

Chapter 2

Exact propagation models on networks: top down

Chapter 1 introduced SIS and SIR diseases and some weaknesses of compartmental models that can be remedied by considering networks. In this chapter, we begin our network-based investigation by setting up the problem we will study. We introduce the full stochastic model and show how to derive exact equations to calculate the probability of the entire network being in a given state. We refer to such models as “top down”. The resulting system will generally have too many equations for practical analysis, so we discuss techniques to derive exact equations at a coarser level.

The diseases occur at the nodes, with the status of a node changing over time. At any given time, we assume the only factors that can affect the probability of a node changing its status are its current status and the statuses of its immediate neighbours. For example, the rate at which a susceptible node becomes infected depends only on how many of its neighbours are infected. Although neighbours can influence a node’s transitions, the rate can also be independent of its neighbours. In particular, an infected node recovers at a rate that does not depend on any neighbour’s status.

If each of the N nodes can have one of m different statuses, then the total number of distinct states of the network is m^N , so for SIS there are 2^N states and for SIR there are 3^N . We refer to the collection of all states as the state space, denoted $\{S_1, S_2, \dots, S_n\}$. Ideally, we would like to predict the state of the network at any time. However, for a stochastic dynamic process, at best we might hope to know each state’s probability. Even this may be impractical, and so we may settle for simply knowing the probability that a given number of individuals have each status.

In this chapter, we will develop exact equations for these probabilities. The full system of equations is generally quite large. Through careful aggregation of states we may find it is easier to calculate the probability that the system is in one of a collection of states. The methods we develop are not specific to SIS or SIR disease, but apply generally to a wide range of dynamic processes spreading on networks. It is simpler to consider a generic process rather than focusing on disease. So we will

develop the mathematical theory for the more general problem, with an emphasis on the aspects relevant to disease spread. To aid the construction of our mathematical models, we make a few explicit assumptions:

1. time is considered to be continuous,
2. a node has only a finite number of possible statuses,
3. the process is stochastic,
4. the inter-event times are exponentially distributed,
5. the parameter of this exponential distribution may depend on the status of the node and on the number of neighbouring nodes of each status,
6. transitions at different nodes are independent.

Ideally, we would like to know the probability the system has a given state at a given time, but this is likely to be impractical. Thus, the aim of the investigation is to determine

- the probability that a node has a given status at a given time,
- the expected number of nodes having a given status at a given time.

These assumptions lead to a continuous-time Markov chain with finite state space. This is a widely used and intensively studied field of mathematics with an extensive literature both from the theoretical and applied points of view. This book is not aimed at introducing Markov chains in general. For this, any of the following provides a good point of reference [124, 157, 161, 162, 171, 259]. Our topic is restricted to a special class of Markov chains which originate from exact propagation models on networks.

We note that relaxing the first requirement above leads to discrete-time models, which are partially investigated in Chapter 6. Further discussion of discrete-time models in the context of network epidemics can be found in [97, 102]. Relaxing the fourth requirement leads to non-Markovian models, where the transition times can be non-exponential. These will be studied in Chapter 9. If the fifth assumption is relaxed, then network models will turn into hypergraph models, where the processes evolve via hyperedges instead of edges (see, for example, [38, 111, 193]).

The methods we develop in this Chapter allow us to significantly simplify the mathematical models we study, without using any approximations. However, we will see that this process is not always easy, and the simplified models may still be quite complex. Later in the book we will explore ways to develop approximate models which are more tractable.

2.1 An introductory example

To motivate our approach and illustrate the processes we consider, we will analyse the state space of an SIS disease propagating on a triangle. We will derive equations governing the probabilities that the system is in each state. Then, we will derive a reduced system that captures the important details of the model. The remainder of the chapter develops techniques for more general cases.

Example 2.1. The state space of the Markov chain for an SIS disease in a triangle is

$$\{SSS, SSI, SIS, ISS, SII, ISI, IIS, III\},$$

where, for example, SSI represents the state where nodes 1 and 2 are susceptible and node 3 is infected. Figure 2.1 shows the possible states and the possible transitions between those states, highlighting the SII state. At most, one transition can happen at a time (though the time between transitions can be arbitrarily small).

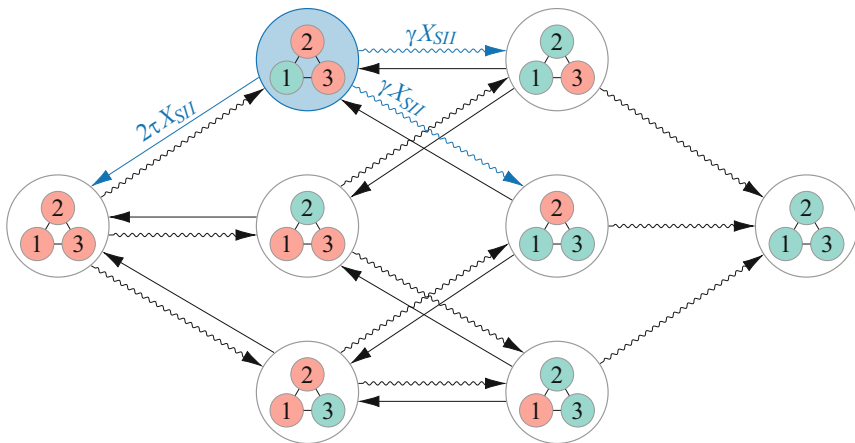


Fig. 2.1: Illustration of all eight network states and associated transitions for an SIS disease spreading in the fully connected network with 3 nodes. Susceptible (●) and infected (●) nodes are denoted by filled circles of different colours. Note that the SSS state is an absorbing state: there is no path out. The SII state and the fluxes of probability going out are highlighted (but not the fluxes in).

We define X_{ABC} to be the probability that the state of the network is ABC , where A , B and C may be S or I. If the transition corresponds to recovery of a single node, it occurs at the *recovery rate* γ , while if it corresponds to infection of a single node, it occurs at the *per-contact infection or transmission rate* τ times the number of infected neighbours. For example, if the system is in state SII, the rate at which it moves to SIS is γ . In contrast, the rate at which the system moves to III is 2τ . From this and following Fig. 2.1, we note that the flux of probability from state ABC to another is given by the rate at which that transition happens times X_{ABC} . Summarising the above yields

$$\begin{aligned}\dot{X}_{SSS} &= \gamma(X_{SSI} + X_{SIS} + X_{ISS}), \\ \dot{X}_{SSI} &= \gamma(X_{SII} + X_{ISI}) - (2\tau + \gamma)X_{SSI}, \\ \dot{X}_{SIS} &= \gamma(X_{SII} + X_{IIS}) - (2\tau + \gamma)X_{SIS}, \\ \dot{X}_{ISS} &= \gamma(X_{ISI} + X_{IIS}) - (2\tau + \gamma)X_{ISS}, \\ \dot{X}_{SII} &= \gamma X_{III} + \tau(X_{SSI} + X_{SIS}) - 2(\tau + \gamma)X_{SII},\end{aligned}$$

$$\begin{aligned}
\dot{X}_{ISI} &= \gamma X_{III} + \tau(X_{SSI} + X_{ISS}) - 2(\tau + \gamma)X_{ISI}, \\
\dot{X}_{IIS} &= \gamma X_{III} + \tau(X_{SIS} + X_{ISS}) - 2(\tau + \gamma)X_{IIS}, \\
\dot{X}_{III} &= -3\gamma X_{III} + 2\tau(X_{SII} + X_{ISI} + X_{IIS}).
\end{aligned}$$

These equations are the *forward Kolmogorov equations* of the system and are also called *master equations*. A solution to the master equations gives the probability that the system is in each state at each given time.

The equations become simpler if we are willing to accept knowing just the probability a given number of nodes have each status. Rather than calculating a given state's probability, we calculate the probability the system is in one of several states collected or grouped based on how many nodes are infected. Define Y_i to be the probability exactly i nodes are infected; that is, $Y_0 = X_{SSS}$, $Y_1 = X_{ISS} + X_{SIS} + X_{SSI}$, $Y_2 = X_{IIS} + X_{ISI} + X_{SII}$ and $Y_3 = X_{III}$; the equations become

$$\dot{Y}_0 = \gamma Y_1, \tag{2.1a}$$

$$\dot{Y}_1 = 2\gamma Y_2 - \gamma Y_1 - 2\tau Y_1, \tag{2.1b}$$

$$\dot{Y}_2 = 2\tau Y_1 - 2\gamma Y_2 - 2\tau Y_2 + 3\gamma Y_3, \tag{2.1c}$$

$$\dot{Y}_3 = 2\tau Y_2 - 3\gamma Y_3. \tag{2.1d}$$

This simplification works for a triangle, but it often fails for more general networks.

Exercise 2.1. Starting from $Y_1 = X_{ISS} + X_{SIS} + X_{SSI}$ for SIS disease in a triangle, find an equation in terms of the X_{ABC} variables for \dot{Y}_1 . Then, simplify this by using Y_1 and Y_2 to derive equation (2.1b). Continue using this approach to complete the derivation of system (2.1).

Exercise 2.2. Using the same variables Y_0, Y_1, Y_2 and Y_3 as for the triangle, attempt to repeat Exercise 2.1 to derive a system like system (2.1) if the 1–3 edge does not exist. What goes wrong? [You will have to modify the equations for X_{ABC} to account for the fact that 1 and 3 cannot transmit to each other.]

In this chapter, we give a more rigorous basis for what we have just done. This will give us the mathematical tools needed to derive master equations for more complicated systems and to identify when it is possible to simplify these, without approximation, by collecting or *lumping* states together. We will see that for large networks lumping often will not reduce the system of equations enough. Even for small networks lumping often leaves us with a large system of equations. The process will generally only be practical for special networks. So later chapters show how to systematically simplify the dynamics to arrive at tractable approximate equations.

2.2 Continuous-time Markov chains

We briefly summarise the basics of continuous-time Markov chains, which we will use to derive master equations. Let the state space of the Markov chain be the set $\{\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_n\}$. For the 3-node SIS system of Fig. 2.1, $n = 2^3 = 8$.

Definition 2.1 *If the system is in state \mathcal{S}_i , the rate at which it transitions to state $\mathcal{S}_j \neq \mathcal{S}_i$ is defined to be $h(\mathcal{S}_i, \mathcal{S}_j)$. We define $h(\mathcal{S}_i, \mathcal{S}_i) = -\sum_{j \neq i} h(\mathcal{S}_i, \mathcal{S}_j)$.*

So $-h(\mathcal{S}_i, \mathcal{S}_i)$ is the total rate at which the system would transition from \mathcal{S}_i to any other state. Thus for each i

$$\sum_j h(\mathcal{S}_i, \mathcal{S}_j) = 0. \quad (2.2)$$

As a shorthand, we often use $a_{ij} = h(\mathcal{S}_i, \mathcal{S}_j)$.

If δt is the length of a short time interval, then the probability of transition from \mathcal{S}_i to \mathcal{S}_j in the interval $(t, t + \delta t)$ is $h(\mathcal{S}_i, \mathcal{S}_j)\delta t + \mathcal{O}(\delta t)$, where $\mathcal{O}(\delta t)$ represents an error such that $\mathcal{O}(\delta t)/\delta t \rightarrow 0$ as δt decreases to 0. Similarly, with probability $1 - h(\mathcal{S}_i, \mathcal{S}_j)\delta t + \mathcal{O}(\delta t)$, that event will not take place. Hence, if the system state at time t is denoted by $\mathcal{S}(t)$, then

$$P(\mathcal{S}(t + \delta t) = \mathcal{S}_j | \mathcal{S}(t) = \mathcal{S}_i) = h(\mathcal{S}_i, \mathcal{S}_j)\delta t + \mathcal{O}(\delta t).$$

This relation enables us to formulate master equations for the probabilities of each state. Let $X_i(t) = P(\mathcal{S}(t) = \mathcal{S}_i)$ denote the probability that the system is in state i at time t . Then, the law of total probability leads to

$$\begin{aligned} X_j(t + \delta t) &= P(\mathcal{S}(t + \delta t) = \mathcal{S}_j) = \sum_{i=1}^n P(\mathcal{S}(t + \delta t) = \mathcal{S}_j | \mathcal{S}(t) = \mathcal{S}_i) P(\mathcal{S}(t) = \mathcal{S}_i) \\ &= \left(\sum_{i \neq j} h(\mathcal{S}_i, \mathcal{S}_j)\delta t X_i(t) \right) + (1 - h(\mathcal{S}_j, \mathcal{S}_j)\delta t) X_j(t) + \mathcal{O}(\delta t), \end{aligned}$$

Subtracting $X_j(t)$, replacing $h(\mathcal{S}_i, \mathcal{S}_j)$ with a_{ij} , dividing by δt and taking $\delta t \rightarrow 0$ yields the master equation

$$\dot{X}_j(t) = \sum_{i=1}^n a_{ij} X_i(t).$$

This is a linear system of ordinary differential equations of the form

$$\dot{X} = PX \quad (2.3)$$

where the matrix P is the transpose of the matrix of transition rates, that is $P_{ji} = a_{ij}$ for $j \neq i$ and $P_{jj} = -\sum_{k \neq j} a_{jk}$. The entries in each column sum to zero, representing the fact that if the system leaves one state, it enters another, so every increase in one state's probability is balanced by a decrease in the probability of another. We note that often the transpose of P is used, and then X is a row vector, not a column. However, we use this formulation since it is more convenient from a dynamical system point of view. The master equations of a network process are formulated in the next section.

