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Obtaining the long-term behavior of master equations with finite state space from the structure of the associated state transition network

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Abstract

The master equation describes the time evolution of the probabilities of a system with a discrete state space. This time evolution approaches for long times a stationary state that will in general depend on the initial probability distribution. Conditions under which the stationary state is unique are usually given as remarks appended to more comprehensive theories in the mathematical literature. We provide a direct and complete derivation of a necessary and sufficient criterion for when this steady state is unique. We translate this problem into the language of graph theory and show that there is a one-to-one correspondence between minimal absorbing sets within the state-transition network and linearly independent stationary states of the master equation.

Keywords: master equation, relaxing, steady states, connectivity, absorbing subnetworks

(Some figures may appear in colour only in the online journal)

1. Introduction

Master equations appear in many different context in chemistry, biology and physics. Examples are biochemical reaction networks, stochastic population dynamics based on deaths and births, and various statistical physics problems.

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Master equations describe the time evolution of the probabilities of the different states of a system, with the dynamics being due to transitions between these states [1, 2]. The most common form is an initial value problem of a linear differential equation. The picture behind a master equation is that of probabilities flowing between states like a fluid, where their total amount is being conserved. The probability flow along a directed link depends linearly on the strength of the link and the amount of probability at the source. Of particular interest is the long-time behavior of the solution, as this determines the states where a system will eventually be, together with their probabilities. Unlike discrete-time Markov chains, which can lead to long-term oscillations of the probabilities, the solution of the master equation for a finite state space will always converge to a stationary solution where the probability distribution does not change any more. In general, this steady state will depend on the initial distribution of the probabilities, i.e. on the initial condition of the corresponding differential equation.

In this paper we focus on the question under which conditions a finite-size master equation has a unique steady state, in which case the master equation is called *relaxing* [3]. If this steady state has only strictly positive entries, the corresponding state transition network is called *ergodic* [4].

The mathematical literature contains necessary and sufficient conditions for the stationary state to be unique, but these are only hinted at or given as a remark appended to theorems within major treatises on topics such as master equations, Markov chains or directed graphs [4–6]. What these all lack is a clear statement and proof that is based on first principles.

In the physical literature, usually more special situations are discussed. For instance, the master equation for the microcanonical ensemble of statistical physics can be shown to be relaxing because the transition rates between pairs of states are symmetric. Therefore, the steady state is the uniform distribution [1, 2].

The often-cited review by Schnakenberg on the network theory of master equation systems [7] discusses models where to each transition there exists also the reverse transition. In this specific case, the stationary solution is always unique. A more mathematical paper by Jamiolkowski and Staszewski [8] gives a general criterion for the master equation to be relaxing, however, this criterion is a nonintuitive mathematical expression based on the principal minors of the matrix that contains the transition rates. The probably most broad discussion of the long-term behavior of the master equation that is accessible to physicists can be found in the book by van Kampen [1]. While providing an intuitively plausible reasoning, this reasoning is not always precise and does not constitute a proof.

Our goal in this paper is to provide a direct proof that is accessible for physicists without delving deep into the mathematical literature. This proof proceeds by translating the initial value problem into the language of graph theory. By considering the network of the states of the system and the transitions between them, an intuitive understanding of the meaning of the steps of the proof can be achieved. An important notion is that of *minimal absorbing sets*, which are subsets of states from where the probability cannot escape. We show that the number of linearly independent steady states of the master equation equals the number of minimal absorbing sets in the corresponding transition network. In particular, the steady state of the master equation is unique if and only if there is exactly one minimal absorbing set. While this statement seems intuitively clear, the complete proof is non-trivial, even though it uses only undergraduate mathematics.

2. The master equation and the time evolution operator

We consider a system of $N \in \mathbb{N}$ states and the transitions between them. If there is no transition from state i to state j, the associated transition rate $\gamma_{i\to j}$ vanishes. The states and the nonzero

transition rates form together a network $\mathcal{S} = (\Omega, \mathcal{E})$, with the states $\Omega = \{1, \ldots, N\}$ being the nodes and the transitions being the directed links $\mathcal{E} \subseteq \Omega \times \Omega$ of the network. The transition rates indicate the weights of these links. For all subsets of states $B \subseteq \Omega$ there is a corresponding subnetwork $(B, \mathcal{E}_B)$, where $\mathcal{E}_B := \{(i, j) \in \mathcal{E} : i, j \in B\}$ consists of all links in the subset $B \subseteq \Omega$.

Since transitions occur only between different states, the network has no self-loops, that is $\gamma_{i\to i} = 0$ for all $i \in \Omega$.

We denote with $p_i(t)$ the probability of the system to be in state i at time t. These probabilities are nonnegative and normalized, $\mathbf{p} \in [0, 1]^N$ with $\|\mathbf{p}\|_1 = 1$.

The master equation that describes the change in time of these probabilities is the following initial value problem

$$\begin{aligned} \partial_t p_i(t) &= \sum_{\substack{j=1 \\ j\neq i}}^{N} \left(p_j(t)\gamma_{j\to i} - p_i(t)\gamma_{i\to j} \right) \\ p_i(t=0) &= p_0^{(i)}, \end{aligned} \tag{1}$$

or, in matrix-vector notation,

$$\begin{aligned} \dot{\mathbf{p}} &= \Gamma \mathbf{p} \\ \mathbf{p}(t=0) &= \mathbf{p}_0, \quad \text{with } \Gamma_{ij} = \begin{cases} \gamma_{j\to i}, & i \neq j \\ -\sum_{k=1}^{N} \gamma_{j\to k}, & i = j. \end{cases} \end{aligned} \tag{2}$$

The solution is given by $\mathbf{p}_t := \mathrm{e}^{\Gamma t}\mathbf{p}_0$, with the initial state $\mathbf{p}(t=0) = \mathbf{p}_0$ and the solution operator

$$\mathrm{e}^{\Gamma t} := \sum_{k\in\mathbb{N}_0} \frac{\Gamma^k t^k}{k!} = \lim_{n\to\infty} \left(\mathcal{I} + \frac{\Gamma t}{n} \right)^n. \tag{3}$$

The matrix Γ is called the **generator** or **transition matrix** of the network Ω [5].

In the following, we relate properties of the solution $\mathbf{p}_t := \mathrm{e}^{\Gamma t}\mathbf{p}_0$ to the properties of the network Ω.

Since sum of all columns of Γ is zero $\left(\sum_{i=1}^{N} \Gamma_{ij} = 0 \text{ for all } j \in \{1, \ldots, N\} \right)$, we have $(\underbrace{1, \ldots, 1}_{N \text{ times}}) \cdot \Gamma = (\underbrace{0, \ldots, 0}_{N \text{ times}})$ and hence $\lambda = 0$ is an eigenvalue of the matrix Γ. The eigenvectors to this eigenvalue are stationary states that satisfy $\dot{\mathbf{p}} = 0$. From Gershgorin's circle theorem [9] follows that all non-zero eigenvalues of Γ have a (strictly) negative real part (see appendix A.1).

The column sum of any matrix power of Γ is also zero $\left(\sum_{i=1}^{N} \left(\Gamma^k\right)_{ij} = 0 \text{ for all } j \in \{1, \ldots, N\} \text{ and for all } k \in \mathbb{N} \right)$, as can be shown by induction. Further, a power series expansion yields that the column sums of its matrix exponential $\mathrm{e}^{\Gamma t}$ equals one,

$$\sum_{i=1}^{N} \left(\mathrm{e}^{\Gamma t}\right)_{ij} = 1. \tag{4}$$

Every initial state can be written as a linear combination of generalized eigenvectors of Γ. In the limit $t \to \infty$, only the eigenvectors of the eigenvalue $\lambda = 0$ (the ones lying in the kernel of Γ) remain, while the contributions of the other eigenvectors decay exponentially.

To see this, let $\boldsymbol{h}_{\lambda,m} \in \ker(\Gamma - \lambda\mathcal{I})^m \backslash \ker(\Gamma - \lambda\mathcal{I})^{m-1}$ be a generalized eigenvector of rank $m \in \mathbb{N}$ to the eigenvalue λ. The action of the time evolution operator $\mathrm{e}^{\Gamma t}$ on this vector is

$$\mathrm{e}^{\Gamma t}\boldsymbol{h}_{\lambda,m} = \mathrm{e}^{\lambda t}\sum_{k=0}^{m-1}\frac{t^k}{k!}\boldsymbol{h}_{\lambda,m-k}, \tag{5}$$

where we used the Jordan normal form of the transition matrix Γ (see [10] for details).

For non-zero eigenvalues $\lambda \neq 0$, this tends to zero since $\mathrm{Re}[\lambda] < 0$.

For $\lambda = 0$, we must have $m = 1$ since the solution of the master equation (2) is bounded. If we had $m \geqslant 2$, we could construct a modified initial state $\tilde{\mathbf{p}}_0 = \mathbf{p}_0 + \epsilon\boldsymbol{h}_{\lambda=0,m=2}$ that would evolve according to

$$\mathbf{p}(t) = \underbrace{\mathrm{e}^{\Gamma t}\mathbf{p}_0}_{\in\left(\mathbb{R}_{\geqslant 0}\right)^N} + \epsilon\left(\boldsymbol{h}_{\lambda=0,m=2} + t\boldsymbol{h}_{\lambda=0,m=1},\right)$$

which is unbounded.

This results in

$$\mathrm{e}^{\Gamma t}\boldsymbol{h}_{\lambda=0} = \boldsymbol{h}_{\lambda=0}. \tag{6}$$

As an alternative to the calculation given here, one can deduce the dynamics of the master equation from the structure of the transition matrix Γ alone. In appendix A.6, we show that the algebraic multiplicity of the eigenvalue $\lambda = 0$ equals the geometric multiplicity and hence $m = 1$ in equation (5).

3. Definitions and preparatory considerations

Before we can state and prove the main theorem, we need a few more definitions and theorems.

3.1. Paths

If state b can be reached from state a via a series of transitions, there is a path from a to b, which we indicate by $a \rightsquigarrow b$, and we say that state b is reachable from state a. We denote with

- $\mathcal{R}(^{\rightarrow}a) := \{b \in \Omega | b \rightsquigarrow a\}$ the set of states from where a path **to** a exists and with
- $\mathcal{R}(a^{\rightarrow}) := \{b \in \Omega | a \rightsquigarrow b\}$ the set of states to which a path **from** a exists.

3.2. Weak, unilateral, and strong connectedness

We call Ω

(a) **Weakly** connected if the corresponding undirected graph of Ω is connected;
(b) **Unilaterally** connected if for all $a, b \in \Omega$, b is reachable from a OR a is reachable from b;
(c) **Strongly** connected if for all $a, b \in \Omega$, b is reachable from a and a is reachable from b, $a \rightsquigarrow b$ and $b \rightsquigarrow a$.

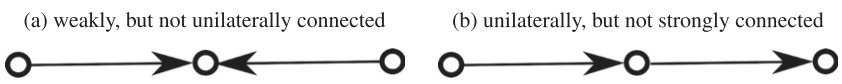

Figure 1. The differences between weak, unilateral and strong connectivity.

