)^{-1}R_{Sb_+}^{\top}R_{b_+S}(S-uId)^{-1} & -(S-uId)^{-1}R_{Sb_+}^{\top} \\ -R_{b_+S}(S-uId)^{-1} & 1 \end{pmatrix}
\end{aligned}$$

with

$$H = \mathfrak{b}_+ + u - R_{b_+S}(S-uId)^{-1}R_{Sb_+}^{\top}. \tag{14}$$

We now obtain from (13):

$$(\mathbf{A_1} - uId)^{-1} = K^{-1}\begin{pmatrix} 1 & -(R_{b_-S}, \lambda_{b_-b_+})\bar{S}_u^{-1} \\ -\bar{S}_u^{-1}\begin{pmatrix} R_{Sb_-}^{\top} \\ \lambda_{b_+b_-} \end{pmatrix} & * \end{pmatrix},$$

where

$$K = \mathfrak{b}_- - u - (R_{b_-S}, \lambda_{b_-b_+})\bar{S}_u^{-1}\begin{pmatrix} R_{Sb_-}^{\top} \\ \lambda_{b_+b_-} \end{pmatrix}.$$

We do not compute the explicit expression for the submatrix $*$ as it is not needed for the completion of the proof. We conclude that

$$e_{b_-}(\mathbf{A_1} - uId)^{-1}e_{b_+}^{\top} = K^{-1}H^{-1}(R_{b_-S}(S-uId)^{-1}R_{Sb_+}^{\top} - \lambda_{b_-b_+}), \tag{15}$$

$$e_{b_+}(\mathbf{A_1} - uId)^{-1}e_{b_-}^{\top} = K^{-1}H^{-1}(R_{b_+S}(S-uId)^{-1}R_{Sb_-}^{\top} - \lambda_{b_+b_-}). \tag{16}$$

K and H are real numbers and cancel out if these expressions are inserted into (9).

■

Remark that K and H are the only quantities in which λ_- or λ_+ do appear. This means that the values of the rates into the absorbing states do not influence Time Duality under bottleneck property.

The identity (11) has a probabilistic interpretation when $\lambda_{b_-b_+} = \lambda_{b_+b_-} = 0$. Suppose we perturb the model by adding another absorbing state c which is reachable from every state in M with rate u, see fig. 4. The matrix $\mathbf{A_1} - uId$ is for every $u \geq 0$ an invertible non conservative infinitesimal generator; in fact only the diagonal entries of $\mathbf{A_1}$ are perturbed. The entry i, j of the matrix $-(\mathbf{A_1} - uId)^{-1}$ is equal to the expectation of the first passage time from i to j in the reduced model, see e.g. [1]. The identity (11) therefore states that the expected first passage time from b_- to b_+ is proportional to the expected first passage time from b_+ to b_- with a ratio which does not depend on the absorption rate u to the added state c.

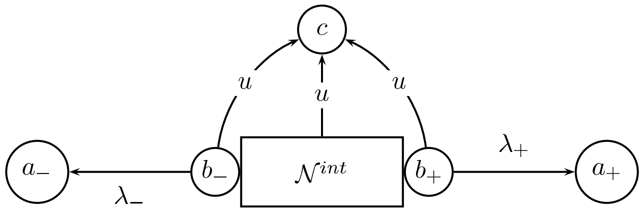

FIGURE 4: The reduced model perturbed by an additional absorbing state c.

4. Permuted balance implies Time Duality in bottleneck case

Reversibility of a CTMC means that in equilibrium any path $\nu = (i, k_0, k_1, \ldots, k_n, j)$ has the same weight as its reversed path $\nu^R = (j, k_n, k_{n-1}, \ldots, k_1, k_0, i)$. It is therefore intuitively clear that reversibility implies Time Duality, since also the time associated to the path ν is identical in distribution to the time associated to the reversed path ν^R. A local description of this behavior is given by the well known *detailed balance conditions*

$$\forall i, j : \ \pi_i q_{ij} = \pi_j q_{ji} \, ,$$

which expresses that in equilibrium the flow from the state i to the neighboring state j can be balanced out by the reversed flow where π is the reversible measure.

In this section we extend the concept of detailed balance by considering a permutation σ on the state space and balance out the flow from i to j by the reversed flow between $\sigma(j)$ to $\sigma(i)$.