2.3 Master equations for arbitrary networks

The aim of this section is to show how to formulate master equations for a process spreading on an arbitrary network, assuming transitions of a node depend only on the statuses of the node and its neighbours.

2.3.1 State space and transition rates for arbitrary dynamics

The network is given by the adjacency matrix of the corresponding undirected graph with N nodes: $G = (g_{ij})_{i,j=1,2,\dots,N}$. Here, $g_{ij} = 1$ if nodes i and j are connected, or $g_{ij} = 0$ otherwise. Plainly, $g_{ij} = g_{ji}$ and we take $g_{ii} = 0$. Let $\{Q_1, Q_2, \dots, Q_m\}$ be the possible statuses nodes can take. Then, a state of the network can be specified by an N -tuple (q_1, q_2, \dots, q_N) , where $q_i \in \{Q_1, Q_2, \dots, Q_m\}$ is the status of node i . The matrix in the master equation Eq. (2.3) is of size $m^N \times m^N$. This is a high-dimensional matrix, but with many zero entries because many transitions are not possible.

Because events happen independently and intervals are exponentially distributed, at most one event happens at any given time. Thus, if the states $S_\alpha = (q_1, q_2, \dots, q_N)$ and $S_\beta = (s_1, s_2, \dots, s_N)$ differ at more than one node, then the transition from S_α to S_β is not possible and $h(S_\alpha, S_\beta) = 0$. If they differ in exactly one node, i , that is $q_i \neq s_i$ but $q_l = s_l$ for all $l \neq i$, then the transition rate depends on the statuses of node i , its neighbours and the process we study. For example, for the specific case of SIS or SIR dynamics, if $q_i = S$, $s_i = I$ and node i has n infected neighbours, then the transition rate is $n\tau$. In other words, node i is infected at rate $n\tau$. In the case of an arbitrary dynamic, let $q_i = Q$ and $s_i = T$, i.e. node i changes from status Q to status T . We take $n_{Q_1}, n_{Q_2}, \dots, n_{Q_m}$ to be the number of neighbours node i has of each status. We define $f_{QT}(n_{Q_1}, n_{Q_2}, \dots, n_{Q_m})$ to be the rate at which node i transitions from status Q to T if it has n_{Q_l} neighbours of status Q_l . Thus, summarising, the rate of transition from state S_α to state S_β can be given as:

$$h(S_\alpha, S_\beta) = \begin{cases} 0 & S_\alpha \text{ and } S_\beta \text{ differ for at least two nodes,} \\ f_{QT}(n_{Q_1}, n_{Q_2}, \dots, n_{Q_m}) & S_\alpha \text{ and } S_\beta \text{ differ in exactly one} \\ -\sum_{l \neq \alpha} h(S_\alpha, S_l) & \text{node } i \\ & S_\alpha = S_\beta. \end{cases} \quad (2.4)$$

2.3.2 State space and transition rates for binary dynamics

To be more specific, we take binary dynamics $m = 2$ as in SIS disease. Nodes can have one of two statuses, say Q and T . In deriving the master equations, we follow ideas developed independently in [288], and [312]. Considering $m = 2$ has many advantages. First, many fundamental processes can be described by two statuses, including the SIS model in epidemiology [4], the QAQ (i.e. quiescent–active–quiescent) model in neuroscience [70], the voter model in social sciences [58, 291, 314] and the Ising model in statistical physics [77, 85, 115, 194], to name just a few. Second, model formulation is clearer and more transparent in this case, and understanding the binary dynamics model provides a direct and simple way to-

wards a generalisation to more than two statuses. The following section will extend this to SIR disease.

We group the 2^N states into $N + 1$ subsets \mathcal{C}^k for $k = 0, 1, \dots, N$. Here, the super-script k is used for indexing and not as an exponent. We take \mathcal{C}^k to be the set of states with k nodes of status T . There are two notable special cases: \mathcal{C}^0 is a subset with a single element, namely the state with all nodes having status Q : $\mathcal{C}^0 = \{QQ \cdots Q\}$, and \mathcal{C}^N is also a subset with a single element, namely the state with all nodes having status T : $\mathcal{C}^N = \{TT \cdots T\}$.

More generally, the states in \mathcal{C}^k are denoted by $S_1^k, S_2^k, \dots, S_{c_k}^k$, where $c_k = \binom{N}{k}$ is the number of different ways in which k nodes of status T can be placed on the network. The status of the l th node of state S_j^k will be denoted by $S_j^k(l)$; thus, $S_j^k(l) = Q$ or $S_j^k(l) = T$. For example, when an SIS epidemic is considered on a triangle network, then $\mathcal{C}^0 = \{SSS\}$, $\mathcal{C}^1 = \{SSI, SIS, ISS\}$, $\mathcal{C}^2 = \{SII, ISI, IIS\}$ and $\mathcal{C}^3 = \{III\}$.

The state of the system can change as follows:

Transition of a node from status Q to T : A node of status Q transitions to status T , that is an $S_j^k \rightarrow S_i^{k+1}$ type transition, where j and i are chosen such that there exists l for which $S_j^k(l) = Q$, $S_i^{k+1}(l) = T$ and $S_j^k(m) = S_i^{k+1}(m)$ for all $m \neq l$. The rate of this transition is given by $f_{QT}(n)$, where n denotes the number of neighbours of node l of status T when the system is in state S_j^k . We note that in the general case, as given in Subsection 2.3.1, the transition rate f_{QT} may depend on the numbers of all types of neighbours. For simplicity, we assume that f_{QT} depends only on the number of neighbours of status T and not on the number of neighbours of status Q .

Transition of a node from status T to Q : A node of status T transitions to status Q , that is an $S_j^k \rightarrow S_i^{k-1}$ type transition, where j and i are chosen such that there exists l for which $S_j^k(l) = T$, $S_i^{k-1}(l) = Q$ and $S_j^k(m) = S_i^{k-1}(m)$ for all $m \neq l$. This means that states S_j^k and S_i^{k-1} differ only at the l 'th position. We assume that the T to Q transition depends only on the number of neighbours of status Q . Thus, the transition rate is $f_{TQ}(n)$, where n denotes the number of neighbours of node l of status Q .

For illustration, we consider three different processes: SIS, QAQ with a hyperbolic tangent transition rate and a voter-like model with two statuses, where both transitions depend on the status of the neighbours.

Example 2.2. Consider an SIS disease propagating on a network. A node can be susceptible S or infected I . Using the above notation, let Q be S and T be I . There are two transitions: infection and recovery. In order to specify the dynamics, the transition rates f_{SI} and f_{IS} have to be specified. In this case, $f_{SI}(n) = \tau n$ with τ the per-contact infection rate, $f_{IS}(n) = \gamma$, with γ , the recovery rate. That is, the infection rate is proportional to the number of infected neighbours, while the recovery rate is independent of the statuses of the neighbours.

Example 2.3. A network of neurones is considered with purely excitatory connections. Within the network, neurones are considered to be either quiescent (Q) or active (A) with the following two types of transitions. A quiescent neurone with n

active neighbours becomes active with rate $f_{QA}(n) = \omega \tanh(n)$, with some parameter ω , which is called synaptic weight, while an active neurone becomes quiescent with rate $f_{AQ}(n) = \alpha$ with some parameter α , which is called the deactivation rate. That is, the activation rate depends in a non-linear way on the number of active neighbours, while the deactivation rate is independent of the statuses of the neighbours.

Example 2.4. Consider a voter-like model, where the nodes of the network represent the voters, which can be of status A or B , and the neighbours of a node can change their status as follows. A node of status A becomes B at rate $f_{AB}(n) = an$ with some parameter a , where n denotes the number of B neighbours of the node. Similarly, a node of status B becomes A at rate $f_{BA}(n) = bn$ with some parameter b , where n denotes the number of A neighbours of the node. Thus, in this case both transitions depend on the statuses of the neighbours.

We note that an alternative rate function is widely used: $f_{AB}(n_A, n_B) = a \frac{n_B}{n_A + n_B}$, where n_A and n_B denote the number of neighbours of status A and B , respectively. The corresponding $B \rightarrow A$ transition rate is $f_{BA}(n_A, n_B) = b \frac{n_A}{n_A + n_B}$, expressing the fact that the rate depends on the ratio of the number of different neighbours.

2.3.3 Master equations for binary dynamics

We begin our derivation of master equations in the special case of SIS disease spreading on a triangle. We then show how this generalises for the derivation of an arbitrary binary process spreading on a network.

Example 2.5. In Fig. 2.1, we have $N = 3$ nodes. There are $2^3 = 8$ distinct states the system can take. We write X_{ABC} to be the probability that the system state is $S = ABC$. We have already seen that the master equations are

$$\begin{aligned}\dot{X}_{SSS} &= \gamma(X_{SSI} + X_{SIS} + X_{ISS}), \\ \dot{X}_{SSI} &= \gamma(X_{SII} + X_{ISI}) - (2\tau + \gamma)X_{SSI}, \\ \dot{X}_{SIS} &= \gamma(X_{SII} + X_{IIS}) - (2\tau + \gamma)X_{SIS}, \\ \dot{X}_{ISS} &= \gamma(X_{ISI} + X_{IIS}) - (2\tau + \gamma)X_{ISS}, \\ \dot{X}_{SII} &= \gamma X_{III} + \tau(X_{SSI} + X_{SIS}) - 2(\tau + \gamma)X_{SII}, \\ \dot{X}_{ISI} &= \gamma X_{III} + \tau(X_{SSI} + X_{ISS}) - 2(\tau + \gamma)X_{ISI}, \\ \dot{X}_{IIS} &= \gamma X_{III} + \tau(X_{SIS} + X_{ISS}) - 2(\tau + \gamma)X_{IIS}, \\ \dot{X}_{III} &= -3\gamma X_{III} + 2\tau(X_{SII} + X_{ISI} + X_{IIS}).\end{aligned}$$

These can be rewritten as $\dot{X} = PX$, where $X = (X_{SSS}, X_{SSI}, X_{SIS}, X_{ISS}, X_{SII}, X_{ISI}, X_{IIS}, X_{III})$ is a vector and

$$P = \begin{pmatrix} 0 & \gamma & \gamma & \gamma & 0 & 0 & 0 & 0 \\ 0 & -2\tau - \gamma & 0 & 0 & \gamma & \gamma & 0 & 0 \\ 0 & 0 & -2\tau - \gamma & 0 & \gamma & 0 & \gamma & 0 \\ 0 & 0 & 0 & -2\tau - \gamma & 0 & \gamma & \gamma & 0 \\ 0 & \tau & \tau & 0 & -2\tau - 2\gamma & 0 & 0 & \gamma \\ 0 & \tau & 0 & \tau & 0 & -2\tau - 2\gamma & 0 & \gamma \\ 0 & 0 & \tau & \tau & 0 & 0 & -2\tau - 2\gamma & \gamma \\ 0 & 0 & 0 & 0 & 2\tau & 2\tau & 2\tau & -3\gamma \end{pmatrix}.$$

As noted following equation (2.3), the columns sum to 0. The vector X can be divided into four parts, $X = ((X_{SSS}), (X_{SSI}, X_{SIS}, X_{ISS}), (X_{SIH}, X_{ISH}, X_{IHS}), (X_{III}))$, based on the number of nodes infected. Thus, $X = (X^0, X^1, X^2, X^3)$, where X^k is a sub-vector whose entries all correspond to k infections. Performing the corresponding division of the rows and columns of P leads to the block-tridiagonal form

$$P = \begin{pmatrix} B^0 & C^0 & 0 & 0 \\ A^1 & B^1 & C^1 & 0 \\ 0 & A^2 & B^2 & C^2 \\ 0 & 0 & A^3 & B^3 \end{pmatrix},$$

where

$$\begin{aligned} B^0 &= (0), & C^0 &= (\gamma, \gamma, \gamma), \\ A^1 &= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, & B^1 &= \begin{pmatrix} -2\tau - \gamma & 0 & 0 \\ 0 & -2\tau - \gamma & 0 \\ 0 & 0 & -2\tau - \gamma \end{pmatrix}, & C^1 &= \begin{pmatrix} \gamma & \gamma & 0 \\ \gamma & 0 & \gamma \\ 0 & \gamma & \gamma \end{pmatrix}, \\ A^2 &= \begin{pmatrix} \tau & \tau & 0 \\ \tau & 0 & \tau \\ 0 & \tau & \tau \end{pmatrix}, & B^2 &= \begin{pmatrix} -2\tau - 2\gamma & 0 & 0 \\ 0 & -2\tau - 2\gamma & 0 \\ 0 & 0 & -2\tau - 2\gamma \end{pmatrix}, & C^2 &= \begin{pmatrix} \gamma \\ \gamma \\ \gamma \end{pmatrix}, \\ A^3 &= (2\tau, 2\tau, 2\tau), & B^3 &= (-3\gamma). \end{aligned}$$

We have

$$\dot{X}^k = A^k X^{k-1} + B^k X^k + C^k X^{k+1}, \quad k = 0, 1, 2, 3.$$

We return now to a general binary dynamic process and formulate the master equations with Q replacing S and T replacing I . Let $X_j^k(t)$ be the probability the system is in state S_j^k at time t . Let

$$X^k(t) = (X_1^k(t), X_2^k(t), \dots, X_{c_k}^k(t))$$

be a c_k -dimensional vector for $k = 0, 1, \dots, N$. The above transitions determine the master equations in the form of (2.3) for the probability functions $X_j^k(t)$. However, as before, the matrix P is block-tridiagonal

$$P = \begin{pmatrix} B^0 & C^0 & 0 & 0 & \cdots & 0 \\ A^1 & B^1 & C^1 & 0 & \vdots & \vdots \\ 0 & A^2 & B^2 & C^2 & \vdots & \vdots \\ 0 & 0 & A^3 & B^3 & \ddots & 0 \\ \vdots & \cdots & \cdots & \ddots & \ddots & C^{N-1} \\ 0 & \cdots & \cdots & 0 & A^N & B^N \end{pmatrix}. \quad (2.5)$$

and

$$\dot{X}^k = A^k X^{k-1} + B^k X^k + C^k X^{k+1}, \quad k = 0, 1, \dots, N, \quad (2.6)$$

where A^0 and C^N are zero matrices. Thus, equation (2.6) is in the form (2.3) with X a column vector made up of the entries of X^0 , followed by X^1, X^2, \dots, X^N .