Figure 1 illustrates the difference.

3.3. Relaxing networks

We call Ω **relaxing** if there exists a unique stationary state $\mathbf{p}_\infty$ such that for all initial conditions $\mathbf{p}_0$ the dynamics of the master equation converges to this stationary state, that is $\lim_{t\to\infty} \mathbf{p}_t = \mathbf{p}_\infty$. This means that the eigenspace of Γ corresponding to the eigenvalue 0 is one-dimensional, $\dim(\mathrm{kern}(\Gamma)) = 1$.

3.4. Absorbing subsets

We write $\mathbf{p} \in B$ if all mass of the probability distribution is restricted to a subset $B \in \Omega$, that is $\sum_{i\in B} p_i = 1$. We call a subset $B \subseteq \Omega$ absorbing if there are no edges pointing out of B, that is if $\gamma_{i\to j} = 0$ for all $i \in B$ and $j \in B^C$. This means that probability cannot flow out of B, so when the mass of the probability distribution of the initial state is in B ($\mathbf{p}_0 \in B$), then it will stay in B for all times: $\mathbf{p}_t \in B$ for all $t \geqslant 0$.

Note that the intersection of absorbing sets is again absorbing. This follows directly from the definition.

Later, we will use the fact that $\mathcal{R}(^{\to}a)^C$ and $\mathcal{R}(a^{\to})$ are absorbing subsets. The two statements are shown as follows:

- If $\mathcal{R}(^{\to}a)^C$ were not absorbing, there would be a state $c \in \mathcal{R}(^{\to}a)^C$ and a $b \in \mathcal{R}(^{\to}a)$ such that $c \rightsquigarrow b$. However, this would imply $c \rightsquigarrow b \rightsquigarrow a$, which is a contradiction.
- If $\mathcal{R}(a^{\to})$ were not absorbing, there would be a state $b \in \mathcal{R}(a^{\to})$ and a state $c \in \mathcal{R}(a^{\to})^C$ such that $b \rightsquigarrow c$. However, this would imply $a \rightsquigarrow b \rightsquigarrow c$, which is a contradiction.

3.5. Minimal absorbing subsets

An absorbing subset $B \subseteq \Omega$ is called **minimal** if for all absorbing subsets $C \subseteq \Omega$ with $C \subseteq B$, we have $B = C$. In particular, there can be more than one minimal absorbing subset.

Every minimal absorbing subset B is strongly connected. To see this, assume that there are two states $i, j \in B$ with $i \nrightsquigarrow j$.. Then $i \in \left(\mathcal{R}(^{\to}j)^C \cap B\right)$ and $j \notin \left(\mathcal{R}(^{\to}j)^C \cap B\right)$. This implies that $\left(\mathcal{R}(^{\to}j)^C \cap B\right)$ is a non-empty intersection of two minimal absorbing sets which is strictly less than B, in contradiction with the premise that B is minimal.

Every state $\omega \in \Omega$ leads to a (not necessarily unique) minimal absorbing subnetwork B_ω, that is, there exists a path $\omega \to b$ to some element $b \in B_\omega$ of some minimal absorbing subset B_ω. This follows from the result in the previous subsection that the set $\mathcal{R}(\omega^{\to})$ is absorbing. This set must contain a minimal absorbing set $B_\omega \subseteq \mathcal{R}(\omega^{\to})$, and (since minimal absorbing subnetworks are strongly connected) every state of B_ω is reachable from ω, that is $\omega \rightsquigarrow b$ for all states $b \in B_\omega \subseteq \mathcal{R}(\omega^{\to})$.

3.6. Diagonal dominance

Let $B \in \mathbb{C}^{N\times N}$ be a complex matrix.

- For $i \in \{1,\dots,N\}$, we call the ith row of B **strictly diagonal dominant** (SDD) if $|B_{ii}| > \sum_{\substack{j=1,\\ j\neq i}}^{N} |B_{ij}|$.
- We call the matrix B SDD if every row of B is SDD. Due to the Gershgorin circle theorem [9], an SDD matrix is non-singular.
- The definition of a **weakly diagonal dominant** (WDD) matrix is the same as the previous one, but with a '$\geqslant$' sign instead of a '$>$' sign.
- We call B **weakly chained diagonal dominant** (WCDD) if B is WDD and for all rows $i \in \{1,\dots,N\}$ that are not (SSD), there exists a $k \in \{1,\dots,N\}$ and a path $i = i_0 \to \cdots \to i_k = j$ in the directed graph associated to B to a (SSD) row $j \in \{1,\dots,N\}$ of B.

It can be shown that WCDD matrices are non-singular (see appendix A.2 for a proof).

3.7. Structure of the matrix Γ

Below, we will use the matrix Γ in a specific form that can be obtained by re-numbering the states.

Let $\mathcal{B} = \{B_1,\dots,B_n\}$, $n \leqslant N$ be the set of minimal absorbing subsets and define $M := N - \sum_{i=1}^{n} |B_i|$. We number the states as follows: the first M states are those not contained in minimal absorbing networks. Then we count the states which lie in minimal absorbing networks block-wise, that is

$$\begin{aligned} B_0 &:= \Omega \backslash \bigcup_{i=1}^{n} B_i = \{1,\dots,M\} \\ B_i &= \left\{ M + \sum_{j=1}^{i-1} |B_j| + 1, \dots, M + \sum_{j=1}^{i} |B_j| \right\}, \quad \text{for } i \in \{1,\dots,n\}. \end{aligned} \tag{7}$$

To keep the notation simple, we did not distinguish between the index $i \in \{1,\dots,N\}$ and the state $\omega_i \in \Omega$ with index i:

$$\begin{aligned} \omega_i &\hat{=} i \\ \Omega &\hat{=} \{1,\dots,N\}. \end{aligned} \tag{8}$$

After this re-numbering of the states, we can write Γ in the following form

$$\Gamma = \begin{pmatrix} \Gamma_{B_0} & 0^{M\times|B_1|} & \dots & 0^{M\times|B_n|} \\ \Gamma_{B_0\to B_1} & \Gamma_{B_1} & & 0^{|B_1|\times|B_n|} \\ \vdots & & \ddots & \\ \Gamma_{B_0\to B_n} & 0^{|B_n|\times|B_1|} & & \Gamma_{B_n} \end{pmatrix} \quad \text{with the matrices} \tag{9}$$

$$\Gamma_{B_0} \in \mathbb{R}^{M\times M}, \quad \Gamma_{B_i} \in \mathbb{R}^{|B_i|\times|B_i|} \quad \text{and} \quad \Gamma_{B_0\to B_i} \in \mathbb{R}^{|B_i|\times M}, \quad \text{for } i \in \{1,\dots,n\}$$

If there is no matrix Γ_{B_0} ($M = 0$) and there is only one minimal absorbing set ($n = 1$), then Γ is called **irreducible** [9, 10], otherwise it is called **reducible**.

Figure 2 gives an illustrating example.

The matrices of the absorbing subnetworks and the full matrix Γ for this example are

$$\Gamma_{B_1} = 0, \quad \Gamma_{B_2} = \begin{pmatrix} -\gamma_{4\to5} & \gamma_{5\to4} \\ \gamma_{4\to5} & -\gamma_{5\to4} \end{pmatrix}, \quad \Gamma_{B_3} = \begin{pmatrix} -\gamma_{6\to7} & 0 & \gamma_{8\to6} \\ \gamma_{6\to7} & -\gamma_{7\to8} & 0 \\ 0 & \gamma_{7\to8} & -\gamma_{8\to6} \end{pmatrix}$$

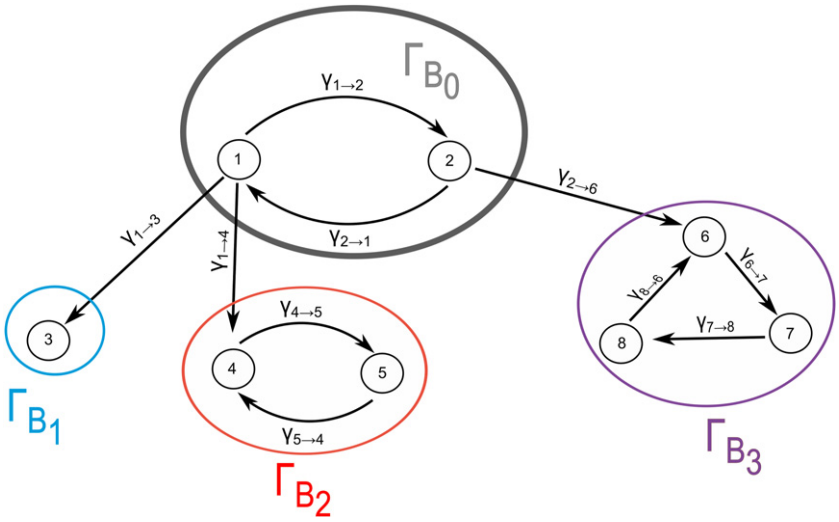

Figure 2. Example of a network/directed graph with the minimal absorbing sets being $B_1 = \{3\}$, $B_2 = \{4, 5\}$ and $B_3 = \{6, 7, 8\}$.

and

$$\Gamma = \begin{pmatrix} \Gamma_{B_0} & 0 & 0 & 0 \\ \Gamma_{B_0 \to B_1} & \Gamma_{B_1} & 0 & 0 \\ \Gamma_{B_0 \to B_2} & 0 & \Gamma_{B_2} & 0 \\ \Gamma_{B_0 \to B_3} & 0 & 0 & \Gamma_{B_3} \end{pmatrix} = \begin{pmatrix} -\gamma_{1\to2} - \gamma_{1\to3} - \gamma_{1\to4} & \gamma_{2\to1} & 0 & 0 & 0 & 0 & 0 & 0 \\ \gamma_{1\to2} & -\gamma_{2\to1} - \gamma_{2\to6} & 0 & 0 & 0 & 0 & 0 & 0 \\ \gamma_{1\to3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \gamma_{1\to4} & 0 & 0 & -\gamma_{4\to5} & \gamma_{5\to4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma_{4\to5} & -\gamma_{5\to4} & 0 & 0 & 0 \\ 0 & \gamma_{2\to6} & 0 & 0 & 0 & -\gamma_{6\to7} & 0 & \gamma_{8\to6} \\ 0 & 0 & 0 & 0 & 0 & \gamma_{6\to7} & -\gamma_{7\to8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \gamma_{7\to8} & -\gamma_{8\to6} \end{pmatrix}$$

3.8. If the matrix Γ_{B_0} exists, it is invertible

In order to show that the matrix Γ_{B_0} is invertible, it suffices to show that Γ_{B_0} is WCDD (see appendix A.2 and section 3.6 for a definition of WCDD).

We assume that Γ is of the form (9) and $\mathcal{B} = \{B_1, \ldots, B_n\}$ is the set of minimal absorbing subsets.