Definition 4. Let $X := (X_t)_{t \geq 0}$ be a CTMC on a finite state space E with irreducible infinitesimal generator $Q = (q_{ij})_{i,j \in E}$. X is called *balanced under permutation* if there exists a permutation σ on E and a positive stochastic vector π invariant under σ such that

$$\forall i,j \in E, \quad \pi_i q_{ij} = \pi_{\sigma(j)} q_{\sigma(j)\sigma(i)}. \tag{17}$$

Then π is called *permuted balanced measure* with respect to the permutation σ.

Invariance of the measure π under a permutation σ means $\pi_i = \pi_{\sigma(i)}$ for all $i \in E$. Thus the system of equations (17), called *permuted balance equations*, reduce to

$$\forall i,j \in E,\ \pi_i q_{ij} = \pi_j q_{\sigma(j)\sigma(i)}. \tag{18}$$

Remark 1.

(i) If $\sigma = id$, balance under permution reduces to the usual reversibility.

(ii) The choice of σ is not unique.

(iii) The choice of π is unique, since it is equal to the unique invariant measure under Q: By summing (18) on both sides over $j \in E$, one obtains

$$\forall i \in E, \quad \pi_i \sum_{j\in E} q_{ij} = 0 = \sum_{j \in E} \pi_j q_{\sigma(j)\sigma(i)},$$

which implies that $\pi Q = 0$.

(iv) One can write equations (18) as the following matrix equation:

$$\mathrm{diag}(\pi) Q = P_\sigma Q^\top P_\sigma^{-1} \mathrm{diag}(\pi),$$

or equivalently

$$Q = (P_\sigma^{-1}\mathrm{diag}(\pi))^{-1} Q^\top P_\sigma^{-1} \mathrm{diag}(\pi), \tag{19}$$

where the permutation matrix P_σ is given by

$$P_\sigma := (p_{ij})_{ij} := \begin{cases} 1 & \text{if } j = \sigma(i), \\ 0 & \text{else.} \end{cases}$$

(v) Let π be permuted balanced for $Q = (q_{ij})_{i,j\in E}$. Then, by iteration of (17), for each path $\nu = (i_0, i_1, \dots, i_n)$:

$$\pi_{i_0} \prod_{k=0}^{n-1} q_{i_k i_{k+1}} = \pi_{\sigma(i_n)} \underbrace{\left[\prod_{k=1}^{n-1} \frac{\pi_{\sigma(i_k)}}{\pi_{i_k}}\right]}_{=1} \prod_{k=0}^{n-1} q_{\sigma(i_{k+1})\sigma(i_k)} = \pi_{\sigma(i_n)} \prod_{k=0}^{n-1} q_{\sigma(i_{k+1})\sigma(i_k)},$$

that is the weight of ν is equal to the weight of the image under σ of its reversed path.

We now treat an example of CTMC which illustrates the notion of balanced under permutation.

Example 1. Let $(X_t)_{t\geq 0}$ be the CTMC on $\{1,2,3,4\}$ associated with the infinitesimal generator

$$Q = \begin{pmatrix} -\alpha-\gamma & \alpha & 0 & \gamma \\ \delta & -\beta-\delta & \beta & 0 \\ 0 & \gamma & -\gamma-\alpha & \alpha \\ \beta & 0 & \delta & -\delta-\beta \end{pmatrix},$$

with three free parameters $\alpha, \beta, \gamma > 0$ and $\delta := \frac{\gamma\beta}{\alpha}$. Its transition graph is given in fig. 5. This model is reversible if and only if Kolmogorov criterion is satisfied

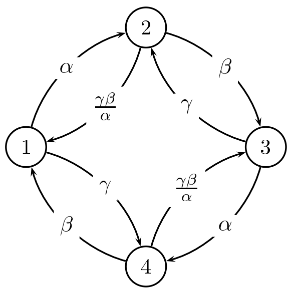

FIGURE 5: Example for permuted balance.

(see [3] 1.22), that is if the product of rates on any cycle of states $(i_1, i_2, \ldots, i_n, i_1)$ satisfies $q_{i_1 i_2} \ldots q_{i_{n-1} i_1} = q_{i_1 i_{n-1}} \ldots q_{i_2 i_1}$. For this example it is the case if and only if $\alpha\beta = \gamma\delta \Leftrightarrow \gamma = \alpha$ and then $\delta = \beta$.