The A^k matrices capture the transition from Q to T , while the C^k matrices describe the transition from T to Q . These matrices depend on the structure of the network and the transition rates f_{QT} and f_{TQ} . We now investigate the structure of these matrices.

Exercise 2.3. Show that if $S_i^{k-1} \in \mathcal{C}^{k-1}$ differs from $S_j^k \in \mathcal{C}^k$ at only a single node, l , then $S_i^{k-1}(l) = Q$ and $S_j^k(l) = T$.

In class \mathcal{C}^{k-1} , there are c_{k-1} elements, and in class \mathcal{C}^k , there are c_k elements; hence, matrix A^k has c_k rows and c_{k-1} columns. The entry in the i th row and j th column of the matrix A^k is denoted by $A_{i,j}^k$. It gives the transition rate from S_j^{k-1} to S_i^k , which is non-zero only in the case where the states differ at only a single node l with $S_j^{k-1}(l) = Q$ and $S_i^k(l) = T$. The rate depends on the number of status T neighbours of node l , that is $A_{i,j}^k = h(S_j^{k-1}, S_i^k)$, yielding

$$A_{i,j}^k = \begin{cases} 0 & S_j^{k-1} \text{ and } S_i^k \text{ differ in more than one node,} \\ f_{QT}(n_T(l, S_j^{k-1})) & S_j^{k-1} \text{ and } S_i^k \text{ differ only for node } l, \end{cases} \quad (2.7)$$

where $n_T(l, S)$ is the number of status T neighbours of node l in state S .

In order to better understand the role of the A^k matrix, consider its j th column, which corresponds to the system leaving S_j^{k-1} . Let $\Omega_Q(S_j^{k-1})$ denote the set of nodes l which have status Q , that is, $\Omega_Q(S_j^{k-1}) = \{l : S_j^{k-1}(l) = Q\}$. For each $l \in \Omega_Q(S_j^{k-1})$, define $i(l)$ so that $S_{i(l)}^k$ is the (unique) state that would result from changing only node l 's status to T . Then, equation (2.7) becomes

$$A_{i,j}^k = \begin{cases} 0 & i \neq i(l) \text{ for any } l \in \Omega_Q(S_j^{k-1}), \\ f_{QT}(n_T(l, S_j^{k-1})) & i = i(l) \text{ for (a unique) } l \in \Omega_Q(S_j^{k-1}). \end{cases}$$

We conclude that the sum of the elements in the j th column of matrix A^k is

$$\sum_{i=1}^{c_k} A_{i,j}^k = \sum_{l \in \Omega_Q(\mathcal{S}_j^{k-1})} f_{QT}(n_T(l, \mathcal{S}_j^{k-1})). \quad (2.8)$$

In the simple case when f_{QT} is of the form $f_{QT}(n) = \tau n$, this reduces to

$$\sum_{i=1}^{c_k} A_{i,j}^k = \tau N_{QT}(\mathcal{S}_j^{k-1}), \quad (2.9)$$

where $N_{QT}(\mathcal{S}_j^{k-1})$ denotes the number of (Q, T) edges in state \mathcal{S}_j^{k-1} .

Similarly, the entry in the i th row and j th column of matrix C^k is denoted by $C_{i,j}^k$ and gives the transition rate from \mathcal{S}_j^{k+1} to \mathcal{S}_i^k . In the \mathcal{C}^{k+1} class, there are c_{k+1} elements, and in the \mathcal{C}^k class, there are c_k elements; hence, matrix C^k has c_k rows and c_{k+1} columns. The entry $C_{i,j}^k$ is non-zero only in the case when the states \mathcal{S}_j^{k+1} and \mathcal{S}_i^k differ at one position, say at position l . The transition rate depends on the number of status Q neighbours of node l , that is $C_{i,j}^k = h(\mathcal{S}_j^{k+1}, \mathcal{S}_i^k)$, yielding

$$C_{i,j}^k = \begin{cases} 0 & \mathcal{S}_j^{k+1} \text{ and } \mathcal{S}_i^k \text{ differ in more than one node} \\ f_{TQ}(n_Q(l, \mathcal{S}_j^{k+1})) & \mathcal{S}_j^{k+1} \text{ and } \mathcal{S}_i^k \text{ differ only for node } l, \end{cases} \quad (2.10)$$

where $n_Q(l, \mathcal{S})$ is the number of status Q neighbours of node l in state \mathcal{S} .

In the simple case of $f_{TQ}(n) = \gamma$, it follows that $C_{i,j}^k$ is either zero or γ . In state \mathcal{S}_j^{k+1} , $k+1$ nodes of the graph have status T ; hence, in the j th column of matrix C^k there are $k+1$ entries that are equal to γ and the remaining entries are zero. Hence, for all $j \in \{1, 2, \dots, c_{k+1}\}$ we have

$$\sum_{i=1}^{c_k} C_{i,j}^k = \gamma(k+1). \quad (2.11)$$

The matrix B^k is a diagonal matrix with c_k rows and columns. This is because B^k accounts only for the rate of $\mathcal{S}_i^k \rightarrow \mathcal{S}_j^k$ type transitions. The rate of a transition from \mathcal{S}_i^k to \mathcal{S}_j^k is zero if $\mathcal{S}_i \neq \mathcal{S}_j$. If $\mathcal{S}_i = \mathcal{S}_j$, then we get

$$B_{i,i}^k = - \sum_{j=1}^{c_{k+1}} A_{j,i}^{k+1} - \sum_{j=1}^{c_{k-1}} C_{j,i}^{k-1}, \quad (2.12)$$

because the sum of the entries in any column is 0.

These rules can be implemented computationally to automatically generate and numerically solve the full set of differential equations. The following exercises encourage the reader to apply these rules.

Exercise 2.4. Find the matrices A^k , B^k and C^k for the SIS dynamics on a line graph with $N = 3$ nodes (see Fig. 2.2a). Write down the full system of master equations and verify that there are 2^N equations.

| **Exercise 2.5.** Do the same for a line graph with $N = 4$ nodes (see Fig. 2.2b).

| **Exercise 2.6.** Do the same for a star graph with $N = 4$ nodes (see Fig. 2.2c).

| **Exercise 2.7.** Write down the system of master equations for the QAQ dynamics given in Example 2.3 on a line graph with $N = 3$ nodes (see Fig. 2.2a).

| **Exercise 2.8.** Write down the system of master equations for the voter-like model given in Example 2.4 on a line graph with $N = 3$ nodes (see Fig. 2.2a).

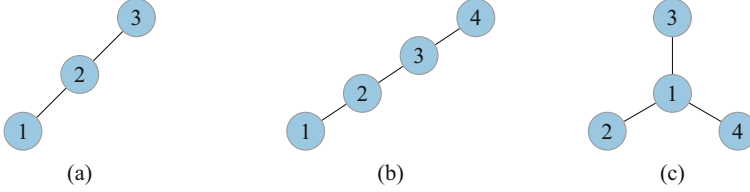


Fig. 2.2: Line with 3 (a) and 4 (b) nodes, respectively. (c) Star network with 4 nodes.

After formulating master equations for different binary dynamics and different graphs, we can write down the master equations for arbitrary binary dynamics on an arbitrary graph with $N = 3$ nodes. The state space consists of the states

$$\{QQQ, TQQ, QTQ, QQT, TTQ, TQT, QTT, TTT\}.$$

All potential transitions are depicted in Fig. 2.3. The rates depend on the process, which determines f_{QT} and f_{TQ} , and the graph, with adjacency matrix $G = (g_{ij})_{i,j=1,2,3}$, which determines how many neighbours of each status a given node has.

For example, for the transition from state QQT to QQQ node 3 moves from status T to Q . This rate depends on how many status Q neighbours it has. As both 1 and 2 have status Q , this is 0 if neither edge exists from node 3, 1 if only one edge exists and 2 if both edges exist. A convenient shorthand for the number of status Q neighbours 3 has, given that the state is QQT , is $g_{13} + g_{23}$. Thus, the transition rate from QQT to QQQ is $f_{TQ}(g_{13} + g_{23})$.

Similarly, the transition rate from state QQT to QTT happens at rate $f_{QT}(g_{32})$, because node 2 transitions from status Q to T , and this depends on whether node 2 is connected to the single node of status T , i.e. node 3. Determining the transition rates for all 24 possible transitions, indicated by arrows in Fig. 2.3, the master equations can be formulated as

$$\begin{aligned} \dot{X}_{QQQ} &= f_{TQ}(g_{13} + g_{23})X_{QQT} + f_{TQ}(g_{12} + g_{32})X_{QTQ} \\ &\quad + f_{TQ}(g_{21} + g_{31})X_{TQQ} - 3f_{QT}(0)X_{QQQ}, \\ \dot{X}_{QQT} &= f_{QT}(0)X_{QQQ} + f_{TQ}(g_{12})X_{QTT} + f_{TQ}(g_{21})X_{TQT} - q_{QQT}X_{QQT}, \\ \dot{X}_{QTQ} &= f_{QT}(0)X_{QQQ} + f_{TQ}(g_{13})X_{QTT} + f_{TQ}(g_{31})X_{TTQ} - q_{QTQ}X_{QTQ}, \end{aligned}$$

$$\begin{aligned}
\dot{X}_{TQQ} &= f_{QT}(0)X_{QQQ} + f_{TQ}(g_{23})X_{TQT} + f_{TQ}(g_{32})X_{TTQ} - q_{TQQ}X_{TQQ}, \\
\dot{X}_{QTT} &= f_{TQ}(0)X_{TTT} + f_{QT}(g_{32})X_{QQT} + f_{QT}(g_{23})X_{QTT} - q_{QTT}X_{QTT}, \\
\dot{X}_{TQT} &= f_{TQ}(0)X_{TTT} + f_{QT}(g_{31})X_{QQT} + f_{QT}(g_{13})X_{TQQ} - q_{TQT}X_{TQT}, \\
\dot{X}_{TTQ} &= f_{TQ}(0)X_{TTT} + f_{QT}(g_{21})X_{QTT} + f_{QT}(g_{12})X_{TQQ} - q_{TTQ}X_{TTQ}, \\
\dot{X}_{TTT} &= f_{QT}(g_{21} + g_{31})X_{QTT} + f_{QT}(g_{12} + g_{32})X_{TQT} \\
&\quad + f_{QT}(g_{13} + g_{23})X_{TTQ} - 3f_{TQ}(0)X_{TTT},
\end{aligned}$$

where

$$\begin{aligned}
q_{QQT} &= f_{TQ}(g_{13} + g_{23}) + f_{QT}(g_{31}) + f_{QT}(g_{32}), \\
q_{QTT} &= f_{TQ}(g_{12} + g_{32}) + f_{QT}(g_{21}) + f_{QT}(g_{23}), \\
q_{TQQ} &= f_{TQ}(g_{21} + g_{31}) + f_{QT}(g_{12}) + f_{QT}(g_{13}), \\
q_{QTT} &= f_{QT}(g_{21} + g_{31}) + f_{TQ}(g_{13}) + f_{TQ}(g_{12}), \\
q_{TQT} &= f_{QT}(g_{12} + g_{32}) + f_{TQ}(g_{23}) + f_{TQ}(g_{21}), \\
q_{TTQ} &= f_{QT}(g_{13} + g_{23}) + f_{TQ}(g_{31}) + f_{TQ}(g_{32}).
\end{aligned}$$

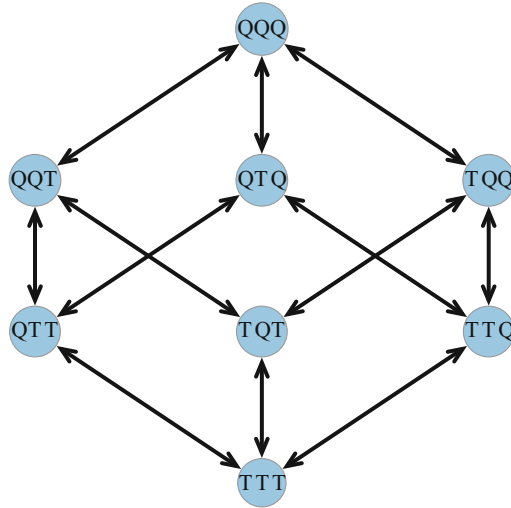


Fig. 2.3: The state space and all possible transitions for an arbitrary binary dynamics on an arbitrary graph with 3 nodes.