(a) Γ_{B_0} is WDD, since

$$\sum_{\substack{i=1,\\ i\neq j}}^{M} \underbrace{|(\Gamma_{B_0})_{ij}|}_{|\Gamma_{ij}|} \leqslant \sum_{\substack{i=1,\\ i\neq j}}^{N} |\Gamma_{ij}| = |\Gamma_{jj}| = |(\Gamma_{B_0})_{jj}|.$$

(b) Let $x \in B_0$ be an arbitrary state in B_0. Then there are two cases:

1. If $\gamma_{x\to b} > 0$ for some $b \in B_i$, then the xth row is SDD, since

$$\sum_{\substack{i=1,\\ i\neq x}}^{M} \underbrace{|(\Gamma_{B_0})_{i,x}|}_{|\Gamma_{i,x}|} < \sum_{\substack{i=1,\\ i\neq x}}^{M} |\Gamma_{i,x}| + \underbrace{|\Gamma_{b,x}|}_{\gamma_{x\to b}} \leqslant \sum_{\substack{i=1,\\ i\neq x}}^{N} |\Gamma_{i,x}| = |\Gamma_{x,x}| = |(\Gamma_{B_0})_{x,x}|.$$

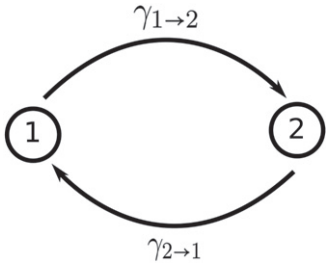

Figure 3. Illustrating the difference between the adjacency matrix A and Γ.

2. If the xth column is not SSD ($\gamma_{x\to b} = 0$ for all $b \in \Omega\backslash B_0$), we know from section 3.5 that there exists a path from the state x to a minimal absorbing set B_i, that is $x \to \cdots \to x' \to b$ for some $i \in \{1, \ldots, n\}$ and some state $b \in B_i$ and $x' \in B_0$. But this again means that if the x-column is not SDD, there is a path from x to the SDD column x' (where $\gamma_{x'\to b} > 0$, for some $b \in B_i$).

4. A simplified version of the main theorem

Before stating the general condition for a network Ω to be relaxing, we first consider the important special case that Ω is strongly connected. Our goal in this section is to prove that a strongly connected network is relaxing (which is a corollary of the theorem of Perron–Frobenius [9–11]). We proceed in three steps.

4.1. A directed graph Ω is strongly connected if and only if its adjacency matrix A is irreducible

Here, we use a different but equivalent characterization of irreducibility than above: a matrix $A \in \mathbb{R}^{N\times N}$ with non-negative entries ($A_{ij} \geqslant 0$ for all i, j) is irreducible if and only if for all $i, j \in \{1, \ldots, N\}$ there exists a natural number $k = k_{ij} \in \mathbb{N}$ such that the i–jth entry of the k_{ij}th matrix power of A is strictly greater zero, that is $\left(A^{k_{ij}}\right)_{ij} > 0$.

The adjacency matrix A of the directed graph Ω is defined by

$$A_{ij} = \begin{cases} 1 & \gamma_{j\to i} > 0 \\ 0 & \text{else.} \end{cases} \tag{10}$$

In contrast to Γ, the adjacency matrix A has zeros on the main diagonal and only tells *qualitatively* whether two links j and i are directly connected. It contains no *quantitative* information about the strength of the links.

Figure 3 shows an example of a strongly connected network. The corresponding adjacency matrix is $A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and the generator is $\Gamma = \begin{pmatrix} -\gamma_{1\to2} & \gamma_{2\to1} \\ \gamma_{1\to2} & -\gamma_{2\to1} \end{pmatrix}$. Unlike the adjacency matrix A, all the column sums of the generator Γ equal zero.

The statement is proven by showing that a state $i \in \{1, \ldots, N\}$ is reachable from another state $j \in \{1, \ldots, N\}$ in $k_{ij} \in \mathbb{N}$ steps if and only if $\left(A^{k_{ij}}\right)_{ij} > 0$, which can be proven by induction.

Below, we will make use of a modified version of this result: we define $\tilde{A} := A + \mathcal{I}$, which is the adjacency matrix of the directed graph $\tilde{\Omega}$ that is obtained by adding a self-loop to every state

of Ω. Then $\tilde{\Omega}$ (and therefore also Ω) is strongly connected if and only if $\tilde{A}$ is irreducible. But when $\tilde{\Omega}$ is strongly connected and every state has a self-loop, then there exists a natural number $k \in \mathbb{N}$ such that there is a path of length $n \in \mathbb{N}$ from state j to state i for all $n \geqslant k$. Hence, we can choose k (defined at the beginning of section 4.1) to be independent of i and j. In particular, when Ω is strongly connected the matrix power of the adjacency matrix $\tilde{A}^k = (\mathcal{I} + A)^k$ has strictly positive entries when k is large enough.

This does not necessarily apply to the adjacency matrix A, as is obvious from the example of figure 3 with $A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Here, the sequence $(A^m)_{m\in\mathbb{N}}$ of matrix powers of A oscillates between the two matrices $A^{2m} = \mathcal{I}$ and $A^{2m+1} = A$.

4.2. When Ω is strongly connected, then for times $t > 0$ all entries of the solution operator $\mathrm{e}^{\Gamma t}$ are strictly positive, that is $\left(\mathrm{e}^{\Gamma t}\right)_{ij} > 0$, for all $i, j \in \{1, \ldots, N\}$, where Γ is the corresponding generator of the network Ω

We know the following two statements to be true:

Firstly, since Ω is strongly connected, the entries of $(\mathcal{I} + \mathrm{Adj}(\Omega))^n$ are strictly positive when n is large enough.

Secondly, the entry of $(\mathcal{I} + \mathrm{Adj}(\Omega))_{ij}$ is strictly positive if and only if the entry of

$$\left(\mathcal{I} + \frac{\Gamma t}{n}\right)_{ij} \overset{(2)}{=\!=} \begin{cases} 1 - \dfrac{t}{n}\displaystyle\sum_{\substack{m=1 \\ m\neq j}}^{N} \gamma_{j\to m}, & \text{if } i = j \\ \dfrac{t}{n}\gamma_{j\to i}, & \text{if } i \neq j, \end{cases}$$

is strictly positive for large enough n.

Hence, the entries of $\left(\mathcal{I} + \frac{\Gamma t}{n}\right)^n$ are strictly positive when n is large enough.

Since by section A.3 in the appendix A the sequence $\left(\left[\left(\mathcal{I} + \frac{\Gamma t}{n}\right)^n\right]_{ij}\right)_{n\in\mathbb{N}}$ has a strictly positive lower bound for all $i, j \in \{1, \ldots, N\}$, we conclude that the components of the solution operator $\left(\mathrm{e}^{\Gamma t}\right)_{ij} := \lim_{n\to\infty}\left[\left(\mathcal{I} + \frac{\Gamma t}{n}\right)^n\right]_{ij}$ are strictly positive.

The ijth entry of $\left(\mathrm{e}^{\Gamma t}\right)$ can be interpreted as the probability for being in state i after the time $t > 0$, provided that the system was in state j at time $t = 0$. So when all entries of the matrix $\left(\mathrm{e}^{\Gamma t}\right)$ are strictly positive, after an arbitrary small time $t > 0$ every state has a non-zero probability (probability vectors $\mathbf{p}_t$ are strictly positive), independent of the initial condition.

4.3. When Ω is strongly connected, then Ω is relaxing and all components of the unique steady state are strictly positive, $\mathbf{p}_\infty \in (\mathbb{R}_{>0})^N$. In this case, the network Ω is called ergodic [4–6]

Proof. Let $\mathbf{v}$ be an eigenvector of Γ to a real eigenvalue $\lambda \in \mathbb{R}$, that is $\Gamma\mathbf{v} = \lambda\mathbf{v}$. Then we have

$$\mathrm{e}^{\lambda t}\|\mathbf{v}\|_1 = \|\mathrm{e}^{\lambda t}\mathbf{v}\|_1 = \|\mathrm{e}^{\Gamma t}\mathbf{v}\|_1 = \sum_{i=1}^{N}\left|\sum_{j=1}^{N}\left(\mathrm{e}^{\Gamma t}\right)_{ij} v_j\right| \overset{(*)}{\leq} \sum_{i,j=1}^{N}\underbrace{\left|\left(\mathrm{e}^{\Gamma t}\right)_{ij}\right|}_{\geq 0}\cdot|v_j| = \sum_{j=1}^{N}|v_j|\underbrace{\left(\sum_{i=1}^{N}\left(\mathrm{e}^{\Gamma t}\right)_{ij}\right)}_{=1} = \|\mathbf{v}\|_1.$$

The identity $\sum_{i=1}^{N}\left(\mathrm{e}^{\Gamma t}\right)_{ij} = 1$ was obtained above (see: equation (4)). Now, let $\mathbf{v} \in \ker(\Gamma)$, which implies $\lambda = 0$ and we have equality in the above estimation. But on the other hand, we

have equality in (*) if and only if

$$\left(\left(\mathrm{e}^{\Gamma t}\right)_{i1} v_1, \ldots, \left(\mathrm{e}^{\Gamma t}\right)_{iN} v_N\right) \in \left(\mathbb{R}_{\geqslant 0}\right)^N \cup \left(\mathbb{R}_{\leqslant 0}\right)^N, \tag{11}$$

that is, when the vector on the right-hand side of equation (11) has either only non-negative or non-positive entries.

Since we assumed that Ω is strongly connected, we know from the previous subsection that the solution operator $\mathrm{e}^{\Gamma t}$ has only strictly positive entries, so from equation (11) follows that $\begin{pmatrix} v_1 \\ \vdots \\ v_N \end{pmatrix} = \mathbf{v} \in \left(\mathbb{R}_{\geqslant 0}\right)^N \cup \left(\mathbb{R}_{\leqslant 0}\right)^N$.

This means that $\ker(\Gamma) \subseteq \left(\mathbb{R}_{\geqslant 0}\right)^N \cup \left(\mathbb{R}_{\leqslant 0}\right)^N$. But a vector space that contains only vectors where all entries have the same sign must be one-dimensional. If it were more than one-dimensional, one could create a vector with positive and negative entries by building a suitable linear combination of the two basis vectors.

This proves that Ω is relaxing. It remains to be shown that the states have strictly positive entries.

So let $\mathbf{p}_\infty \in \ker(\Gamma) \cap \left(\mathbb{R}_{\geqslant 0}\right)^N$ be the unique steady state, with non-negative entries and $\|\mathbf{p}_\infty\| = 1$. Then $\mathbf{p}_\infty$ has only strictly positive components since we have equality in (12) if and only if all components of $\mathbf{p}_\infty$ are zero:

$$p_\infty^{(i)} = \frac{\sum_{\substack{j=1,\\ j\neq i}}^{N} p_\infty^{(j)} \gamma_{j\to i}}{\sum_{\substack{j=1,\\ j\neq i}}^{N} \gamma_{i\to j}} \geqslant 0. \tag{12}$$

□

5. Statement of the main theorem and its proof

The theorem that we will prove in the following states:

The master equation (2) of a network Ω is relaxing if and only if there is exactly one minimal absorbing set.