If $\gamma \neq \alpha$, the model is not reversible but permuted balanced for $\sigma = (24)$. Indeed, the system of equations (17) reduce to

$$\pi_2 = \frac{\alpha}{\beta}\pi_1, \qquad \pi_3 = \pi_1, \qquad \pi_4 = \frac{\gamma}{\delta}\pi_1 = \frac{\alpha}{\beta}\pi_1,$$

which admits as unique solution

$$\pi = \frac{1}{2(\alpha+\beta)}(\beta, \alpha, \beta, \alpha), \tag{20}$$

the unique invariant measure of Q (independent of the value of γ).
Note that the model is also permuted balanced with respect to the permutations $(13), (14)(23)$ and $(12)(34)$.

We can now apply the notion of permuted balance to the irreducible matrix $\mathbf{A}$ defined in (1), which takes the form

$$\mathbf{A} = \mathbf{A_1} + \mathrm{diag}((\mathbf{A_0} + \mathbf{A_2})\mathbf{1}^\top) = \mathbf{A_1} + \mathrm{diag}(\lambda_-, 0, \dots, 0, \lambda_+) \tag{21}$$

under bottleneck property.

Theorem 2. *Let $(X_t)_{t\geq 0}$ be a CTMC on the state space $E = \{a_-\} \cup M \cup \{a_+\}$ $(= \{a_-, b_-\} \cup \mathcal{N}^{int} \cup \{b_+, a_+\})$ with infinitesimal generator (4). Suppose that $\mathbf{A}$ defined in (21) admits a permuted balanced measure π with respect to some permutation σ on M which has b_- and b_+ as fixed points. Then Time Duality follows.*

Proof. Define for the permuted balanced measure π on M

$$\pi =: (\pi_{b_-}, \pi_{\mathcal{N}^{int}}, \pi_{b_+}).$$

By assumption b_- and b_+ are fixed points of σ, so

$$\mathrm{diag}(\pi) = \begin{pmatrix} \pi_{b_-} & 0 & 0 \\ 0 & \mathrm{diag}(\tilde{\pi}) & 0 \\ 0 & 0 & \pi_{b_+} \end{pmatrix} \text{ and } P_\sigma = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \tilde{P_\sigma} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

where $\tilde{\pi}$ is the restriction of π to the states in $\mathcal{N}^{int}$, analogue for $\tilde{P_\sigma}$.
The only difference between $\mathbf{A}$ and $\mathbf{A}_1$ are the first and last entry of the diagonal. Thus, using the partition (10) of the matrix $\mathbf{A}_1$ and equation (19) applied to $\mathbf{A}$ we gain:

$$S = (\tilde{P_\sigma}^{-1}\mathrm{diag}(\tilde{\pi}))^{-1} \cdot S^\top \cdot \tilde{P_\sigma}^{-1}\mathrm{diag}(\tilde{\pi}), \qquad \pi_{b_-}\lambda_{b_-b_+} = \pi_{b_+}\lambda_{b_+b_-},$$
$$R_{b_-S} = \frac{1}{\pi_{b_-}} R_{Sb_-}\mathrm{diag}(\tilde{\pi})\tilde{P_\sigma}, \qquad R^\top_{Sb_+} = \pi_{b_+}(\mathrm{diag}(\tilde{\pi})\tilde{P_\sigma})^{-1}R^\top_{b_+S}.$$

Furthermore

$$\begin{aligned}
R_{b_-b_+}(u) + \lambda_{b_-b_+} &= \lambda_{b_-b_+} - R_{Sb_+}(S - uId)^{-1} R_{b_-S}^\top \\
&= \frac{\pi_{b_+}}{\pi_{b_-}} \left(\lambda_{b_+b_-} - R_{Sb_-} \mathrm{diag}(\tilde{\pi}) \tilde{P_\sigma} (S - uId)^{-1} \tilde{P_\sigma}^{-1} \mathrm{diag}(\tilde{\pi})^{-1} R_{b_+S}^\top \right) \\
&= \frac{\pi_{b_+}}{\pi_{b_-}} \left(\lambda_{b_+b_-} - R_{b_+S} \mathrm{diag}(\tilde{\pi})^{-1} \tilde{P_\sigma} (S^\top - uId)^{-1} \tilde{P_\sigma}^{-1} \mathrm{diag}(\tilde{\pi}) R_{Sb_-}^\top \right) \\
&= \frac{\pi_{b_+}}{\pi_{b_-}} \left(\lambda_{b_+b_-} - R_{b_+S} (\underbrace{\mathrm{diag}(\tilde{\pi})^{-1} \tilde{P_\sigma} S^\top \tilde{P_\sigma}^{-1} \mathrm{diag}(\tilde{\pi})}_{=S} - uId)^{-1} R_{Sb_-}^\top \right) \\
&= \frac{\pi_{b_+}}{\pi_{b_-}} (R_{b_+b_-}(u) + \lambda_{b_+b_-})
\end{aligned}$$