2.3.4 Master equations for SIR dynamics

The theory developed so far extends in a natural way to non-binary dynamics. To minimise technicalities, we consider just SIR disease propagation.

Example 2.6. As a first example, we write down the master equation for the simple network of two nodes connected by an edge. The state space is given by

$$\mathcal{C} = \{RR, RS, SR, SS, RI, IR, SI, IS, II\},$$

where the order indicates which node has each status. We will see later that it is useful to divide the states according to the number of I and S nodes. Let $\mathcal{C}^{i,j}$ denote the class of states in which there are i status I nodes and j status S nodes:

$$\begin{aligned} \mathcal{C}^{00} &= \{RR\}, & \mathcal{C}^{01} &= \{RS, SR\}, & \mathcal{C}^{02} &= \{SS\}, \\ \mathcal{C}^{10} &= \{RI, IR\}, & \mathcal{C}^{11} &= \{SI, IS\}, & \mathcal{C}^{20} &= \{II\}. \end{aligned}$$

The master equations follow by accounting for all possible transitions and their rates. They are

$$\begin{aligned} \dot{X}_{RR} &= \gamma(X_{RI} + X_{IR}), & \dot{X}_{SS} &= 0, & \dot{X}_{SI} &= -(\gamma + \tau)X_{SI}, \\ \dot{X}_{RS} &= \gamma X_{IS}, & \dot{X}_{RI} &= \gamma X_{II} - \gamma X_{RI}, & \dot{X}_{IS} &= -(\gamma + \tau)X_{IS}, \\ \dot{X}_{SR} &= \gamma X_{SI}, & \dot{X}_{IR} &= \gamma X_{II} - \gamma X_{IR}, & \dot{X}_{II} &= \tau(X_{SI} + X_{IS}) - 2\gamma X_{II}. \end{aligned}$$

Example 2.7. For a network with $N = 3$ nodes, the classes of the state space are

$$\begin{aligned} \mathcal{C}^{00} &= \{RRR\}, & \mathcal{C}^{01} &= \{RRS, RSR, SRR\}, & \mathcal{C}^{02} &= \{RSS, SRS, SSR\}, \\ \mathcal{C}^{03} &= \{SSS\}, & \mathcal{C}^{10} &= \{RRI, RIR, IRR\}, \\ \mathcal{C}^{11} &= \{RSI, RIS, SRI, SIR, IRS, ISR\}, & \mathcal{C}^{12} &= \{SSI, SIS, ISS\}, \\ \mathcal{C}^{20} &= \{RII, IRI, IIR\}, & \mathcal{C}^{21} &= \{SII, ISI, IIS\}, & \mathcal{C}^{30} &= \{III\}. \end{aligned}$$

In particular, for a line network with 3 nodes, the master equations are

$$\begin{aligned} \dot{X}_{RRR} &= \gamma(X_{IRR} + X_{RRI} + X_{RIR}), & \dot{X}_{RSS} &= \gamma X_{ISS}, \\ \dot{X}_{RRS} &= \gamma(X_{IRS} + X_{RIS}), & \dot{X}_{SRS} &= \gamma X_{SIS}, \\ \dot{X}_{RSR} &= \gamma(X_{ISR} + X_{RSI}), & \dot{X}_{SSR} &= \gamma X_{SSI}, \\ \dot{X}_{SRR} &= \gamma(X_{SIR} + X_{SRI}), & \dot{X}_{SSS} &= 0, \end{aligned}$$

for the \mathcal{C}^{00} , \mathcal{C}^{01} , \mathcal{C}^{02} and \mathcal{C}^{03} states;

$$\begin{aligned} \dot{X}_{RRI} &= \gamma(X_{IRI} + X_{RII}) - \gamma X_{RRI}, & \dot{X}_{SIR} &= \gamma X_{SII} - (\gamma + \tau)X_{SIR}, \\ \dot{X}_{RIR} &= \gamma(X_{IIR} + X_{RII}) - \gamma X_{RIR}, & \dot{X}_{IRS} &= \gamma X_{IIS} - \gamma X_{IRS}, \\ \dot{X}_{IRR} &= \gamma(X_{IIR} + X_{IRI}) - \gamma X_{IRR}, & \dot{X}_{ISR} &= \gamma X_{ISI} - (\gamma + \tau)X_{ISR}, \\ \dot{X}_{RSI} &= \gamma X_{ISI} - (\gamma + \tau)X_{RSI}, & \dot{X}_{SSI} &= -(\gamma + \tau)X_{SSI}, \\ \dot{X}_{RIS} &= \gamma X_{IIS} - (\gamma + \tau)X_{RIS}, & \dot{X}_{SIS} &= -(\gamma + 2\tau)X_{SIS}, \\ \dot{X}_{SRI} &= \gamma X_{SII} - \gamma X_{SRI}, & \dot{X}_{ISS} &= -(\gamma + \tau)X_{ISS}, \end{aligned}$$

for the \mathcal{C}^{10} , \mathcal{C}^{11} and \mathcal{C}^{12} states; and finally

$$\begin{aligned}
\dot{X}_{RII} &= \tau(X_{RSI} + X_{RIS}) + \gamma X_{III} - 2\gamma X_{RII}, & \dot{X}_{SII} &= \tau(X_{SSI} + X_{SIS}) - (2\gamma + \tau)X_{SII}, \\
\dot{X}_{IRI} &= \gamma X_{III} - 2\gamma X_{IRI}, & \dot{X}_{ISI} &= -(2\gamma + 2\tau)X_{ISI}, \\
\dot{X}_{IIR} &= \tau(X_{SIR} + X_{ISR}) + \gamma X_{III} - 2\gamma X_{IIR}, & \dot{X}_{IIS} &= \tau(X_{SIS} + X_{ISS}) - (2\gamma + \tau)X_{IIS}, \\
\dot{X}_{III} &= \tau X_{IIS} + 2\tau X_{ISI} + \tau X_{SII} - 3\gamma X_{III},
\end{aligned}$$

for the \mathcal{C}^{20} , \mathcal{C}^{21} and \mathcal{C}^{30} states. In general, the system can move from a \mathcal{C}^{ij} state to a $\mathcal{C}^{i+1,j-1}$ state by infection or to a $\mathcal{C}^{i-1,j}$ state by recovery.

We emphasise that \mathcal{C}^{ij} is not a state but a collection (or class) of states of the system. In Fig. 2.4, we give the possible paths that an arbitrary network with 4 nodes can take between the different classes. Although we group these states together into classes by how many individuals of each status there are, the transition rates into or out of different states in the same class may vary. Hence, the transition rates in the figure cannot be explicitly given without breaking the classes down into their individual states, as they depend on the choice of the state in a given class.

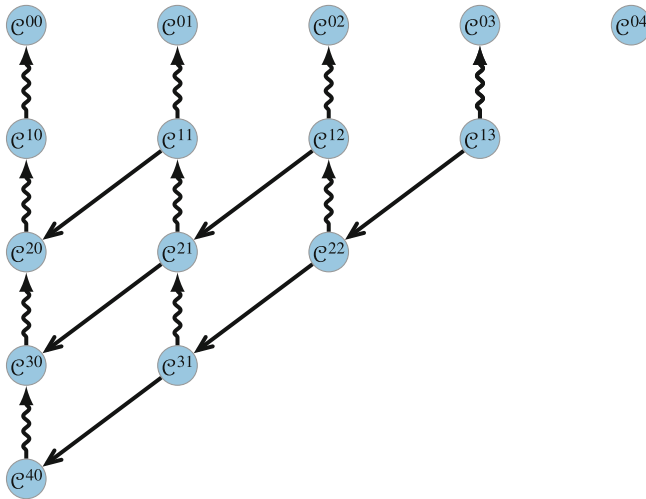


Fig. 2.4: Potential transitions for an SIR model for an arbitrary 4-node network. Straight lines correspond to transmissions and sinuous lines correspond to recoveries.

Exercise 2.9. Write down the full system of master equations for SIR dynamics on a triangle, i.e. on a complete graph with $N = 3$ nodes.

Finally, we investigate the structure of the matrix yielding the system of master equations. We introduce a coarser classification of the state space. Let \mathcal{C}^i denote the class made up of states where there are i nodes of status I. Then, obviously

$$\mathcal{C}^i = \bigcup_{j=0}^{N-i} \mathcal{C}^{ij}$$

and the system can move from a state in class \mathcal{C}^i to a state in class \mathcal{C}^{i+1} by infection or to a state in class \mathcal{C}^{i-1} by recovery. The number of states in class \mathcal{C}^{ij} is $\binom{N}{i} \binom{N-i}{j}$; hence, a simple summation shows that the number of states in class \mathcal{C}^i is $2^{N-i} \binom{N}{i}$. For example, in the case of a network with $N = 3$ nodes in the class \mathcal{C}^0 , there are 8 states, in the class \mathcal{C}^1 there are 12 states, in the class \mathcal{C}^2 there are 6 states and in the class \mathcal{C}^3 there is a single state, as can be explicitly checked by using the list of states above.

To formulate the system of master equations, let $X^i(t)$ be a $2^{N-i} \binom{N}{i}$ dimensional vector, the coordinates of which yield the probability of the system being in the states of class \mathcal{C}^i , for $i = 0, 1, \dots, N$. Since the possible transitions from class \mathcal{C}^i are to classes \mathcal{C}^{i+1} and \mathcal{C}^{i-1} , the system takes the form

$$\dot{X}^i = A^i X^{i-1} + B^i X^i + C^i X^{i+1}, \quad i = 0, 1, \dots, N, \quad (2.13)$$

where A^0 and C^N are zero matrices. Thus, Eq. (2.13) is in the form (2.3), with a matrix P that can be written in block tridiagonal form as

$$P = \begin{pmatrix} B^0 & C^0 & 0 & 0 & \dots & 0 \\ A^1 & B^1 & C^1 & 0 & \vdots & \vdots \\ 0 & A^2 & B^2 & C^2 & \vdots & \vdots \\ 0 & 0 & A^3 & B^3 & \ddots & 0 \\ \vdots & \dots & \dots & \ddots & \ddots & C^{N-1} \\ 0 & \dots & \dots & 0 & A^N & B^N \end{pmatrix}.$$

2.4 Lumping

We return to the case of general binary dynamics. The system of master equations given by (2.6) consists of 2^N linear differential equations, so the number of equations grows exponentially with N . This quickly becomes impractical or impossible to solve at large N . However, it is not always necessary to determine all probabilities. Particularly, when the number of nodes is large, the expected number or proportion of nodes of status Q and status T may be more useful. We denote these expected values at time t by $[Q](t)$ and $[T](t)$. They are expressed as

$$[Q](t) = \sum_{k=0}^N \left((N-k) \sum_{j=1}^{c_k} X_j^k(t) \right), \quad [T](t) = \sum_{k=0}^N \left(k \sum_{j=1}^{c_k} X_j^k(t) \right).$$

There are different approaches to determine or approximate these expected values. Conceptually, the simplest way is through individual-based stochastic simulation, using methods such as the Gillespie algorithm [112, 113] (or other methods

we present for SIS and SIR disease in Appendix A.1). However, this offers limited scope for a deeper understanding of the interactions between network topology and node dynamics, and results based on simulation are difficult to generalise. An alternative is the derivation of mean-field-like equations using pair or triple approximations [166, 256], heterogenous mean-field approximations [244], edge-based compartmental models [215, 222, 316] and effective degree-type models [115, 197, 300]. Chapters 4 to 7 give an extensive treatment of these modelling frameworks and show how different models are related. However, most of these models are approximate, and if we want an exact reduction, these mean-field-like approaches are insufficient. For networks with sufficient symmetry, the technique of lumping [100, 171, 268] can be used to reduce the exponential number of equations to a tractable number that are exact at a coarser scale. Ideally, the lumped system should have enough variables so that its solution provides relevant and significant information about the system. For example, the reduced system should be able to provide the expected number of nodes of each status.