We prove the forward direction by contraposition. Suppose there exists two distinct minimal absorbing subsets $B_1, B_2 \subseteq \Omega$. Then Ω cannot be relaxing since the stationary state will lie in B_1 (B_2) when the initial condition is in B_1 (B_2), that is $\mathbf{p}_0 \in B_{1,2} \Longrightarrow \mathbf{p}_\infty \in B_{1,2}$.

For the backward direction, we start from the assumption that there is exactly one minimal absorbing set B_1. We show that Ω is relaxing by proving $\dim\ker(\Gamma) = 1$. We write Γ in the form (9),

$$\Gamma = \begin{pmatrix} \Gamma_{B_0} & 0 \\ \Gamma_{B_0\to B_1} & \Gamma_{B_1} \end{pmatrix}.$$

Let $\mathbf{v}^* = \begin{pmatrix} \mathbf{u}^* \\ \mathbf{w}^* \end{pmatrix} \in \ker(\Gamma)$ with $\mathbf{u}^* \in \mathbb{R}^M$ and $\mathbf{w}^* \in \mathbb{R}^{(N-M)}$. Then we have

$$0 \stackrel{!}{=} \Gamma \boldsymbol{v}^* = \begin{pmatrix} \Gamma_{B_0} & 0 \\ \Gamma_{B_0\to B_1} & \Gamma_{B_1} \end{pmatrix} \begin{pmatrix} \mathbf{u}^* \\ \boldsymbol{w}^* \end{pmatrix} = \begin{pmatrix} \Gamma_{B_0}\mathbf{u}^* \\ \Gamma_{B_0\to B_1}\mathbf{u}^* + \Gamma_{B_1}\boldsymbol{w}^* \end{pmatrix}. \tag{13}$$

Since we know from section 3.8 that Γ_{B_0} is invertible, we have $\mathbf{u}^* = \mathbf{0}$ and $\mathbf{v}^* = \begin{pmatrix} 0 \\ \mathbf{w}^* \end{pmatrix}$. But $\mathbf{w}^*$ must lie in the kernel of Γ_{B_1}, which is one-dimensional, since B_1 is strongly connected (see: section 4.3). This means that $\dim \ker(\Gamma) = \dim \ker(\Gamma_{B_1}) = 1$ which completes the proof.

6. Generalized main theorem: the number of minimal absorbing sets equals the dimension of the kernel of Γ

Proof. Let $\mathcal{B} = \{B_1, \ldots, B_n\}$, $n \leqslant N$ be the set of minimal absorbing sets and let Γ be of the form (9), that is

$$\Gamma = \begin{pmatrix} \Gamma_{B_0} & 0^{M\times|B_1|} & \cdots & 0^{M\times|B_n|} \\ \Gamma_{B_0\to B_1} & \Gamma_{B_1} & & 0^{|B_1|\times|B_n|} \\ \vdots & & \ddots & \\ \Gamma_{B_0\to B_n} & 0^{|B_n|\times|B_1|} & & \Gamma_{B_n} \end{pmatrix}. \tag{14}$$

Let $\mathbf{q}_i \in \ker(\Gamma_{B_i}) \cap (\mathbb{R}_{>0})^{|B_i|}$ with $\|\mathbf{q}_i\|_1 = 1$ for all $i \in \{1, \ldots, n\}$. We know from section 3.5 that all B_i are strongly connected and from section 4.3 that all $\mathbf{q}_i$ are well defined and uniquely determined.

Further, define $\mathbf{p}_i := (0_M, 0_{|B_1|}, \ldots, \mathbf{q}_i, \ldots, 0_{|B_n|})^{\mathrm{T}}$ and note that the vectors $\{\mathbf{p}_i : i \in \{1, \ldots, n\}\}$ are linearly independent. Then we have

$$\Gamma\mathbf{p}_i = \begin{pmatrix} 0 \\ \Gamma_{B_i}\mathbf{q}_i \\ 0 \end{pmatrix} = 0_N \tag{15}$$

and hence $\operatorname{span}\left(\{\mathbf{p}_i : i \in \{1, \ldots, n\}\}\right) \subseteq \ker(\Gamma)$.

On the other hand, let $\mathbf{v} \in \ker(\Gamma)$ be an arbitrary element of the kernel of Γ. We write $\mathbf{v}$ as

$$\mathbf{v} = (\mathbf{u}_0, \mathbf{w}_1, \ldots, \mathbf{w}_n) \in \mathbb{R}^M \times \mathbb{R}^{|B_1|} \times \cdots \times \mathbb{R}^{|B_n|}. \tag{16}$$

Then we know that

$$0_N \overset{v\in\ker(\Gamma)}{=\!=} \Gamma\mathbf{v} = \begin{pmatrix} \Gamma_{B_0}\mathbf{u}_0 \\ \Gamma_{B_0\to B_1}\mathbf{u}_0 + \Gamma_{B_1}\mathbf{w}_1 \\ \vdots \\ \Gamma_{B_0\to B_n}\mathbf{u}_0 + \Gamma_{B_n}\mathbf{w}_n \end{pmatrix} = \begin{pmatrix} 0_M \\ \Gamma_{B_1}\mathbf{w}_1 \\ \vdots \\ \Gamma_{B_n}\mathbf{w}_n \end{pmatrix}. \tag{17}$$

The last equality holds because Γ_{B_0} is invertible. Moreover, since $\dim \ker(\Gamma_{B_i}) = 1$ for all $i \in \{1, \ldots, n\}$ we conclude that $\mathbf{u}_0 = \mathbf{0}_M$ and $\mathbf{w}_i \in \ker(\Gamma_{B_i}) = \operatorname{span}(\mathbf{q}_i)$, that is $\mathbf{w}_i = \lambda_i\mathbf{q}_i$, for some $\lambda \in \mathbb{R}$.

It then follows that

$$\mathbf{v} = \begin{pmatrix} 0_M \\ \lambda_1 \mathbf{q}_1 \\ \vdots \\ \lambda_n \mathbf{q}_n \end{pmatrix} = \sum_{i=1}^{n} \lambda_i \mathbf{p}_i, \quad \text{and hence} \tag{18}$$

$$\ker(\Gamma) \subseteq \operatorname{span}\left(\{\mathbf{p}_i : i \in \{1, \ldots, n\}\}\right).$$

□

This means that we can construct a basis of steady states from the set of minimal absorbing sets, with every basis vector corresponding to exactly one minimal absorbing set.

For the example given in figure 2, the basis vectors are

$$\mathbf{p}_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \mathbf{p}_2 = \frac{1}{\gamma_{4\to5} + \gamma_{5\to4}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ \gamma_{5\to4} \\ \gamma_{4\to5} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \mathbf{p}_3 = \frac{1}{\gamma_{7\to8}\gamma_{8\to6} + \gamma_{8\to6}\gamma_{6\to7} + \gamma_{6\to7}\gamma_{7\to8}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \gamma_{7\to8}\gamma_{8\to6} \\ \gamma_{8\to6}\gamma_{6\to7} \\ \gamma_{6\to7}\gamma_{7\to8} \end{pmatrix}. \tag{19}$$

7. Discussion and conclusions

We have shown that the information about the number of linearly independent steady states of a finite-size master equation is encoded in the directed network of transitions: there is a one-to-one correspondence between minimal absorbing sets and basis vectors of the kernel of the generator that span the space of steady states. In particular, the dimension of the space of steady states equals the number of minimal absorbing sets. Moreover, for every minimal absorbing set $B_i \subseteq \Omega$ we can construct a normalized basis vector $\mathbf{p}_i \in \left(\mathbb{R}_{\geqslant 0}\right)^N \cap \ker(\Gamma)$ according to equation (29) in appendix A.4, where the strictly positive entries correspond to the states lying in the minimal absorbing set B_i.

The questions remains how to proceed in practice. Given a system $\mathcal{S} = (\Omega, \mathcal{E})$ composed of a finite number of states Ω and transition rates $\mathcal{E}$, how does one determine whether this system is relaxing and, if not, how many steady states there are?

The standard way would be to determine the dimension and the span of the kernel of Γ, which can be done in $\mathcal{O}(|\Omega|^3)$ steps. The alternative, however, is to search for the strongly connected components, which is possible in $\mathcal{O}(|\Omega| + |\mathcal{E}|)$ steps, and merge each of these strongly connected components into a single 'macrostate', see figure 4 where this is done for the example from figure 2.

Every absorbing macrostate in the resulting coarse-grained network is a minimal absorbing set in the original network. Their number determines whether Ω is relaxing or not.

In order to find a basis of vectors spanning the space of steady states, it suffices now to determine the steady state $\mathbf{p}_i$ for each minimal absorbing set B_i, based on equation (29) in the appendix A.

The stationary state $\mathbf{p}_\infty$ for the whole network Ω when starting from the initial state $\mathbf{p}_0$ is the projection of $\mathbf{p}_0$ onto the span of the steady states of the minimal absorbing sets $\mathbf{p}_i$.

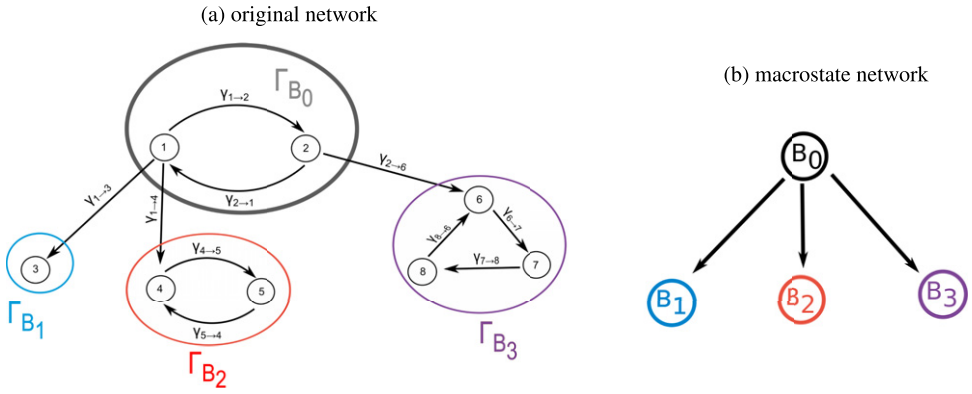

Figure 4. Merging of the strongly connected components of a network into 'macrostates'.

Writing the initial state as

$$\mathbf{p}_0 = \sum_{i=1}^{n} \mu_i \mathbf{p}_i + \sum_{i=n+1}^{N} \mu_i \boldsymbol{h}^{(i)}_{\lambda\neq 0}, \tag{20}$$

(with $\boldsymbol{h}_{\lambda\neq 0,i}$ being the generalized eigenvectors (see equation (5) and appendix A.5) then $\mathbf{p}_\infty$ is given by

$$\mathbf{p}_\infty \overset{\text{(A.5)}}{=\!=} S \begin{pmatrix} \mathcal{I}_n & 0^{n\times(N-n)} \\ 0^{(N-n)\times n} & 0^{(N-n)\times(N-n)} \end{pmatrix} S^{-1}\mathbf{p}_0 = \sum_{i=1}^{n} \mu_i \mathbf{p}_i, \tag{21}$$

where the columns of the matrix S are the generalized eigenvectors of the transition matrix Γ (see equation (31) in appendix A.5 for a formal definition.)