and thus

$$\frac{R_{b_-b_+}(u) + \lambda_{b_-b_+}}{R_{b_+b_-}(u) + \lambda_{b_+b_-}} = \frac{\pi_{b_+}}{\pi_{b_-}}$$

which implies Time Duality by Theorem 1.

■

As we noticed in Remark 1 (iv), Time Duality holds since we can replace each path $(b_+, i_0, i_1, \ldots, i_n, b_-)$ by $(b_-, \sigma(i_n), \sigma(i_{n-1}), \ldots, \sigma(i_0), b_+)$, its reversed image under σ.

Example 2. Define

$$\mathbf{A}_1 = \begin{pmatrix} -\alpha - \gamma - 1 & \alpha & 0 & \gamma \\ \delta & -\beta - \delta & \beta & 0 \\ 0 & \gamma & -\gamma - \alpha & \alpha \\ \beta & 0 & \delta & -\delta - \beta - 1 \end{pmatrix},$$

for $\alpha, \beta, \gamma, \delta > 0$ and $\lambda_- = 1 = \lambda_+$. Here the boundary states b_- and b_+ are labelled 1 and 3, see also fig. 6.

Clearly $\mathbf{A} = \mathbf{A_1} + \mathrm{diag}(1, 0, 0, 1)$ is equal to the infinitesimal generator given in Example 1 if $\delta = \frac{\gamma\beta}{\alpha}$. In this case, the permuted balanced measure π with respect to the permutation which only exchanges 2 and 4 is given by (20) and, by Theorem 2, Time Duality holds.

Another type of condition for Time Duality is the less restrictive invariance of the matrix S – describing the transitions inside of $\mathcal{N}^{int}$ – under simultaneous swap of

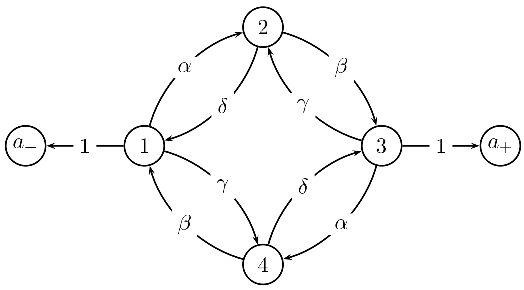

FIGURE 6: Transition graph considered in example 2 and 3.

some rows and some columns or, with other words, the commutativity of S with a permutation matrix P_σ.

Theorem 3. *Let $(X_t)_{t\geq 0}$ be a CTMC on the state space $E = \{a_-\} \cup M \cup \{a_+\}$ with infinitesimal generator (4). If there exists a permutation σ on $M \setminus \{b_-, b_+\}$ and $\kappa_1, \kappa_2 > 0$ such that*

$$S = P_\sigma S P_\sigma^{-1}, \qquad \lambda_{b_+b_-} = \kappa_1\kappa_2\lambda_{b_-b_+},$$
$$R_{b_-S} = \frac{1}{\kappa_1} R_{b_+S} P_\sigma^{-1}, \qquad R_{Sb_-}^\top = \kappa_2 P_\sigma^{-1} R_{Sb_+}^\top,$$

then Time Duality follows.

Proof. For any $u \geq 0$,

$$\begin{aligned} R_{b_-b_+}(u) + \lambda_{b_-b_+} &= \lambda_{b_-b_+} - R_{b_-S}(S + uId)^{-1} R_{Sb_+}^\top \\ &= \frac{1}{\kappa_1\kappa_2}\lambda_{b_+b_-} - \left(\frac{1}{\kappa_1} R_{b_+S} P_\sigma^{-1}\right) P_\sigma (S + uId)^{-1} P_\sigma^{-1} \left(\frac{1}{\kappa_2} P_\sigma R_{Sb_-}^\top\right) \\ &= \frac{1}{\kappa_1\kappa_2}(R_{b_+b_-}(u) + \lambda_{b_+b_-}). \end{aligned}$$

We complete the proof using Theorem 1.

■

Let us present an application of Theorem 3.