Lumping, in general, is a method for coarse-graining Markov chains by partitioning, or lumping, the state space. The problem is to partition the state space in such a way that the Markov property is not lost in the aggregated process. Lumping of Markov chains is studied in [171, 268]; the particular case of random walks on networks is examined in [100]. Spectral properties of the transition matrix are related to the lumpability of the system [25, 155]. However, due to the exponentially large state space, in the case of network processes, these spectral methods have limited efficiency. This leads us to use another way to find partitions, namely exploiting the symmetries of the underlying network, as presented below.

The remainder of this section is structured as follows. First, we introduce a few definitions which help our analysis. Then, the idea of lumping is illustrated by motivating examples. Next, the lumping of linear systems of ODEs is dealt with in general. This is followed by the presentation of lumping system (2.6) and showing how this is related to the automorphisms (symmetries) of the graph. Finally, the lumping procedure is carried out for small networks and for arbitrarily large networks with special structure.

2.4.1 Partition of the state space

Consider a system with n states $\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_n$. For the class of problems we study, we can represent the probability of state \mathcal{S}_i by $X_i(t)$, with the vector $X = (X_1, X_2, \dots, X_n)$ denoting all of the probabilities. We can think of transitions from \mathcal{S}_r to \mathcal{S}_j in terms of probability flowing between the states. The amount of this flux is given by $P_{jr}X_r$.

Sometimes, we do not need to know X_i for every state i , or calculating the full solution may simply be too difficult. In such cases, we would like to use a coarser scale. This means partitioning (or lumping) some states together, creating m classes

$\{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_m\}$ of states. To make our terminology clear, we introduce some definitions.

Definition 2.2 *Given a set of objects $\Sigma = \{\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_n\}$, a partition of Σ is a set $\mathcal{C}^* = \{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_m\}$ of classes having two properties:*

- *Each class \mathcal{C}_j is a nonempty subset of Σ .*
- *Every $\mathcal{S}_i \in \Sigma$ belongs to exactly one \mathcal{C}_j .*

Typically, we have some collection of indices for our objects, usually integers, although in Example 2.8 below the states are indexed by a list giving the status of every node. There is a clear relation between a partition of the states and a partition of the indices. It will often be useful to have a shorthand for the set of indices associated with a class in the partition.

Definition 2.3 *Given a set of objects indexed by some indices $\Sigma = \{\mathcal{S}_{i_1}, \mathcal{S}_{i_2}, \dots, \mathcal{S}_{i_n}\}$, let $\mathcal{C}^* = \{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_m\}$ be a partition of Σ . The induced partition on the index set $\{i_1, i_2, \dots, i_n\}$ is $L = \{L_1, L_2, \dots, L_m\}$, where each L_k is the set of indices appearing in \mathcal{C}_k . That is, $L_k = \{i_j : \mathcal{S}_{i_j} \in \mathcal{C}_k\}$. We refer to L_k as the induced class of indices associated with \mathcal{C}_k .*

We write $Y_j = \sum_{i \in L_j} X_i$ to be the combined probability of all states in \mathcal{C}_j . In many cases, the correct choice of partition leads to a significant simplification of the equations. In such cases, we arrive at a linear system for Y_j having fewer equations.

2.4.2 A motivating example

Looking back at Example 2.1 of Section 2.1, we see that lumping several states together into larger classes can significantly reduce the number of equations. However, Exercise 2.2 shows that this does not always work. We will see that the success of a lumping depends strongly on the symmetries of the network. We now consider a more complex network structure to demonstrate more clearly how symmetries simplify the equations.

Example 2.8. We investigate an SIS disease spreading in a star network with four nodes. The states and flows between them are represented by the flow diagram in Fig. 2.5. For this specific case, we use the notation \mathcal{S}_{ABCD} to represent the state in which the central node has status A , the leftmost node status B , the top node status C and the rightmost node status D , where these are each either S or I .

The probability of state \mathcal{S}_{ABCD} is denoted X_{ABCD} . An arrow from state \mathcal{S}_i to state \mathcal{S}_j means that the system can move directly from \mathcal{S}_i to \mathcal{S}_j , either through recovery of a node or a transmission. An arrow from X_i to X_j has an associated flux, and this flux appears in the equations as an additive term for \dot{X}_j and a subtracted term for \dot{X}_i . Many arrows in Fig. 2.5 are bidirected, but some are not.

When we group those states that are symmetric together, we arrive at a partition made up of classes \mathcal{C}^{ik} , where the superscript i is 0 if the central node is susceptible and 1 if infected, and the superscript k gives the number of peripheral nodes that are infected.

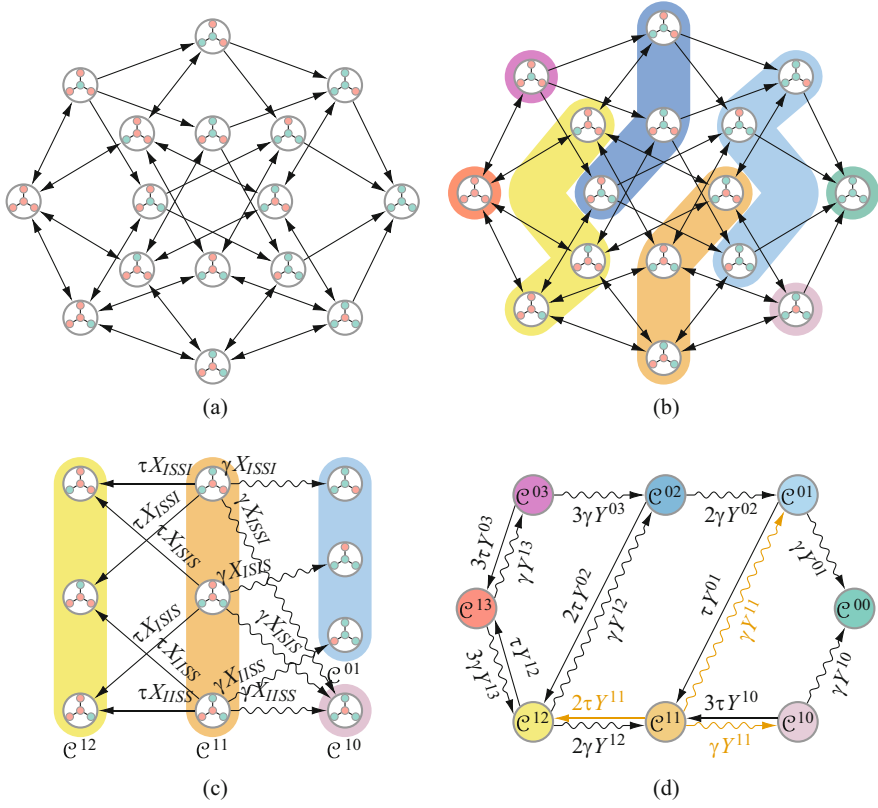


Fig. 2.5: Lumping for the spread of an SIS disease in a star with four nodes. Susceptible (●) and infected (●) nodes are denoted by filled circles of different colours. (a) The possible transitions in the original state space. (b) A partition formed by grouping symmetric states together. (c) The fluxes from each state \mathcal{S} in \mathcal{C}^{11} to the adjacent classes are proportional to the probability of \mathcal{S} , with the same coefficients for all $\mathcal{S} \in \mathcal{C}^{11}$. (d) The final lumped system. In (c) and (d), recoveries are denoted by sinusoidal paths. Note the relation between the highlighted fluxes out of \mathcal{C}^{11} in (d) and fluxes out of states within \mathcal{C}^{11} in (c).

$$\begin{aligned}
 \mathcal{C}^{00} &= \{\mathcal{S}_{SSSS}\} & \mathcal{C}^{02} &= \{\mathcal{S}_{SIIS}, \mathcal{S}_{SISI}, \mathcal{S}_{SSII}\} & \mathcal{C}^{12} &= \{\mathcal{S}_{ISII}, \mathcal{S}_{IISI}, \mathcal{S}_{IIIS}\} \\
 \mathcal{C}^{01} &= \{\mathcal{S}_{SISS}, \mathcal{S}_{SSIS}, \mathcal{S}_{SSSI}\} & \mathcal{C}^{11} &= \{\mathcal{S}_{IISS}, \mathcal{S}_{ISIS}, \mathcal{S}_{ISSI}\} & \mathcal{C}^{13} &= \{\mathcal{S}_{IIII}\} \\
 \mathcal{C}^{10} &= \{\mathcal{S}_{IISS}\} & \mathcal{C}^{03} &= \{\mathcal{S}_{SIII}\}
 \end{aligned}$$

For notational convenience, we will use L_{ik} to denote the subscripts associated with the states in \mathcal{C}^{ik} . Then, the probability Y^{ik} of the class \mathcal{C}^{ik} is given by

$$Y^{ik} = \sum_{j \in L_{ik}} X_j$$

Consider the class \mathcal{C}^{11} consisting of all states in which the central node and a single peripheral node are infected. The central node can transmit to either of the two remaining peripheral nodes, each with an associated rate τ . Looking in particular at \mathcal{S}_{IIS} , the transitions are to \mathcal{S}_{IIIS} and \mathcal{S}_{IISI} . The flux from X_{IIS} to X_{IIIS} is τX_{IIS} and the flux to X_{IISI} is also τX_{IIS} . Thus, the total flux from X_{IIS} into \mathcal{C}^{12} is $2\tau X_{IIS}$. Similarly, the fluxes from X_{ISIS} and X_{ISSI} into \mathcal{C}^{12} are also proportional to X_{ISIS} and X_{ISSI} , respectively, with the same proportionality constant. Thus, the total flux from \mathcal{C}^{11} to \mathcal{C}^{12} is simply $2\tau Y^{11}$.

With the chosen partition, all classes \mathcal{C}^{ij} have the property that, given another class \mathcal{C}^{kl} , the flow from any $\mathcal{S}_r \in \mathcal{C}^{ij}$ into the states in \mathcal{C}^{kl} is proportional to X_r , and that same proportionality constant holds for every $\mathcal{S}_r \in \mathcal{C}^{ij}$. Thus, the total flux from \mathcal{C}^{ij} to \mathcal{C}^{kl} is proportional to Y^{ij} with the same constant of proportionality.

Because this holds for every pair of classes, we can reduce our system to just considering the classes, rather than the individual states. Our final equations are

$$\begin{aligned} \dot{Y}^{00} &= \gamma(Y^{10} + Y^{01}), & \dot{Y}^{11} &= 3\tau Y^{10} + \tau Y^{01} + 2\gamma Y^{12} - (2\gamma + 2\tau)Y^{11}, \\ \dot{Y}^{01} &= 2\gamma Y^{02} + \gamma Y^{11} - (\gamma + \tau)Y^{01}, & \dot{Y}^{03} &= \gamma Y^{13} - (3\gamma + 3\tau)Y^{03}, \\ \dot{Y}^{10} &= \gamma Y^{11} - (\gamma + 3\tau)Y^{10}, & \dot{Y}^{12} &= 3\gamma Y^{13} + 2\tau(Y^{02} + Y^{11}) - (3\gamma + \tau)Y^{12}, \\ \dot{Y}^{02} &= 3\gamma Y^{03} + \gamma Y^{12} - (2\gamma + 2\tau)Y^{02}, & \dot{Y}^{13} &= 3\tau Y^{03} + \tau Y^{12} - 4\gamma Y^{13}. \end{aligned}$$

The system for the X variables would have 16 equations. Here, we have reduced this to 8, at the cost that we can no longer resolve individual states.

Exercise 2.10. Consider a different partition of the states in Fig. 2.5, where \mathcal{C}^k is made up of all states with k infected nodes. Let Y_k be the probability that k nodes are infected. Show that we cannot write down a system of linear differential equations just in terms of Y_k . [Hint: Assume that initially $X_{SSS} = 1$ and calculate the initial rate of change of Y_2 . Repeat with $X_{SSS} = 1$.]

2.4.3 Lumping of linear systems

In Example 2.8, the lumping worked because it provided a partition such that for any two classes \mathcal{C}_i and \mathcal{C}_j we could express the total flow of probability from \mathcal{C}_i to \mathcal{C}_j as some constant times the amount of probability in \mathcal{C}_i . In fact, a stronger condition holds: each state $\mathcal{S}_r \in \mathcal{C}_i$ has the property that the combined flow from it to the states in \mathcal{C}_j gave the same value, regardless of \mathcal{S}_r . This motivates the following definition.

Definition 2.4 A Markov process is called lumpable if there is a partition of the states $\{\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_n\}$ into a set of classes $\mathcal{C} = \{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_m\}$ such that for any two classes \mathcal{C}_j and \mathcal{C}_l the sum

$$\bar{A}_{jl} = \sum_{\mathcal{S}_i \in \mathcal{C}_j} h(\mathcal{S}_r, \mathcal{S}_i)$$

takes the same value for any $S_r \in \mathcal{C}_l$. Then, the partition $\{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_m\}$ is called a lumping of the state space.