The proof provided in this paper is based on the assumption that the state space is finite. The theorems that served as templates for our proof, such as the Perron–Frobenius theorem [9]), have no version for the infinite-dimensional case. There are, however, good reasons to assume that the results are valid also for some models with an infinite state space.

There are systems which show the same behavior (qualitative and approximately quantitative) as a reduced system $\Omega_{<\infty} \subsetneq \Omega_\infty$ with a finite state space, for which the above considerations hold. Examples are systems with a finite number of minimal absorbing sets for each connected component and chemical reaction systems where unusually large numbers of molecules are extremely unlikely. For these systems, we expect that given an initial state $\mathbf{p}_0$ and an $\epsilon > 0$, it is possible to choose a finite sub-system $\Omega_{<\infty}$ of Ω_∞ such that the apart from an arbitrary small probability mass ϵ dynamics takes places in the finite sub-system.

Acknowledgments

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Data availability statement

No new data were created or analysed in this study.

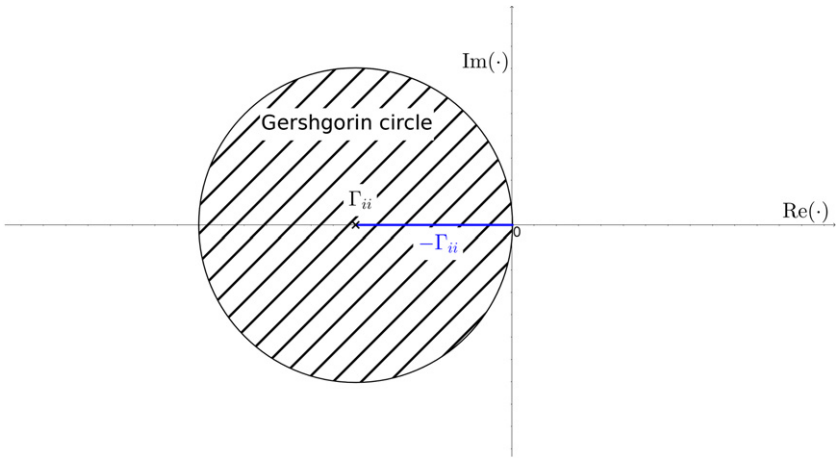

Figure 5. The union of all Gershgorin circles containing all eigenvalues of Γ. Hence $\mathrm{Re}(\sigma(\Gamma)) \subseteq \mathbb{R}_{\leqslant 0}$ and $\sigma(\Gamma) \cap (i\mathbb{R}) = \{0\}$.

Appendix A

A.1. Gershgorin circle theorem and consequences for the eigenvalues of Γ

Let $\mathcal{B}(z, r) := \{x \in \mathbb{C} : |z - x| \leqslant r\}$ denote the closed ball around the complex number z with radius $r > 0$. For an $N \times N$ complex matrix ($N \in \mathbb{N}$), the spectrum $\sigma(A)$ of A (that is the set of all eigenvalues of A) lies within the union of all Gershgorin circles:

$$\sigma(A) \subseteq \bigcup_{i=1}^{N} \mathcal{B}\left(A_{ii}, \sum_{\substack{j=1,\\ j\neq i}}^{N} |A_{ji}|\right)$$

Proof. Let $\mathbf{v}$ be an eigenvector of the matrix $A \in \mathbb{C}^{N\times N}$ to the eigenvalue λ, that is $A\mathbf{v} = \lambda\mathbf{v}$. We can choose that for some component $i \in \{1, \ldots, N\}$ the corresponding entry in the eigenvector equals one, $v_i = 1$, and for all other components $j \in \{1, \ldots, N\}$ we have $|v_j| \leqslant 1$. Now we make the following estimation:

$$\lambda = \lambda \underbrace{v_i}_{1} = (\lambda\mathbf{v})_i = (A\mathbf{v})_i = \sum_{\substack{j=1,\\ j\neq i}}^{N} A_{ij}v_j + A_{ii}\underbrace{v_i}_{1}$$

$$\Longrightarrow |\lambda - A_{ii}| = \left|\sum_{\substack{j=1,\\ j\neq i}}^{N} A_{ij}v_j\right| \leqslant \sum_{\substack{j=1,\\ j\neq i}}^{N} |A_{ij}| \cdot \underbrace{|v_j|}_{\leqslant 1} \leqslant \sum_{\substack{j=1,\\ j\neq i}}^{N} |A_{ij}|$$

□

When we apply the Gershgorin circle theorem to the transition matrix Γ, we get the following result:

Γ has only eigenvalues with a non-positive real part $\left(\mathrm{Re}\,(\sigma(\Gamma)) \subseteq \mathbb{R}_{\leqslant 0}\right)$ and $\lambda = 0$ is the only eigenvalue of Γ where the real part equals zero $\left(\sigma(\Gamma) \cap (i\mathbb{R}) = \{0\}\right)$.

This follows directly from figure 5 and the fact that $-\Gamma_{ii} = \sum_{\substack{j=1,\\ j\neq i}}^{N} |\Gamma_{ji}|$ for all $i \in \{1,\dots,N\}$: the origin is the only point in the intersection of the Gershgorin circle and the half-space $\{z \in \mathbb{C} | \mathrm{Re}(z) \geqslant 0\}$.

A.2. WCDD matrices are non-singular

Proof. The fact that SDD matrices are non-singular follows from Gershgorin's circle theorem [9] (for a proof, see appendix A.1).

Now let A be WCDD and assume that A is singular. Let $\boldsymbol{x} \in \mathrm{kern}(A)$, w.l.o.g. assume that there is an $i \in \{1,\dots,N\}$ such that $1 = |x_i| \geqslant |x_k| \forall k \in \{1,\dots,N\}, k \neq i$. Then we have

$$0 = (A\boldsymbol{x})_i = \sum_{\substack{k=1,\\ k\neq i}}^{N} A_{ik}x_k + A_{ii}x_i \Longrightarrow -A_{ii}x_i = \sum_{\substack{k=1,\\ k\neq i}}^{N} A_{ik}x_k \tag{22}$$

$$\begin{aligned} \Longrightarrow |A_{ii}| = |-A_{ii}x_i| &\overset{(26)}{=} \left| \sum_{\substack{k=1,\\ k\neq i}}^{N} A_{ik}x_k \right| \\ &\leqslant \sum_{\substack{k=1,\\ k\neq i}}^{N} |A_{ik}| \underbrace{|x_k|}_{\leqslant 1} \overset{(*)}{\leqslant} \sum_{\substack{k=1,\\ k\neq i}}^{N} |A_{ik}| \overset{A\ldots\mathrm{WDD}}{\leqslant} |A_{ii}|. \end{aligned} \tag{23}$$

Hence, in line (23) we have equality everywhere. In particular:

(a) The last equality tells us that the i-the row is not SDD.
(b) Equality in $(*)$ means that whenever $A_{ik} \neq 0 \Longrightarrow |x_k| = 1$.

Since A is WCDD we know there exists a path $i = i_0 \to i_1 \to \cdots \to i_k = j$ to the SDD row number j. In particular, we have $A_{i_0,i_1} \neq 0 \overset{(b)}{\Rightarrow} |x_{i_1}| = 1$. Repeating the argument from the beginning, we get from (a) that the i_1th row is not SDD. When we keep iterating, we finally get, that the jth row is not SDD which is a contradiction. □

A.3. When Ω is strongly connected, the sequence $\left(\left[\left(\mathcal{I} + \frac{\Gamma t}{n}\right)^n\right]_{ij}\right)_{n\in\mathbb{N}}$ has a strictly positive lower bound

Proof. Define

$$\begin{aligned} \Gamma_{\min} &\coloneqq \min\{\Gamma_{ll} : l \in \{1,\dots,N\}\} < 0 \\ d &\coloneqq \text{length of the shortest path from } j \text{ to } i \\ \gamma^{(j\to i)} &\coloneqq \begin{cases} 1, & \text{if } j = i \\ \min\left\{ \prod_{l=1}^{d} \gamma_{m_l \to m_{l+1}} : (m_1,\dots,m_d) \in \{1,\dots,N\}^d, m_1 = j, m_d = i, \gamma_{m_l\to m_{l+1}} \neq 0 \right\}, & \text{if } j \neq i \end{cases} \end{aligned} \tag{24}$$

The interpretation of $\gamma^{(j\to i)}$ is the following: for all path ($j = m_i \to \cdots \to m_k = i$) of length $d \in \mathbb{N}$ from state j to state i, multiply the rates $\gamma_{m_l \to m_{l+1}}$ of the edges that constitute the path and take the minimum over all paths.

Then we can make the following estimate:

$$\left(\mathrm{e}^{\Gamma t}\right)_{ij} = \lim_{n\to\infty}\left(\left(\mathcal{I}+\frac{\Gamma t}{n}\right)^n\right)_{ij} = \lim_{n\to\infty}\sum_{k_1=1}^{N}\cdots\sum_{k_{n-1}=1}^{N}\left(\mathcal{I}+\frac{\Gamma t}{n}\right)_{i,k_1}\cdots\left(\mathcal{I}+\frac{\Gamma t}{n}\right)_{k_{n-1},j} \geq$$
$$\overset{(*)}{\geq} \lim_{n\to\infty}\underbrace{\frac{n!}{(n-d)!\,n^d}}_{\xrightarrow{n\to\infty}1}\frac{\gamma^{(j\to i)}\,t^d}{d!}\underbrace{\left(1+\frac{\Gamma_{min}\,t}{n}\right)^{n-d}}_{\xrightarrow{n\to\infty}\mathrm{e}^{\Gamma_{min}\,t}} = \frac{\gamma^{(j\to i)}\,t^d}{d!}\,\mathrm{e}^{\Gamma_{min}\,t} > 0, \tag{25}$$

where we used in (*) the following calculation:

$$\begin{aligned}
&\sum_{k_1=1}^{N}\cdots\sum_{k_{n-1}=1}^{N}\left(\mathcal{I}+\frac{\Gamma t}{n}\right)_{i,k_1}\cdots\left(\mathcal{I}+\frac{\Gamma t}{n}\right)_{k_{n-1},j} \\
&\quad\geqslant \binom{n}{d}\underbrace{\left(\frac{\gamma_{j\to m_2}t}{n}\right)\cdots\left(\frac{\gamma_{m_{d-1}\to i}t}{n}\right)}_{d\text{ times}}\underbrace{\left(1+\frac{\Gamma_{\square\square}t}{n}\right)\cdots\left(1+\frac{\Gamma_{\square\square}t}{n}\right)}_{n-d\text{ times}} \\
&\quad\geqslant \frac{n!}{(n-d)!n^d}\frac{\gamma^{(j\to i)}t^d}{d!}\left(1+\frac{\Gamma_{\min}t}{n}\right)^{n-d}
\end{aligned} \tag{26}$$

□

A.4. Explicit expression for the stationary state of a strongly connected network

In the following, we derive an analytical expression for the stationary state in the case that the network is strongly connected. In this case, the kernel of the generator is one-dimensional (see: section 4.3) and $\mathbf{p}_\infty \in \ker(\Gamma) \cap (\mathbb{R}_{>0})^N$ has strictly positive entries and is uniquely determined by $\|\mathbf{p}_\infty\|_1 = 1$.