Example 3. We use the model introduced in Example 2 fig. 6, and identify

$$R_{b_-S} = (\alpha, \gamma),\ R_{b_+S} = (\gamma, \alpha),\ R_{Sb_-} = (\delta, \beta),\ R_{Sb_+} = (\beta, \delta),\ \lambda_{b_-b_+} = 0,\ \lambda_{b_+b_-} = 0$$

and $S = -(\beta+\delta)Id$. The matrix S is trivially invariant under any 2×2-permutation matrix, but only for

$$P_\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

we can fulfil $R^\top_{Sb_-} = \kappa_2 P_\sigma^{-1} R^\top_{Sb_+}$ with $\kappa_2 = 1$. Also $R_{b_-S} = \frac{1}{\kappa_1} R_{b_+S} P_\sigma^{-1}$ holds if and only if $\kappa_1 = 1$. Therefore the assumptions of Theorem 3 are fulfilled and Time Duality follows for any values of α, β, γ and δ.

This underlines that assumptions of Theorem 3 are sometimes less restrictive than the ones of Theorem 2, and that Time Duality can hold even if the chain is not permuted balanced.

5. The case without bottleneck

For general continuous time QBD's which do not have the bottleneck form, the technique used in Theorem 1 is not fruitful any more. The matrix $\mathbf{A_1}$ decomposes as before into blocks according to the sets $\mathcal{N}^-$, $\mathcal{N}^{int}$ and $\mathcal{N}^+$

$$\mathbf{A_1} = \begin{pmatrix} \Gamma_- & R_{\mathcal{N}^-\mathcal{N}^{int}} & \Lambda_{\mathcal{N}^-\mathcal{N}^+} \\ R_{\mathcal{N}^{int}\mathcal{N}^-} & S & R_{\mathcal{N}^{int}\mathcal{N}^+} \\ \Lambda_{\mathcal{N}^+\mathcal{N}^-} & R_{\mathcal{N}^+\mathcal{N}^{int}} & \Gamma_+ \end{pmatrix}$$

and, instead to compare (15) with (16), we have to compare

$$e_i (R_{\mathcal{N}^-\mathcal{N}^-}(u) + \Gamma_-)^{-1} (R_{\mathcal{N}^-\mathcal{N}^+}(u) + \Lambda_{\mathcal{N}^-\mathcal{N}^+}) K^{-1} e_j^\top$$

with

$$e_j K^{-1} (R_{\mathcal{N}^+\mathcal{N}^-}(u) + \Lambda_{\mathcal{N}^+\mathcal{N}^-})(R_{\mathcal{N}^-\mathcal{N}^-}(u) + \Gamma_-)^{-1} e_i^\top$$

for $i \in \mathcal{N}^-, j \in \mathcal{N}^+$ and $R_{ij} = -R_{iS}(S + uId)^{-1} R_{Sj}$. Unfortunately the quantities which appear in these expressions are now matrices which do not commute with the others. Therefore the derivation of a simple criterion seemed hopeless. Nevertheless we construct a modified CTMC with bottleneck and show that if the modified model fulfills Theorem 2 or Theorem 3 then Time Duality follows for the original model. Now the initial conditions μ_- and μ_+ play an important role and we will describe them as the solution of a linear system.

We assume in the rest of this section that $(X_t)_{t\geq 0}$ denotes a CTMC on $E = \{a_-\} \cup M \cup \{a_+\}$ with infinitesimal generator (2) and that μ_- resp. μ_+ are probability measures with support in $\mathcal{N}^-$ resp. $\mathcal{N}^+$. We construct a new CTMC $(\tilde{X}_t)_{t\geq 0}$ on the state space

$$\tilde{E} := \{c_-\} \cup E \cup \{c_+\} = \{c_-, a_-\} \cup M \cup \{a_+, c_+\}$$

with infinitesimal generator

$$\tilde{Q} := \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & -1 - \mu_-\mathbf{H}_-^{-1}\mathbf{1}^\top & \mu_-\mathbf{H}_-^{-1} & 0 & 0 \\ 0 & \mathbf{A_2}\mathbf{1}^\top & \mathbf{A_1} & \mathbf{A_0}\mathbf{1}^\top & 0 \\ 0 & 0 & \mu_+\mathbf{H}_+^{-1} & -1 - \mu_+\mathbf{H}_+^{-1}\mathbf{1}^\top & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{22}$$

where $\mathbf{H}_+$ is defined in (7).