The sum represents the combined transition rate from S_r to any state in \mathcal{C}_j .

We now explore the mathematical concept of lumping for a general system, which can be expressed in the form

$$\dot{X} = AX,$$

where A is an arbitrary $n \times n$ matrix. If we think of the components of X as measuring the probability (or some other quantity) of the states of a system, then our goal is to partition the states in such a way that if we take Y to be a vector whose entries give the sum of X_i for each class, we can arrive at a new linear system for Y . The key detail that guaranteed this previously is that given two classes, \mathcal{C}_l and \mathcal{C}_j , and any state $S_r \in \mathcal{C}_l$, the combined flux from S_r into all of the states in \mathcal{C}_j is proportional to X_r , with the same proportionality constant holding for all $S_r \in \mathcal{C}_l$.

We now express this condition in terms of the matrix A . The following definition goes back to the so-called Dynkin criterion [100].

Definition 2.5 *The linear system $\dot{X} = AX$ is called lumpable if there is a partition $L = \{L_1, L_2, \dots, L_m\}$ of the set $\{1, 2, \dots, n\}$ satisfying the following property: for any classes L_j and L_l , there exists a number \bar{A}_{jl} such that*

$$\bar{A}_{jl} = \sum_{i \in L_j} A_{ir}, \text{ for } r \in L_l,$$

that is, the sum does not depend on r whenever $r \in L_l$. The $m \times m$ matrix \bar{A} is called a lumping of matrix A , and the partition L is called a lumping of $\{1, 2, \dots, n\}$.

If the linear system corresponds to a Markov process, then either both the system and the process are lumpable or both are not. This follows by taking L to be the induced partition of the classes.

We will define $Y_j = \sum_{i \in L_j} X_i$ and set Y to be the vector whose entries are Y_j . Then, taking \bar{A} we will show that

$$\dot{Y} = \bar{A}Y. \quad (2.14)$$

We derive equation (2.14) in several steps. First, consider a lumping $\{L_1, L_2, \dots, L_m\}$ of $\{1, 2, \dots, n\}$. We define the vectors U_j for $j = 1, \dots, m$ such that the i th entry of U_j is 1 if $i \in L_j$ and 0 otherwise. Then, the dot product of U_j with X gives $Y_j = \sum_{i \in L_j} X_i$. Taking the matrix U whose j th row is U_j , we have

$$Y = UX.$$

where Y is the vector whose entries are Y_j .

The following simple result about UA holds.

Proposition 2.1 *If matrix \bar{A} is a lumping of matrix A and U is as defined above, then $UA = \bar{A}U$.*

Proof. The element in the j th row and r th column of UA is

$$(UA)_{jr} = \sum_{i=1}^n U_{ji}A_{ir} = \sum_{i \in L_j} A_{ir} = \bar{A}_{jl},$$

where l is the index for which $r \in L_l$. The element in the j th row and r th column of $\bar{A}U$ is

$$(\bar{A}U)_{jr} = \sum_{k=1}^m \bar{A}_{jk}U_{kr} = \bar{A}_{jl},$$

where l is the index such that $r \in L_l$, since every column of U has a single unit entry, the rest being zero. Thus, the two expressions are equal. \square

We are now able to prove that $\dot{Y} = \bar{A}Y$.

Proposition 2.2 *Let \bar{A} be a lumping of matrix A and let U be the matrix for which $UA = \bar{A}U$ holds. Based on this, we introduce the new, m -dimensional (lumped) variable $Y = UX$. This lumped variable satisfies the lumped linear ODE system $\dot{Y} = \bar{A}Y$.*

Proof. We already have $Y = UX$ and U is a constant matrix. Thus, $\dot{Y} = U\dot{X}$, but $\dot{X} = AX$. So we have $\dot{Y} = UAX$. As $UA = \bar{A}U$, our system becomes $\dot{Y} = \bar{A}UX$. Substituting for UX , we finally have

$$\dot{Y} = \bar{A}Y.$$

\square

The crucial step in lumping is finding the partition of the state space. This can either be derived intuitively through the symmetries of the network or by attempting to identify partitions that satisfy the properties stated in Definition 2.4 or 2.5. Once the partition is known, both \bar{A} and U follow. The lumpability condition on A is a non-trivial requirement, and not all systems will be lumpable.

It should be noted that the results we have proven are more general than what we need. For the systems we consider, we are always considering vectors X that represent probabilities. The proofs did not rely on this, and so the same procedure will work for more general systems, but we do not investigate this further.

2.4.4 The use of graph symmetries to lump a binary dynamic network model

We found the partition for the star network SIS system of Example 2.8 by identifying states that were symmetric and lumping them into a single class. In this section, we see that this approach works in general. It should be noted that this is not the only option for lumping a system to get simpler equations. As a trivial example

for any disease, there is always the option to create a partition with just a single class \mathcal{C}^* containing all states, then we would arrive at the equation $\dot{Y}^* = 0$. This is mathematically simple, but it has no informational value beyond stating that the quantity we are measuring (probability in this case) is preserved. There is a balance between simplicity and information content.

Our goal after lumping the states is to recover information about the number of nodes of each status. So all states that are lumped together must have the same number of nodes of each status. In this section, we show a procedure for finding lumpings that respect this property if there are symmetries. We focus our attention on binary processes to keep the indexing simple, but the approach is more general.

Consider now an arbitrary binary dynamic process spreading in a network, such as SIS disease. We will arbitrarily set the node statuses to be Q and T . For a network of N nodes, there are 2^N possible states. We recall the important partition

$$\{\mathcal{C}^0, \mathcal{C}^1, \dots, \mathcal{C}^N\},$$

where \mathcal{C}^k denotes the class made up of all states with k nodes of status T . There are $c_k = \binom{N}{k}$ states in \mathcal{C}^k , denoted $\mathcal{S}_1^k, \mathcal{S}_2^k, \dots, \mathcal{S}_{c_k}^k$. We set X_i^k to be the probability of state \mathcal{S}_i^k and use X^k to be a vector whose entries are the probabilities of each state of \mathcal{C}^k . That is, $X^k = (X_1^k, X_2^k, \dots, X_{c_k}^k)$, and we use X to be the vector formed by taking the entries of X^0 , then of X^1 and so forth until X^N .

We have already seen that we cannot necessarily write down a consistent system of equations if we choose $\mathcal{C}^0, \mathcal{C}^1, \dots, \mathcal{C}^N$ to be our partition (Exercises 2.2 and 2.10). We will have to refine this partition. However, equation (2.6) shows that for this partition, the equations for a given X^k can be expressed entirely in terms of X^{k-1} , X^k and X^{k+1}

$$\dot{X}^k = A^k X^{k-1} + B^k X^k + C^k X^{k+1}, \quad k = 0, 1, \dots, N$$

for some matrices A^k, B^k and C^k , with B^k being a diagonal matrix. Then, $\dot{X} = PX$, where

$$P = \begin{pmatrix} B^0 & C^0 & 0 & \dots & 0 \\ A^1 & B^1 & C^1 & \dots & \vdots \\ 0 & A^2 & B^2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & C^{N-1} \\ 0 & \dots & \dots & A^N & B^N \end{pmatrix}.$$

The specific form of these submatrices depends on the network structure and the spreading binary process.

Definition 2.6 Given a set and a partition of that set $J = \{J_1, J_2, \dots, J_{m_J}\}$, a second partition $L = \{L_1, L_2, \dots, L_{m_L}\}$ is a refinement of J if for every L_l there is a J_j such that $L_l \subseteq J_j$.

If L is a refinement of J , and we denote all of the L_i that are a subset of J_j by $L_1^j, L_2^j, \dots, L_{l_j}^j$, then these form a partition of J_j .

For simplicity, we will assume that the states are indexed from 1 to 2^N , so that if $i < j$, then the number of nodes in state S_i having status T is less than or equal to the number of nodes in S_j having status T . If the number of nodes with status T is the same, the ordering is arbitrary, but it is unchanging.

We now turn specifically to partitions of our state space. There are 2^N possible states S_1, S_2, \dots, S_{2^N} .

Definition 2.7 *Given the partition of $\{S_1, S_2, \dots, S_{2^N}\}$ into $\{\mathcal{C}^0, \mathcal{C}^1, \dots, \mathcal{C}^N\}$, we say that a lumping respects $\{\mathcal{C}^0, \mathcal{C}^1, \dots, \mathcal{C}^N\}$ if the partition for the lumping is a refinement of $\{\mathcal{C}^0, \mathcal{C}^1, \dots, \mathcal{C}^N\}$.*

In Example 2.8, the lumping respected the partition $\{\mathcal{C}^0, \mathcal{C}^1, \mathcal{C}^2, \mathcal{C}^3, \mathcal{C}^4\}$, with $\mathcal{C}^1, \mathcal{C}^2$ and \mathcal{C}^3 each divided into two smaller classes. Our goal is to find a lumping \bar{P} of P that respects the partition $\{\mathcal{C}^0, \mathcal{C}^1, \mathcal{C}^2, \dots, \mathcal{C}^N\}$.

Consider a refinement of $\{\mathcal{C}^0, \mathcal{C}^1, \mathcal{C}^2, \dots, \mathcal{C}^N\}$. For every k , let $\{\mathcal{C}_1^k, \mathcal{C}_2^k, \dots, \mathcal{C}_{l_k}^k\}$ denote those classes in the refined partition that are a subset of \mathcal{C}^k . To test whether this partition provides a lumping, we check that Definition 2.4 is satisfied. Let \mathcal{C}_j^h and \mathcal{C}_l^k be any two classes in the partition of the state space. If the number of nodes of status T differ by two or more, then the flow between these states is zero. Alternately, if the number of nodes of each status is the same and the classes are not the same, then again the flow between these classes is zero. So the properties of the definition are immediately satisfied for these cases. Thus, we only need to consider \mathcal{C}_j^h and \mathcal{C}_l^k if the number of nodes in status T differ by exactly 1 or if $\mathcal{C}_j^h = \mathcal{C}_l^k$.

Lemma 2.8 *The binary Markov process described by equation (2.6) has a lumping that respects $\{\mathcal{C}^0, \mathcal{C}^1, \dots, \mathcal{C}^N\}$ if each class \mathcal{C}^k may be partitioned into $\{\mathcal{C}_1^k, \mathcal{C}_2^k, \dots, \mathcal{C}_{l_k}^k\}$ and the following properties hold for any k :*

- For any classes \mathcal{C}_l^{k-1} and \mathcal{C}_j^k , there exists a number \bar{A}_{jl}^k such that

$$\bar{A}_{jl}^k = \sum_{S_i \in \mathcal{C}_j^k} h(S_r, S_i) \quad (2.15)$$

for any $S_r \in \mathcal{C}_l^{k-1}$.

- For any classes \mathcal{C}_l^{k+1} and \mathcal{C}_j^k , there exists a number \bar{C}_{jl}^k such that

$$\bar{C}_{jl}^k = \sum_{S_i \in \mathcal{C}_j^k} h(S_r, S_i) \quad (2.16)$$

for any $S_r \in \mathcal{C}_l^{k+1}$.

Proof. To prove this, we show that Definition 2.4 holds for any \mathcal{C}_j^m and \mathcal{C}_l^k , that is, we just show that for any two classes \mathcal{C}_j^m and \mathcal{C}_l^k , the sum $\sum_{\mathcal{S}_i \in \mathcal{C}_j^m} h(\mathcal{S}_r, \mathcal{S}_i)$ is the same for all $\mathcal{S}_r \in \mathcal{C}_l^k$. We break this into four parts:

- If $|m - k| \geq 2$, then at least two nodes are required to change status of the system to move from any \mathcal{S}_r to \mathcal{S}_i . Thus, the sum is trivially 0.
- If $m = k - 1$, then satisfying the first condition is the same as satisfying Definition 2.4.
- If $m = k + 1$, then satisfying the second condition is the same as satisfying Definition 2.4.
- If $m = k$ and $\mathcal{C}_j^k \neq \mathcal{C}_l^k$, then the system cannot move between states in these classes because any change of state will change the number of nodes with status T . Thus, the only case remaining to check is if $\mathcal{C}_j^k = \mathcal{C}_l^k$. In this case, if $\mathcal{S}_i \neq \mathcal{S}_r$, the result is still zero, so the sum collapses to just a single term:

$$\sum_{\mathcal{S}_i \in \mathcal{C}_j^m} h(\mathcal{S}_i, \mathcal{S}_r) = h(\mathcal{S}_r, \mathcal{S}_r).$$

From equation (2.4) we have

$$h(\mathcal{S}_r, \mathcal{S}_r) = - \sum_{\mathcal{S}_i \in \mathcal{C}^{k+1}} h(\mathcal{S}_r, \mathcal{S}_i) - \sum_{\mathcal{S}_i \in \mathcal{C}_{k-1}} h(\mathcal{S}_r, \mathcal{S}_i).$$

Alternately, we can show this by referring to the diagonal element of B^k . If the conditions of the lemma hold, then this sum will be the same for all $\mathcal{S}_r \in \mathcal{C}_l^k$.