A detailed proof can be found in [12, 13]. The original statement was first formulated in 1948 by Tutte [14].

We denote with $[A]_{ij}$ the first *minor* of the matrix A, that is the determinant of the matrix that results from a matrix $A \in \mathbb{C}^{N\times N}$ by deleting row number i and column number j (for a general definition of minors, see appendix A.7). With this notation, the **adjugate** of the matrix A is defined as

$$\mathrm{adj}(A) := \left((-1)^{j+i}[A]_{ji}\right)_{i,j\in\{1,\ldots,N\}} = \begin{pmatrix} (-1)^{1+1}[A]_{11} & \ldots & (-1)^{N+1}[A]_{N1} \\ \vdots & & \vdots \\ (-1)^{1+N}[A]_{1N} & \ldots & (-1)^{N+N}[A]_{NN} \end{pmatrix}, \tag{27}$$

with the property $A\,\mathrm{adj}(A) = \det(A)\mathcal{I}_N = \mathrm{adj}(A)A$.

Since the transition matrix Γ is singular, we have

$$0^{N\times N} = \underbrace{\det(\Gamma)}_{0}\mathcal{I}_N = \Gamma\,\mathrm{adj}(\Gamma). \tag{28}$$

This means that all columns of the adjugate must lie in the kernel of Γ and are therefore proportional to $\mathbf{p}_\infty$. Hence we have for all $j \in \{1, \ldots, N\}$

$$\mathbf{p}_\infty \overset{(28)}{\propto} \operatorname{adj}(\Gamma)\boldsymbol{e}_j = \left(\underbrace{\operatorname{adj}(\Gamma)_{ij}}_{(-1)^{i+j}[\Gamma]_{ji}} \right)_{i\in\{1,\ldots,N\}} \overset{(27)}{=\!=} (-1)^{i+j} \left(\underbrace{[\Gamma]_{ji}}_{(-1)^{i+j}[\Gamma]_{ii}} \right)_{i\in\{1,\ldots,N\}} \overset{\text{A.7}}{=\!=} \begin{pmatrix} [\Gamma]_{11} \\ \vdots \\ [\Gamma]_{NN} \end{pmatrix}, \tag{29}$$

where we used the fact that the first minors $[\Gamma]_{ji}$ of the transition matrix Γ are connected to the first principal minors $[\Gamma]_{ii}$ via $[\Gamma]_{ji} = (-1)^{i+j}[\Gamma]_{ii}$. This applies to all matrices whose columns sum up to zero and is proven in appendix A.8 below.

The calculation of the principal minors can be done efficiently via in-trees, as derived in appendix A.7 below. This gives the expression

$$\mathbf{p}_\infty \overset{(\text{A.7})}{=\!=} \begin{pmatrix} \sum_{T\in\Theta_1(\Omega)} \prod_{(i,j)\in\mathcal{E}(T)} \gamma_{i\to j} \\ \vdots \\ \sum_{T\in\Theta_N(\Omega)} \prod_{(i,j)\in\mathcal{E}(T)} \gamma_{i\to j} \end{pmatrix}. \tag{30}$$

For the kth component of that vector one has to consider the in-trees T (defined in appendix A.7) rooted in state number k and spanning the whole network Ω. For each such in-tree one multiplies the rates associated with all edges $\mathcal{E}(T)$ and then performs the sum over all in-trees. An illustration of this procedure is given in figure 6.

It is possible to find all in-trees in $\mathcal{O}\left(N + |\mathcal{E}| + |\mathcal{E}| \cdot n\right)$ number of steps [15], where N is the number of states, $|\mathcal{E}|$ the number of edges and n the number of minimal absorbing sets.

As a special case, we consider the microcanonical ensemble of statistical physics [2] where the rates for a transition and the corresponding reverse transition are identical, $\gamma_{i\to j} = \gamma_{j\to i}$ for all $i, j \in \{1, \ldots, N\}$. From equation (29) follows that the stationary probability for each state is the same, i.e. $\mathbf{p}_\infty = \frac{1}{|\Omega|}(1, \ldots, 1)^{\mathrm{T}}$: for every in-tree rooted at a state $i \in \Omega$, it is possible to construct an in-tree rooted at any other state $j \in \Omega$ by inverting the direction of the transitions. The overall product $\prod_{(i,j)\in\mathcal{E}(T))} \gamma_{i\to j}$ stays the same since the rates for forward and backward transitions are symmetric as is the number of in-trees for each state.

A.5. Explicit expression for the stationary state of an arbitrary network

This section provides some details for deriving the explicit expression for the stationary solution given in equation (21) in section 7. We choose a basis $\left(\boldsymbol{h}_\lambda^{(i)}\right)_{i\in\{1,\ldots,N\}}$ of generalized eigenvectors of the transition matrix Γ such that the first n basis vectors $\mathbf{p}_1, \ldots, \mathbf{p}_n$, are given

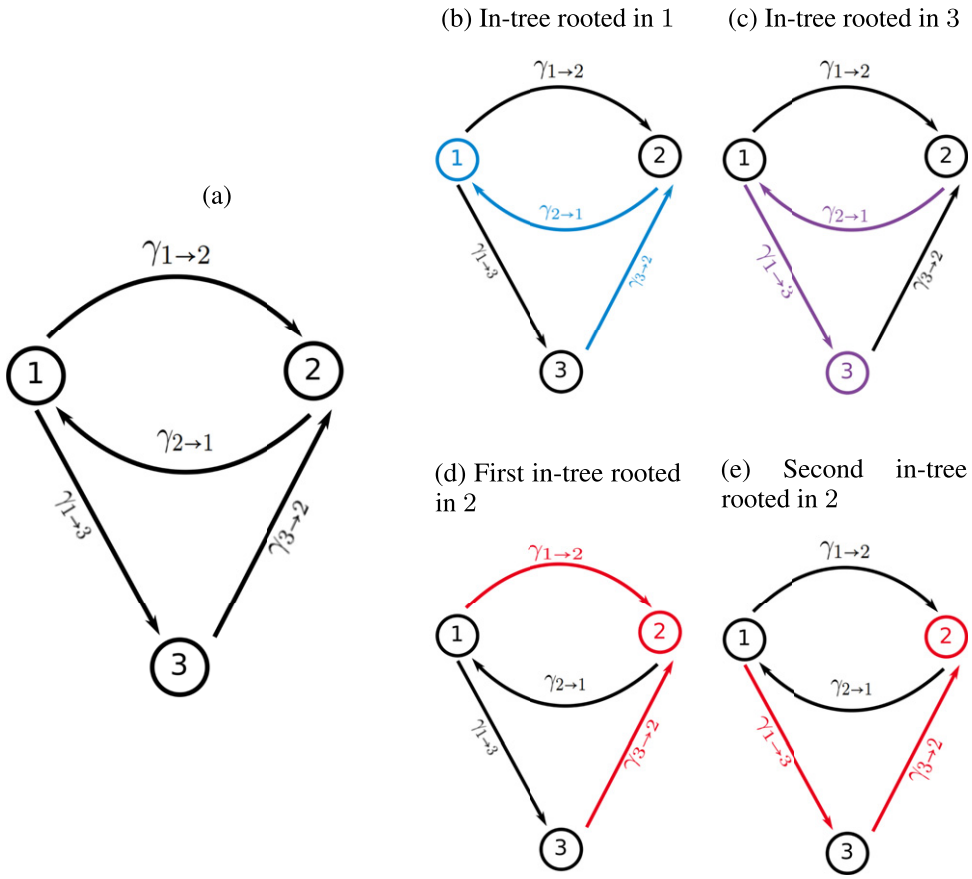

Figure 6. Example of a strongly connected network (a) together with the corresponding in-trees rooted in states number 1 (Figure 6b) and 3 (Figure 6c), and the two in-trees rooted in state number 2 (Figure 6d and 6e). The kernel of Γ is the span of a vector whose ith component is the sum over all in-trees rooted in state number i of the product of the rates of all edges that constitute that particular in-tree. In this example we have:

$$\text{kern}\,(\Gamma) = \text{span}\left\{\begin{pmatrix} \gamma_{3\to2}\cdot\gamma_{2\to1} \\ \gamma_{1\to2}\cdot\gamma_{3\to2} + \gamma_{1\to3}\cdot\gamma_{3\to2} \\ \gamma_{2\to1}\cdot\gamma_{1\to3} \end{pmatrix}\right\}$$

by formula (29), that is $\mathbf{p}_1, \ldots, \mathbf{p}_n$ are forming an (orthogonal) basis of the kernel of Γ with $\mathbf{p}_i \in (\mathbb{R}_{>0})^N$ and $\|\mathbf{p}_i\|_1 = 1$.

Further, let this ordered basis define the columns of the matrix S, where the first n column are $\mathbf{p}_1, \ldots, \mathbf{p}_n$:

$$S := \left(\underbrace{\boldsymbol{h}^{(1)}_{\lambda=0}}_{\mathbf{p}_1}, \ldots, \underbrace{\boldsymbol{h}^{(n)}_{\lambda=0}}_{\mathbf{p}_1}, \boldsymbol{h}^{(n+1)}_{\lambda\neq0} \ldots, \boldsymbol{h}^{(N)}_{\lambda\neq0}\right) = \left(\mathbf{p}_1, \ldots, \mathbf{p}_n, \boldsymbol{h}^{(n+1)}_{\lambda\neq0} \ldots, \boldsymbol{h}^{(N)}_{\lambda\neq0}\right). \tag{31}$$

Writing the initial state $\mathbf{p}_0 = \sum_{i=1}^{N} \mu_i \boldsymbol{h}_\lambda^{(i)}$ as a linear combination of this basis, we can compute the stationary state $\mathbf{p}_\infty$ as follows:

$$\mathbf{p}_\infty = \lim_{t\to\infty} \mathrm{e}^{\Gamma t} \underbrace{\mathbf{p}_0}_{\sum_{i=1}^{N} \mu_i \boldsymbol{h}_\lambda^{(i)}} = \sum_{i=1}^{N} \mu_i \underbrace{\left(\lim_{t\to\infty} \mathrm{e}^{\Gamma t} \boldsymbol{h}_\lambda^{(i)} \right)}_{\delta_{\lambda,0} \boldsymbol{h}_{\lambda=0}^{(i)}} \overset{(*)}{=\!=} \sum_{i=1}^{n} \mu_i \underbrace{\boldsymbol{h}_{\lambda=0}^{(i)}}_{\mathbf{p}_i} = \sum_{i=1}^{n} \mu_i \mathbf{p}_i, \quad (32)$$

where we used in step $(*)$ the fact that the time evolution of a generalized eigenvector of rank $m \leqslant N$ can be explicitly computed to

$$\begin{aligned} \mathrm{e}^{\Gamma t} \boldsymbol{h}_{\lambda,m} &= \left(\mathrm{e}^{\lambda t} \sum_{k=1}^{m-1} \frac{(\Gamma - \lambda \mathcal{I})^k t^k}{k!} \right) \boldsymbol{h}_{\lambda,m} \xrightarrow{t\to\infty} \delta_{\lambda,0} \boldsymbol{h}_{\lambda=0} \\ &= \begin{cases} 0^{(N)} = \left(\overbrace{0, \ldots, 0}^{N \text{ times}} \right), & \text{if } \mathrm{Re}[\lambda] < 0 \\ \boldsymbol{h}_{\lambda=0} \coloneqq \boldsymbol{h}_{\lambda=0,m=1}, & \text{if } \mathrm{Re}[\lambda] = 0 \end{cases} \end{aligned}$$

when we keep in mind that in our case $\mathrm{Re}[\lambda] = 0 \Rightarrow \lambda = 0$.