This modified model satisfies the bottleneck property, see fig. 7.

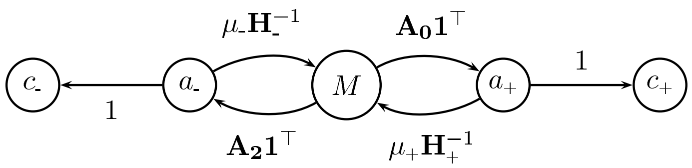

FIGURE 7: The modification of a general model to recover the bottleneck property

Note that the precise values of the absorption rate in c_- and c_+ are irrelevant for the appearance of Time Duality. Theorem 1 states that Time Duality holds for the process $\tilde{X}$ if and only if

$$\frac{-\mu_-\mathbf{H}_-^{-1}(\mathbf{A_1} - uId)^{-1}\mathbf{A_0}\mathbf{1}^\top}{-\mu_+\mathbf{H}_+^{-1}(\mathbf{A_1} - uId)^{-1}\mathbf{A_2}\mathbf{1}^\top} = \frac{\mu_-\mathbf{H}_-^{-1}\overbrace{(-\mathbf{A_1})^{-1}\mathbf{A_0}\mathbf{1}^\top}^{=\mathbf{H}_-\mathbf{1}^\top}}{\mu_+\mathbf{H}_+^{-1}\underbrace{(-\mathbf{A_1})^{-1}\mathbf{A_2}\mathbf{1}^\top}_{=\mathbf{H}_+\mathbf{1}^\top}} = \frac{\mu_-\mathbf{1}^\top}{\mu_+\mathbf{1}^\top} = 1,$$

which is clearly equivalent to the weak Time Duality for $(X_t)_{t\geq 0}$ according to Definition 2.

This observation leads to

Theorem 4. *Let $(X_t)_{t\geq 0}$ be a CTMC on the state space $E = \{a_-\} \cup M \cup \{a_+\}$ with infinitesimal generator (2). Let μ_- resp. μ_+ be initial distributions concentrated on $\mathcal{N}^-$*

resp. $\mathcal{N}^+$*. If the modified process* $(\tilde{X}_t)_{t\geq 0}$ *with infinitesimal generator (22) admits a permuted balanced measure* π*, then* $(X_t)_{t\geq 0}$ *is* (μ_-, μ_+)*-time dual. Moreover the initial laws are related by*

$$\mu_+ = \kappa \cdot \mu_- \mathbf{H}_-^{-1} diag(\pi) P_\sigma \mathbf{H}_+$$

where π *and* σ *satisfy (17) and* κ *is a positive constant.*

In the same spirit we gain

Theorem 5. *Let* $(X_t)_{t\geq 0}$ *be the reduced model associated with a general continuous time QBD with infinitesimal generator (2). Let* μ_- *resp.* μ_+ *be initial distributions concentrated on* $\mathcal{N}^-$ *resp.* $\mathcal{N}^+$*. If there is a permutation* σ *on* M *and* $\kappa > 0$ *such that the following identities hold:*

$$\begin{aligned} \mathbf{A_1} &= P_\sigma \mathbf{A_1} P_\sigma^{-1} & \qquad \lambda_{a_+ a_-} &= \lambda_{a_- a_+} \\ \mathbf{A_2} \mathbf{1}^\top &= \frac{1}{\kappa} P_\sigma \mathbf{A_0} \mathbf{1}^\top & \qquad \mu_- \mathbf{H}_-^{-1} &= \kappa \mu_+ \mathbf{H}_+^{-1} P_\sigma, \end{aligned}$$

then $(X_t)_{t\geq 0}$ *is* (μ_-, μ_+)*-time dual. In this case the initial laws are uniquely determined by*

$$\mu_+^\top = \kappa \cdot \mathbf{H}_+ P_\sigma^{-1} \mathbf{A_0} \mathbf{1}^\top, \qquad \mu_-^\top = \kappa \cdot \mathbf{H}_- P_\sigma^{-1} \mathbf{A_2} \mathbf{1}^\top.$$

In both theorems κ plays the role of a renormalisation constant. The proofs of both theorems are straightforward.

6. Acknowledgments

We thank an anonymous referee of a first version of this paper for mentioning the reference [6] and encouraging us to solve the question of Time Duality in a much more general framework than our former results did. We thank R. Lipowsky for fruitful discussions on these topics.

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