□

Equation 2.15 states that for any state \mathcal{S}_r in the class \mathcal{C}_l^{k-1} , the total flux into \mathcal{C}_j^k is proportional to the probability of state \mathcal{S}_r with the same proportionality constant \bar{A}_{jl}^k . Equation (2.16) is equivalent, but for \mathcal{C}_l^{k+1} to \mathcal{C}_j^k . Thus, for these cases the flux of probability from one class to another is simply a constant times the combined probability in the first class.

We are almost ready to prove the main result of this section, that if we place “symmetric” states into the same partition, then we arrive at a valid lumping. We first need to give a mathematical definition of what “symmetric” means in this context.

Definition 2.9 Let $G = G(V, E)$ be a graph with vertices and edges given by sets $V(G)$ and $E(G)$, respectively. A bijection $\Phi : V(G) \rightarrow V(G)$ such that $(x, y) \in E(G)$ if and only if $(\Phi(x), \Phi(y)) \in E(G)$ is an automorphism of graph G . The set of all automorphisms of G , under the composition of maps, forms the automorphism group denoted by $\text{Aut}(G)$ ([82, 330]).

In less mathematical language, we can think of the graph drawn on paper. Applying the function Φ to the node labels corresponds to relabelling the nodes, so that node x is now labelled with the label $\Phi(x)$ (see Fig. 2.6). If the result of replacing each node name x by $\Phi(x)$ is a graph that is identical to what would be seen after

	1	2	3	4	5
$A_1 = \text{id}$	1	2	3	4	5
$A_2 = \text{rot}$	5	1	2	3	4
$A_3 = \text{rot}$	4	5	1	2	3
$A_4 = \text{rot}$	3	4	5	1	2
$A_5 = \text{rot}$	2	3	4	5	1
$A_6 = \text{ref}$	1	5	4	3	2
$A_7 = \text{ref}$	3	2	1	5	4
$A_8 = \text{ref}$	5	4	3	2	1
$A_9 = \text{ref}$	2	1	5	4	3
$A_{10} = \text{ref}$	4	3	2	1	5

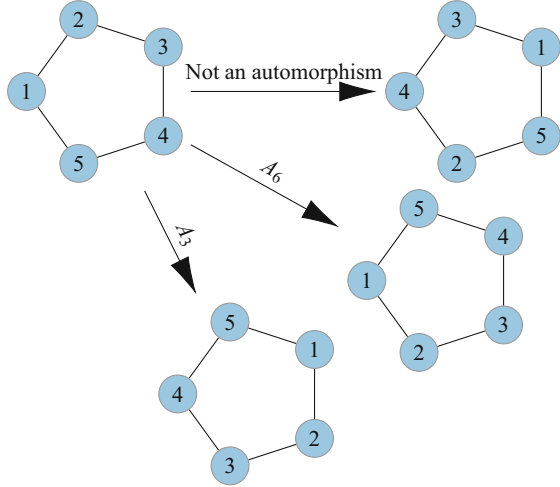


Fig. 2.6: (Left) The automorphism group of the cycle network with 5 nodes, composed from rotations and reflections. (Right) Examples of A_3 , A_6 and a permutation that is not an automorphism.

moving each node $\Phi(x)$ to the current location of x (with any associated edges following), then Φ is an automorphism. It is important to note that if we perform one automorphism to G and then perform another to the result, the combined outcome is also an automorphism of the original graph.

If the nodes of a graph have some status associated with them, then we say that Φ takes the state S_i to state S_j if $S_i(l) = S_j(\Phi(l))$ for all l . In this case, we write $S_j = \Phi(S_i)$.

Definition 2.10 *Given the automorphisms of a graph, the orbit of a state S_j is the class of states of the form $\Phi(S_j)$ for all automorphisms Φ .*

If there is some Φ such that $S_i = \Phi(S_j)$, then the orbits of the two are identical.

We introduce an equivalence relation for \mathcal{C} , saying states are equivalent if they are in the same orbit. We call this the automorphism equivalence relation. The set of orbits form a partition of the states. If we list an orbit in some order $S_{j_1}, S_{j_2}, \dots, S_{j_m}$ and then perform the same automorphism to each state, we get back the same class of states, but in a new order. So the automorphism only permutes the elements of an orbit.

Exercise 2.11.

- Show that all equivalent states have the same number of nodes of status T .
- Show that if we create a partition such that each class is made up of a set of equivalent states, then we have a refinement of $\{\mathcal{C}^0, \mathcal{C}^1, \dots, \mathcal{C}^N\}$.

We can now formulate our main result connecting the automorphism group of the graph to the lumping of the Markov chain.

Theorem 2.11 *If we partition the states by creating classes made up of states that are equivalent under automorphisms, then the resulting partition yields a lumping that respects $\{\mathcal{C}^0, \mathcal{C}^1, \dots, \mathcal{C}^N\}$.*

To prove this theorem, we will rely on the observation that if the flow from state \mathcal{S}_{l_1} to \mathcal{S}_{j_1} is cX_{l_1} for some constant rate c , and if Φ takes \mathcal{S}_{l_1} to \mathcal{S}_{l_2} and \mathcal{S}_{j_1} to \mathcal{S}_{j_2} , then the flow from \mathcal{S}_{l_2} to \mathcal{S}_{j_2} is cX_{l_2} .

Proof. Let the partition be given as $\{\mathcal{C}_j^k \subset \mathcal{C}^k : j = 1, 2, \dots, n_k, k = 0, 1, \dots, N\}$. The assumption of the theorem can be formulated as follows: for any $k \in \{0, 1, \dots, N\}$, $j \in \{1, 2, \dots, n_k\}$ and $\mathcal{S}_r, \mathcal{S}_q \in \mathcal{C}_j^k$, there is an automorphism Φ , for which $\Phi(\mathcal{S}_r) = \mathcal{S}_q$. Lemma 2.8 will be applied to prove the statement. We will check that condition (2.15) holds. Equation (2.16) can be checked similarly. Let \mathcal{C}_l^{k-1} and \mathcal{C}_j^k be arbitrary classes in the partition and $\mathcal{S}_r \in \mathcal{C}_l^{k-1}$ be an arbitrary state. We show that the sum in (2.15) is independent of the choice of the state \mathcal{S}_r .

We first prove that the relation

$$h(\Phi(\mathcal{S}_r), \Phi(\mathcal{S}_i)) = h(\mathcal{S}_r, \mathcal{S}_i) \quad (2.17)$$

holds for any automorphism Φ . If $h(\mathcal{S}_r, \mathcal{S}_i) \neq 0$, then there is a single node x whose status is Q in \mathcal{S}_r and T in \mathcal{S}_i , and all other nodes have the same status in both. The value of $h(\mathcal{S}_r, \mathcal{S}_i)$ is given by some function $f_{QT}(n_Q, n_T)$, where n_Q is the number of neighbours of x having status Q and n_T is the number of nodes with status T in state \mathcal{S}_r . Consider an automorphism Φ . Then, $y = \Phi(x)$ has status Q in $\Phi(\mathcal{S}_r)$ and T in $\Phi(\mathcal{S}_i)$. All other nodes have the same status in both. The number of neighbours of y with each status is again n_Q and n_T , so $h(\Phi(\mathcal{S}_r), \Phi(\mathcal{S}_i)) = f_{QT}(n_Q, n_T)$, which proves (2.17).

Now let $\mathcal{S}_q \in \mathcal{C}_l^{k-1}$ be an arbitrary but fixed state in its class. Let Φ be an automorphism taking \mathcal{S}_r to \mathcal{S}_q , i.e. $\Phi(\mathcal{S}_r) = \mathcal{S}_q$. Using (2.17), we get

$$\sum_{\mathcal{S}_i \in \mathcal{C}_j^k} h(\mathcal{S}_r, \mathcal{S}_i) = \sum_{\mathcal{S}_i \in \mathcal{C}_j^k} h(\Phi(\mathcal{S}_r), \Phi(\mathcal{S}_i)) = \sum_{\mathcal{S}_i \in \mathcal{C}_j^k} h(\mathcal{S}_q, \Phi(\mathcal{S}_i)).$$

This shows that the sum is independent of which r is chosen, completing the proof. \square

2.5 Applications of lumping

We can now take the results of the previous section and use it to develop a recipe for lumping. We begin with the assumption that the network under consideration has symmetries, and that we are able to find them. In practice, there may not be any symmetries, or it may be difficult to identify them (see, e.g., Chapter 3 in [330]). Our approach is restricted to networks for which it is possible to find the symmetries.

Recipe for lumping: Given a network G , and a dynamic process spreading on the network, the steps to derive the reduced master equations are:

1. Identify a group of automorphisms (symmetries) of the network.
2. Partition the states so that two states are in the same class if there is an automorphism that maps one to the other (each is a subset of \mathcal{C}^k for some k).
3. From each class \mathcal{C}_l , choose a single state \mathcal{S}_r . For each other class $\mathcal{C}_j \neq \mathcal{C}_l$, calculate

$$\bar{\mathcal{A}}_{jl} = \sum_{\mathcal{S}_i \in \mathcal{C}_j} h(\mathcal{S}_r, \mathcal{S}_i).$$

4. Define the diagonal element $\bar{\mathcal{A}}_{jj}$ so that the columns sum to zero: $\bar{\mathcal{A}}_{jj} = -\sum_{l \neq j} \bar{\mathcal{A}}_{jl}$.

Then if Y_j measures the total probability of being in \mathcal{C}_j , the lumped equations become

$$\dot{Y} = \bar{\mathcal{A}}Y,$$

where Y is the vector of Y_j .

Fig. 2.7: A method to generate the lumped equations.

We now apply these steps to several examples. Throughout, \mathcal{C}^k denotes the set of states with k infected nodes for SIS disease (or with k “status T ” nodes for other binary processes). For the final lumping partition, we use $\mathcal{C}_1^k, \mathcal{C}_2^k, \dots, \mathcal{C}_{l_k}^k$ to denote the subclasses of \mathcal{C}^k . If there is no subclass, we use $\mathcal{C}_1^k = \mathcal{C}^k$.

2.5.1 Lumping for some small networks

We now show some applications of the recipe in Fig. 2.7 to small networks.

Example 2.9. Consider SIS dynamics on a line graph with $N = 3$ nodes, as in Fig. 2.2a. Then, the state space is $\{SSS, SSI, SIS, ISS, SII, ISI, IIS, III\}$, where, for example, SSI represents the state of the network in which the statuses of nodes 1 and 2 are S and the status of node 3 is I. The states SSI and ISS are equivalent via a reflection around the central node; hence, they are in the same lumping class. However, the state SIS is not equivalent to these as it cannot be mapped into either via a graph automorphism, since in this state the I node has two S neighbours, while in the two other states the I node has only a single S neighbour.

Thus, the class $\mathcal{C}^1 = \{SSI, SIS, ISS\}$ consists of two lumping classes, namely $\{SSI, ISS\}$ and $\{SIS\}$. Similar reasoning leads to the observation that the class $\mathcal{C}^2 = \{SII, ISI, IIS\}$ consists of two lumping classes, namely $\{SII, IIS\}$ and $\{ISI\}$. Thus, the lumping classes are $\mathcal{C}_1^0 = \{SSS\}$, $\mathcal{C}_1^1 = \{SSI, ISS\}$, $\mathcal{C}_2^1 = \{SIS\}$, $\mathcal{C}_1^2 = \{SII, IIS\}$, $\mathcal{C}_2^2 = \{ISI\}$ and $\mathcal{C}_3^3 = \{III\}$.

As an example, we consider \mathcal{C}_1^2 and arbitrarily choose SII . The states reachable from SII are III, SSI and SIS. We have $h(SII, III) = \tau$, $h(SII, SSI) = \gamma$ and

$h(\text{SII}, \text{SIS}) = \gamma$. Thus, the flow from \mathcal{C}_1^2 to \mathcal{C}_1^3 is τY_1^2 , the flow to \mathcal{C}_1^1 is γY_1^2 and the flow to \mathcal{C}_2^1 is γY_1^2 . The terms corresponding to other starting states can be calculated similarly (see Exercise 2.13).

Once the process is complete, we have a single equation for each class. Thus, the full system of $2^3 = 8$ differential equations can be lumped to 6 equations. This is not a large gain, but for similar larger systems the reduction becomes significant.

Exercise 2.12. Using the full system of master equations in Exercise 2.4, for the 3-node line graph, write each Y as a linear combination of the probabilities of states in a given class. Then, differentiating this equation and using careful substitution, derive the lumped system for the above example.

Exercise 2.13. By using the recipe in Fig. 2.7, derive the lumped system for the 3-node line graph.

Choosing another process with binary dynamics, while keeping the same graph, gives the same lumping classes; only the coefficients in the lumped system change. This can be checked by solving the following exercise.