By summing over all entries of the vectors on the left- and right-hand side of (31), we find that the coefficients μ_i for $i \in \{1, \ldots, n\}$ are positive and add up to one.

A.6. The algebraic multiplicity $a_{\lambda=0}$ for the eigenvalue $\lambda = 0$ of the transition matrix Γ equals the number of minimal absorbing sets

Proof. Let the characteristic polynomial of the matrix Γ be given by

$$\det(t\mathcal{I} - \Gamma) = t^N + \chi_1 t^{N-1} + \ldots + \chi_{N-m} t^m + \ldots \chi_{N-1} t^1 + \underbrace{\chi_N}_{0}. \quad (33)$$

We know from [10] that the absolute value of χ_{N-m} for $m \in \{1, \ldots, N-1\}$ is given by the sum over all principal minors of Γ of order m, namely

$$\begin{aligned} |\chi_{N-m}| &= \sum_{J \in \{J \in \mathcal{P}(\{1,\ldots,N\}) : |J| = m\}} [\Gamma]_{J,J} = \\ &\overset{(37)}{=\!=} \sum_{J \in \{J \in \mathcal{P}(\{1,\ldots,N\}) : |J| = m\}} \sum_{\dot{\bigcup}_{\alpha\in J} \Omega_\alpha = \Omega} \sum_{k \in J} \sum_{T_k \in \Theta_k(\Omega_k)} \prod_{(i,j) \in \bigcup_{l=1}^{m} \mathcal{E}(T_l)} \gamma_{i\to j}, \end{aligned} \quad (34)$$

where $\mathcal{P}(\{1, \ldots, N\})$ denotes the power set of $\{1, \ldots, N\}$. Since this sum consists of strictly positive summands, it can only be equal to zero if the index set is empty, which in this case means the network Ω cannot be decomposed into m in-trees. This can only be the case Ω consists of at least $m+1$ minimal absorbing sets.

When $a_{\lambda=0} \geqslant 1$ is the algebraic multiplicity of the eigenvalue $\lambda = 0$, we know that the last $a_{\lambda=0}$ coefficients of equation (33) must vanish, but the next one must not: $\chi_{N-k+1} = 0$ for all $k \in \{1, \ldots, a_{\lambda=0}\}$, but $\chi_{N-a_{\lambda=0}} \neq 0$.

So it is possible, to decompose the network Ω into $a_{\lambda=0}$ in-trees, but it is not possible, to decompose Ω into $a_{\lambda=0} - 1$ in-trees. This is only possible the network Ω has exactly $a_{\lambda=0}$ minimal absorbing sets. Figure 7 serves as an illustration of that argument. □

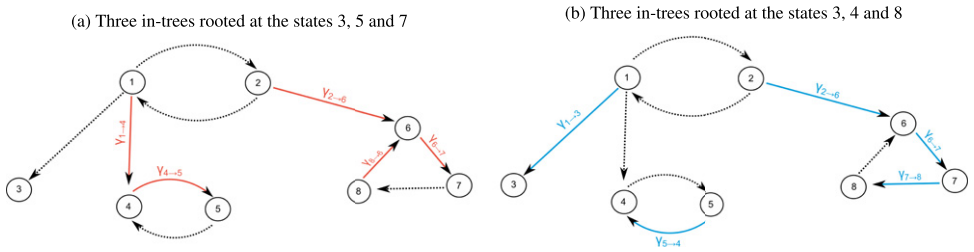

Figure 7. Example of two decomposition of the network Ω into three in-trees. Since Ω has three minimal absorbing sets, it is not possible to decompose it into less than three in-trees. $T_3 = (\Omega_3, \mathcal{E}_3) = \{\{3\}, \varnothing\}$, $T_5 = (\Omega_5, \mathcal{E}_5) = \{\{1,4,5\}, \{(1,4),(4,5)\}\}$, $T_7 = (\Omega_7, \mathcal{E}_7) = \{\{2,6,7,8\}, \{(2,6),(6,7),(8,6)\}\}$, $\prod_{(i,j)\in \bigcup_{l=1}^{3} \mathcal{E}(T_l)} \gamma_{i\to j} = \gamma_{1\to4}\,\gamma_{4\to5}\,\gamma_{2\to6}\,\gamma_{8\to6}\,\gamma_{6\to7}$ $T_3 = (\Omega_3, \mathcal{E}_3) = \{\{1,3\}, \{(1,3)\}\}$, $T_4 = (\Omega_4, \mathcal{E}_4) = \{\{4,5\}, \{(5,4)\}\}$, $T_8 = (\Omega_8, \mathcal{E}_8) = \{\{2,6,7,8\}, \{(2,6),(6,7),(7,8)\}\}$, $\prod_{(i,j)\in \bigcup_{l=1}^{3} \mathcal{E}(T_l)} \gamma_{i\to j} = \gamma_{1\to3}\,\gamma_{5\to4}\,\gamma_{2\to6}\,\gamma_{6\to7}\,\gamma_{7\to8}$

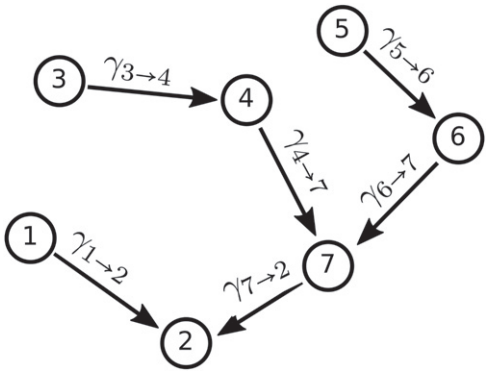

Figure 8. Example of an in-tree rooted at state number 2. There is a unique directed path from each state of the tree leading to state number 2. Its weight equals $\prod_{(i,j)\in\mathcal{E}(T)} \gamma_{i\to j} = \gamma_{1\to2}\gamma_{7\to2}\gamma_{7\to2}\gamma_{4\to7}\gamma_{6\to7}\gamma_{3\to4}\gamma_{5\to6}$.

Since we know from the theorem in section 6 that the number of minimal absorbing sets equals the dimension of the kernel of Γ, we can conclude that for the eigenvalue $\lambda = 0$ of Γ the algebraic multiplicity equals the geometric multiplicity and since all other eigenvalues of Γ have strictly negative real part, we can conclude that the solution of the master equation defined in equation (3) is bounded.

A.7. Calculation of the principal minors of the transition matrix via in-trees

We call a network Ω an **in-tree** (also called **anti-arborescence** [15]) **rooted at state $\omega_0 \in \Omega$** if for all states $\omega \in \Omega$ there is a unique directed path leading from state ω toward the root ω_0. An example is given in figure 8, where the root is state number 2. The *weight* of an in-tree is the product of the link-strength of all edges of the in-tree: $\prod_{(i,j)\in\mathcal{E}(T)} \gamma_{i\to j}$.

Further, we define

$$\Theta_m(\Omega) := \{T \subseteq \mathcal{S} : T \text{ is an } in-\text{tree of } \Omega \text{ root ed in state number } m\} \qquad (35)$$

to be the set of all in-tree of Ω that are rooted in state number $m \in \{1,\dots,N\}$.

A **minor** of a matrix is the determinant of a smaller submatrix:

Let $A \in \mathbb{C}^{M\times N}$ be a matrix and $I \subsetneqq \{1,\dots,M\}, J \subsetneqq \{1,\dots,N\}$ be subsets of the first M (N) natural numbers. We denote by $A_{I,J} \in \mathbb{C}^{M-|I|,N-|J|}$ the submatrix of A that is obtained by deleting all rows $i \in I$ and all columns $j \in J$ and set $[A]_{I,J}$ to be the determinant of $A_{I,J}$ $\left([A]_{I,J} := \det(A_{I,J})\right)$, provided that $A_{I,J}$ is a square matrix.

Example:

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix},$$
$$[A]_{2,3} := [A]_{\{2\},\{3\}} = \begin{vmatrix} a_{11} & a_{12} & \square \\ \square & \square & \square \\ a_{31} & a_{32} & \square \end{vmatrix} = \begin{vmatrix} a_{11} & a_{12} \\ a_{31} & a_{32} \end{vmatrix} = a_{11}a_{32} - a_{12}a_{31} \tag{36}$$

$[A]_{I,J}$ is called a **principal** minor if $I = J$. In the following we want to show that the principal minors of the (negative) transition matrix can be computed via sums of weights of in-trees, namely

$$[-\Gamma]_{J,J} = \sum_{\dot{\bigcup}_{\alpha\in J}\Omega_\alpha=\Omega} \sum_{k\in J} \sum_{T_k\in\Theta_k(\Omega_k)} \prod_{(i,j)\in\bigcup_{l=1}^{|J|}\mathcal{E}(T_l)} \gamma_{i\to j}, \tag{37}$$

where the first sum goes over all partitions of Ω into $|J|$ non-empty, disjoint sets such that $k \in \Omega_k$ for all $k \in J$.

Proof. We follow the proof given in [12]. First, a few definitions:

- We denote by $\mathcal{S}(\Omega\backslash J)$ the set of all permutations of the set $\Omega\backslash J$
- For a permutation $\pi \in \mathcal{S}(\Omega\backslash J)$, we set $\mathcal{F}_\pi := \{\omega \in \{1,\dots,k\} : \pi(\omega) = \omega\}$ to be the set of fixed points of π, $C_\pi := \{\text{cycles of}\pi\}$ the set of all cycles of the permutation π and $c_\pi := |C_\pi|$ the number of cycles of π
- Specific in the context of the network Ω, we set
  - $\Omega_\pi := (\Omega\backslash\mathcal{F}_\pi) :=$ the set of nodes in Ω for which the action of the permutation π is non-trivial
  - $\gamma_{C_\pi} := \prod_{\omega\in\Omega\backslash(J\cup\mathcal{F}_\pi)} \gamma_{\omega\to\pi(\omega)}$.

Consider for example the permutation $\pi = \left(\begin{array}{c|cccccccc} \omega & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \hline \pi(\omega) & 2 & 3 & 1 & 5 & 4 & 6 & 7 & 8 \end{array}\right) =$ (123) (45) for $\pi \in \mathcal{S}_8 = \mathcal{S}\left(\{1,2,\dots,8\}\right)$.

Here, $\mathcal{F}_\pi = \{6,7,8\}$, $C_\pi = \{(123),(45)\}$, $c_\pi = |C_\pi| = 2$ and $\gamma_{C_\pi} = \gamma_{1\to2}\gamma_{2\to3}\gamma_{3\to1}\gamma_{4\to5}\gamma_{5\to4}$.

According to the definition of the determinant, we have:

$$[-\Gamma]_{J,J} = \sum_{\pi\in\mathcal{S}(\Omega\backslash J)} \operatorname{sgn}(\pi) \prod_{\alpha\in\Omega\backslash J} (-\Gamma)_{\pi(\alpha),\alpha}. \tag{38}$$

We will tackle the expression in equation (38) by looking at the summands separately.

(a) π consists of only one cycle, that is $\pi = \begin{pmatrix} \omega_1 & \dots & \omega_k \\ \omega_2 & \dots & \omega_1 \end{pmatrix} =: (\omega_1, \dots, \omega_k)$. Then we have:

$$\begin{aligned}
&\underbrace{\operatorname{sgn}(\pi)}_{(-1)^{k-1}} \quad \underbrace{\prod_{\alpha\in\Omega\setminus J} (-\Gamma)_{\pi(\alpha),\alpha}}_{\prod_{i\in\mathcal{F}_\pi}(-\Gamma_{ii})\cdot \prod_{\beta\in\Omega\setminus(J\cup\mathcal{F}_\pi)}(-\Gamma_{\pi(\beta),\beta})} \\
&\quad = (-1)^{k-1} \prod_{i\in\mathcal{F}_\pi} \underbrace{(-\Gamma_{ii})}_{\sum_{j_i=1}^{N}\gamma_{i\to j_i}} \cdot \prod_{\beta\in\Omega\setminus(J\cup\mathcal{F}_\pi)} \underbrace{(-\Gamma_{\pi(\beta),\beta})}_{(-1)\gamma_{\beta\to\pi(\beta)}} \\
&\quad = (-1)^{k-1} \underbrace{\prod_{i\in\mathcal{F}_\pi}\sum_{j_i=1}^{N}\gamma_{i\to j_i}}_{\sum_{\boldsymbol{j}\in\{1,\dots,N\}^{|\mathcal{F}_\pi|}}\prod_{i\in\mathcal{F}_\pi}\gamma_{i\to j_i}} \cdot \underbrace{\prod_{\beta\in\Omega\setminus(J\cup\mathcal{F}_\pi)}(-1)\gamma_{\beta\to\pi(\beta)}}_{(-1)^k\gamma_{C_\pi}} \overset{|\Omega\setminus(J\cup\mathcal{F}_\pi)|=k}{=\!=\!=\!=\!=\!=\!=\!=} \\
&\quad = (-1)\cdot \sum_{\boldsymbol{j}\in\{1,\dots,N\}^{|\mathcal{F}_\pi|}} \gamma_{C_\pi} \prod_{i\in\mathcal{F}_\pi}\gamma_{i\to j_i}
\end{aligned} \tag{39}$$

(b) π consists of multiple cycles: $\pi = c_1 \dots c_{c_\pi}$, with $c_i = (\omega_1^{(i)}, \dots, \omega_{k_i}^{(i)})$. In this case, the same type of calculation as in (a) yields the result

$$\operatorname{sgn}(\pi)\prod_{\alpha\in\Omega\setminus J}(-\Gamma)_{\pi(\alpha),\alpha} = (-1)^{c_\pi}\cdot \sum_{\boldsymbol{j}\in\{1,\dots,N\}^{|\mathcal{F}_\pi|}} \gamma_{C_\pi}\prod_{i\in\mathcal{F}_\pi}\gamma_{i\to j_i}. \tag{40}$$

Then equation (38) can be reduced to

$$[-\Gamma]_{J,J} \overset{(40)}{=\!=} \sum_{\pi\in\mathcal{S}(\Omega\setminus J)} (-1)^{c_\pi}\cdot \sum_{\boldsymbol{j}\in\{1,\dots,N\}^{|\mathcal{F}_\pi|}} \underbrace{\gamma_{C_\pi}\prod_{i\in\mathcal{F}_\pi}\gamma_{i\to j_i}}_{\text{monomial}}. \tag{41}$$

We call a monomial a product of weights of $N - |J|$ different links, starting at $N - |J|$ different states.

Let c_M be the number of cycles in one monomial.

Note that $c_M \geqslant c_\pi$, since different permutation can result in the same product of links, due to the term $\prod_{i\in\mathcal{F}_\pi}\gamma_{i\to j_i}$.

Now, for a given monomial in equation (41) with at least one cycles ($c_M > 0$) there are $\binom{c_M}{k}$ possible permutation to construct γ_M, all with a sign of $(-1)^k$ for $k \in \{0, \dots, c_M\}$ (see figure 9 for a graphical illustration). But, since

$$\sum_{k=0}^{c_M}\binom{c_M}{k}(1)^{c_M-k}(-1)^k = (1-1)^{c_M} = 0, \tag{42}$$

only monomials without any cycles ($c_M = 0$) remain in the sum of equation (41), the rest cancel out. What remains are sums of products of $N - |J|$ links starting from all $N - |J|$ states of $\Omega\setminus J$ that do not contain any cycles. This means that you consider a partition of Ω into $|J|$ distinct

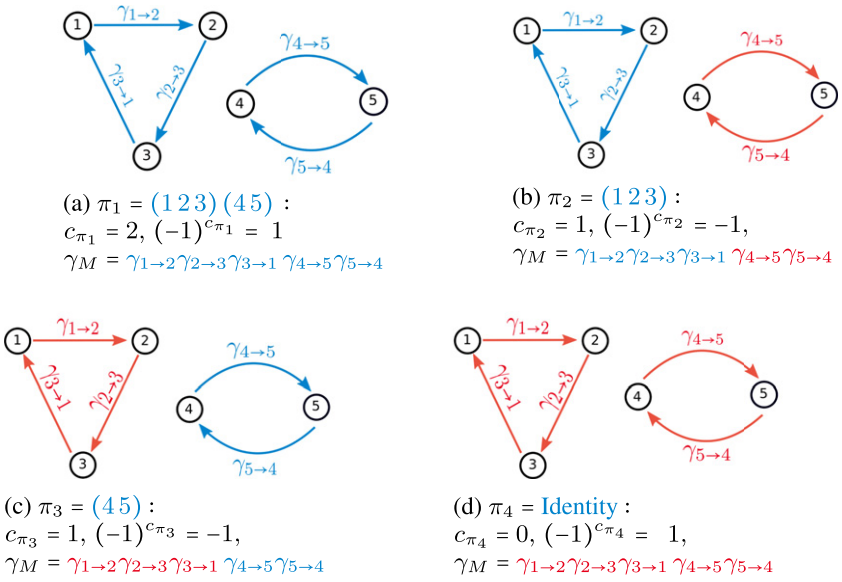

Figure 9. Example of the associated network of two cycles of the monomial $\gamma_{\mathcal{M}} = \gamma_{1\to2}\,\gamma_{2\to3}\,\gamma_{3\to1}\quad\gamma_{4\to5}\,\gamma_{5\to4} = \sum_{\pi\in\mathcal{S}_5}\gamma_{C_\pi}\prod_{i\in\mathcal{F}_\pi}\sum_{j_i=1}^{N=5}\gamma_{i\to j_i}$. There are four different permutations that lead to these cycles with $c_M = 2$. □

in-trees, you take the product of the link strengths of all the edges of theses in-trees and you sum over all such partitions. This results in the final formula (37) for $[-\Gamma]_{J,J}$.

A.8. First minors of the transition matrix

In order to evaluate $[\Gamma]_{i,j}$, we first have a look at a more general case:

Let $A \in \mathbb{C}^{(N-1)\times N}$ be an arbitrary matrix, whose columns sum up to zero ($\boldsymbol{e}_i^{\mathrm{T}}A = 0^{\mathrm{T}}$ for all $i \in \{1,\ldots,N-1\}$). Then the first minors $[A]_{\varnothing,\{i\}}$ of A, which are obtained by deleting column number i and taking the determinant of the resulting sub-matrix, satisfy the relation

$$[A]_{\varnothing,\{i\}} = (-1)^{i-1}[A]_{\varnothing,\{1\}}, \tag{43}$$

with the notation introduced in appendix A.7.

Proof. The statement is trivial for $i = 1$, so let us assume that $i \geqslant 2$. Then the matrix

$$B := \left(A\boldsymbol{e}_1 + A\boldsymbol{e}_i, A\boldsymbol{e}_2, A\boldsymbol{e}_3, \ldots, A\boldsymbol{e}_{i-1}, A\boldsymbol{e}_{i+1}, \ldots, A\boldsymbol{e}_N\right) \tag{44}$$

is also singular, so we have:

$$\begin{aligned} 0 = \det(B) &= \det\left(A_{\{i\},\varnothing}\right) + \underbrace{\det\left(A\boldsymbol{e}_i, A\boldsymbol{e}_2, A\boldsymbol{e}_3, \ldots, A\boldsymbol{e}_{i-1}, A\boldsymbol{e}_{i+1}, \ldots, A\boldsymbol{e}_N\right)}_{(-1)^{i-2}\det(A_{\{1\},\varnothing})}. \\ &= \det(A_{\{i\},\varnothing}) + (-1)^{i-2}\det(A_{\{1\},\varnothing}) \end{aligned} \tag{45}$$

In the last step, we have used the fact that the determinant changes its sign when interchanging two column and we have move the first column ($A\boldsymbol{e}_i$) successively $i-2$-times to the right. □

In particular, the matrix $\Gamma_{\varnothing,\{i\}}$ (that is, deleting the ith row from the transition matrix) fulfills the requirements and hence we can compute:

$$\begin{aligned}[\Gamma]_{ji} &\overset{\text{Def}}{=\!=} \det\left(\left(\Gamma_{\varnothing,\{i\}}\right)_{\{j,\varnothing\}}\right) = (-1)^{j-1}\det\left(\left(\Gamma_{\varnothing,\{i\}}\right)_{\{1,\varnothing\}}\right)\\ &= (-1)^{i-1}(-1)^{j-1}\det\left(\left(\Gamma_{\varnothing,\{i\}}\right)_{\{i,\varnothing\}}\right) = (-1)^{i+j}[\Gamma]_{ii}.\end{aligned} \tag{46}$$

This means that we can compute all first minors $[\Gamma]_{ji}$ of the transition matrix Γ from its first principal minors $[\Gamma]_{ii}$. This can be used to compute the stationary state of a strongly connected network, as done in appendix A.4.

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