Exercise 2.14. Using the recipe in Fig. 2.7, write down the full system of master equations and the lumped system for QAQ dynamics on a line graph with $N = 3$ nodes.

In order to better understand how to find the lumping classes, it is useful to examine the lumping for some graphs with $N = 4$ nodes. The lumping recipe does not depend on the dynamics; hence, in the examples below the dynamic will not be specified: a general binary dynamics with two statuses Q and T will be used. For each graph, the reader is asked to formulate the lumped system for a given dynamics.

Example 2.10. Consider a general binary dynamics with two statuses Q and T on a complete graph with $N = 4$ nodes (see Fig. 2.8b). We again take \mathcal{C}^k to denote the class of states with k nodes of status T . All four states in class \mathcal{C}^1 are equivalent via suitable graph automorphisms, since any permutation of the nodes is an automorphism. For example, state $QTQQ$ can be taken to state $QQQT$ by an automorphism Φ , for which $\Phi(2) = 4$, $\Phi(4) = 2$, $\Phi(1) = 1$ and $\Phi(3) = 3$. Thus, \mathcal{C}^1 is a single lumping class. Similarly, all six states in class \mathcal{C}^2 are equivalent via suitably chosen graph automorphisms. For example, state $QTQT$ is equivalent to state $QQT T$ via the automorphism Φ , for which $\Phi(2) = 3$, $\Phi(3) = 2$, $\Phi(1) = 1$ and $\Phi(4) = 4$; this Φ is not unique. Thus, \mathcal{C}^2 is a single lumping class. The same is true for \mathcal{C}^3 ; hence, the lumping classes are $\mathcal{C}_1^0 = \mathcal{C}^0$, $\mathcal{C}_1^1 = \mathcal{C}^1$, $\mathcal{C}_1^2 = \mathcal{C}^2$, $\mathcal{C}_1^3 = \mathcal{C}^3$ and $\mathcal{C}_1^4 = \mathcal{C}^4$. Thus, the full system of $2^4 = 16$ differential equations can be lumped to 5 equations on a complete graph.

Exercise 2.15. By using the recipe in Fig. 2.7, write down the lumped system for SIS dynamics on a complete graph with $N = 4$ nodes.

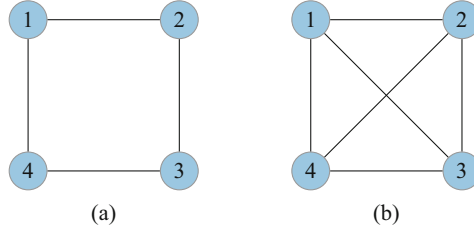


Fig. 2.8: Cycle (a) and fully connected (b) networks with 4 nodes.

Example 2.11. Consider a general binary dynamics with two statuses Q and T on a star graph with $N = 4$ nodes, as in Fig. 2.2c. The central node is numbered 1 and the leaves are numbered 2, 3 and 4. The states $QTQQ$, $QQTQ$ and $QQQT$ of the class \mathcal{C}^1 are all equivalent via suitable graph automorphisms, since for these states, any permutation of the nodes that keeps the central node fixed is an automorphism. For example, state $QTQQ$ is equivalent to state $QQTQ$ via an automorphism, Φ , for which $\Phi(2) = 3$, $\Phi(3) = 2$, $\Phi(1) = 1$ and $\Phi(4) = 4$. However, state $TQQQ$ is not equivalent to any of the above since no such automorphism exists. This is because, in the latter state, the node with status T has three neighbours of status Q , while in the other states it has a single neighbour of status Q . Thus, \mathcal{C}^1 consists of two lumping classes: $\{QTQQ, QQTQ, QQQT\}$ and $\{TQQQ\}$. Similarly, states in class \mathcal{C}^2 for which the central node is of status T are equivalent via appropriately chosen automorphisms. For example, state $TQTQ$ is equivalent to state $TQQT$ via the automorphism Φ , for which $\Phi(3) = 4$, $\Phi(4) = 3$, $\Phi(1) = 1$ and $\Phi(2) = 2$. Thus, \mathcal{C}^2 consists of two lumping classes: $\{TTQQ, TQTQ, TQQT\}$ and $\{QTTQ, QQTT, QTQT\}$. The class \mathcal{C}^3 can also be divided into two lumping classes; hence, the lumping classes are

$$\begin{aligned} \mathcal{C}_1^0 &= \mathcal{C}^0, & \mathcal{C}_1^1 &= \{QTQQ, QQTQ, QQQT\}, & \mathcal{C}_2^1 &= \{TQQQ\}, \\ \mathcal{C}_1^2 &= \{QTTQ, QQTT, QTQT\}, & \mathcal{C}_2^2 &= \{TTQQ, TQTQ, TQQT\}, \\ \mathcal{C}_1^3 &= \{QTTT\}, & \mathcal{C}_2^3 &= \{TTTQ, TTQT, TQTT\}, & \mathcal{C}_1^4 &= \mathcal{C}^4. \end{aligned}$$

These are the partitions seen in Fig. 2.5. The full system of $2^4 = 16$ differential equations can be lumped to 8 equations on the star graph, as we saw in Example 2.8.

Exercise 2.16. By using the recipe in Fig. 2.7, write down the lumped system for the voter model (Example 2.4) on a star graph with $N = 4$ nodes.

Example 2.12. Consider a general binary dynamics with two statuses Q and T on a cycle graph with $N = 4$ nodes, as in Fig. 2.8a. All four states in class \mathcal{C}^1 are equivalent via a suitable rotation. For example, state $QTQQ$ can be taken to state $QQTQ$ via the automorphism Φ , for which $\Phi(2) = 3$, $\Phi(3) = 4$, $\Phi(4) = 1$ and $\Phi(1) = 2$. Thus, \mathcal{C}^1 forms a single lumping class. Similarly, there are four states in class \mathcal{C}^2 (i.e. $\{TTQQ, QTTQ, QQTT, TQQT\}$) that are equivalent via automorphisms, namely

via rotations. For example, state $QTTQ$ is equivalent to state $QQTT$ by the rotation Φ , given by $\Phi(2) = 3$, $\Phi(3) = 4$, $\Phi(4) = 1$ and $\Phi(1) = 2$. Thus, \mathcal{C}^2 consists of two lumping classes: $\{TTQQ, QTTQ, QQTT, TQQT\}$ and $\{QTQT, TQTQ\}$. The class \mathcal{C}^3 forms a single lumping class, because its elements are all equivalent via rotations. Hence, the lumping classes are

$$\begin{aligned}\mathcal{C}_1^0 &= \mathcal{C}^0, & \mathcal{C}_1^1 &= \mathcal{C}^1, & \mathcal{C}_1^2 &= \{TTQQ, QTTQ, QQTT, TQQT\}, \\ \mathcal{C}_2^2 &= \{QTQT, TQTQ\}, & \mathcal{C}_1^3 &= \mathcal{C}^3, & \mathcal{C}_1^4 &= \mathcal{C}^4.\end{aligned}$$

Thus, the full system of $2^4 = 16$ differential equations can be lumped to 6 equations on a cycle graph with 4 nodes. We note that reflections are not needed in building up the lumping classes.

Exercise 2.17. By using the recipe in Fig. 2.7, write down the lumped system for SIS dynamics on a cycle graph with $N = 4$ nodes.

Example 2.13. Consider a general binary dynamics with two statuses Q and T on a line graph with $N = 4$ nodes, as in Fig. 2.2b. States $TQQQ$ and $QQQT$ of class \mathcal{C}^1 are equivalent via a reflection. States $QTQQ$ and $QQTQ$ of class \mathcal{C}^1 are also equivalent via a reflection. However, states $QQQT$ and $QTQQ$ are not equivalent. This is because in state $QQQT$, the node with status T has one neighbour of status Q , while in state $QTQQ$, it has two. There is no automorphism between the states. Thus, \mathcal{C}^1 consists of two lumping classes: $\{TQQQ, QQQT\}$ and $\{QTQQ, QQTQ\}$. Similarly, state $TQQT$ in class \mathcal{C}^2 is not equivalent to any other state of this class. In this state, both nodes of status T have a single neighbour, which is of status Q . However, state $TTQQ$ is equivalent to $QQTT$ via a reflection. Since the only nontrivial automorphism of the graph is the reflection, class \mathcal{C}^2 is divided into four lumping classes: $\{TQQT\}$, $\{QTTQ\}$, $\{TTQQ, QQTT\}$ and $\{TQTQ, QTQT\}$. Class \mathcal{C}^3 can be divided into two lumping classes; hence, the lumping classes are

$$\begin{aligned}\mathcal{C}_1^0 &= \mathcal{C}^0, & \mathcal{C}_1^1 &= \{TQQQ, QQQT\}, & \mathcal{C}_2^1 &= \{QTQQ, QQTQ\}, & \mathcal{C}_1^2 &= \{TQQT\} \\ \mathcal{C}_2^2 &= \{QTTQ\}, & \mathcal{C}_3^2 &= \{TTQQ, QQTT\}, & \mathcal{C}_4^2 &= \{TQTQ, QTQT\}, \\ \mathcal{C}_1^3 &= \{TTTQ, QTTT\}, & \mathcal{C}_2^3 &= \{TTQT, TQTT\}, & \mathcal{C}_1^4 &= \mathcal{C}^4.\end{aligned}$$

Thus, the full system of $2^4 = 16$ differential equations can be lumped to 10 equations on a line graph with 4 nodes.

Exercise 2.18. By using the recipe in Fig. 2.7, write down the lumped system for SIS dynamics on a line graph with $N = 4$ nodes.

Exercise 2.19. Determine the lumping classes for a general binary dynamics on a lollipop network (see Fig. 2.9a).

Exercise 2.20. Determine the lumping classes for a general binary dynamics on a toast network (see Fig. 2.9b).

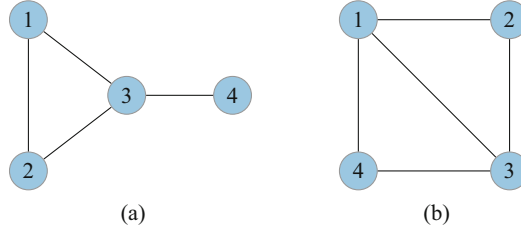


Fig. 2.9: (a) Lollipop and (b) toast networks with 4 nodes.

Exercise 2.21. Consider an SIR disease spreading on a single edge as in Example 2.6. Derive the lumped system.

Exercise 2.22. Consider SIR spread on a fully connected 3-node graph. The states are given in Example 2.7. Derive the lumped system.

Exercise 2.23. Consider SIR spread on the line network with three nodes. The states and master equations are given in Example 2.7. Derive the lumped system.

2.5.2 Lumping for some classes of networks of arbitrary size

In this section, we show applications of the general lumping theorem and demonstrate lumping for some arbitrarily large graphs with special symmetry structure.

Lumping for the complete network

First, we show that for a complete graph the 2^N -dimensional system given by (2.6) can be lumped to an $(N+1)$ -dimensional system. The lumped system is well known in the literature, but so far as we are aware, it was first derived from the full 2^N -dimensional system in [288].

The automorphism group of the complete graph is the permutation group \mathbf{S}_N , that is, any relabelling is an automorphism. Hence, the orbit of any element from \mathcal{C}^k is equal to \mathcal{C}^k itself. All states with k infected nodes can be lumped together. There are $N+1$ lumping classes: \mathcal{C}^k for all $k \in \{0, 1, \dots, N\}$. We have

$$Y^k = \sum_{j=1}^{c_k} X_j^k, \quad k = 1, \dots, N.$$

Proposition 2.3 *If G is a complete graph, then the Y^k functions satisfy the following differential equations:*

$$\dot{Y}^0 = f_{TQ}(N-1)Y^1 - Nf_{QT}(0)Y^0,$$

$$\begin{aligned}
\dot{Y}^k &= (k+1)f_{TQ}(N-k-1)Y^{k+1} + (N-k+1)f_{QT}(k-1)Y^{k-1} \\
&\quad - ((N-k)f_{QT}(k) + kf_{TQ}(N-k))Y^k, \text{ for } k = 1, 2, \dots, N-1, \\
\dot{Y}^N &= f_{QT}(N-1)Y^{N-1} - Nf_{TQ}(0)Y^N.
\end{aligned}$$

Proof. Using the steps of Fig. 2.7, we need only consider a single \mathcal{S}_k chosen from each \mathcal{C}^k . For simplicity, we choose the state $T \cdots T Q \cdots Q$, where nodes 1 through k have status T and the remaining $(N-k)$ nodes have status Q .

For state \mathcal{S}_k , each of the $(N-k)$ nodes of status Q has k neighbours of status T . So the rate of moving from \mathcal{S}_k to any state in \mathcal{C}^{k+1} is $(N-k)f_{QT}(k)$. Similarly, each of the k neighbours of status T has $(N-k)$ neighbours of status Q . Thus, the rate of moving from \mathcal{S}_k to \mathcal{S}_{k-1} is $kf_{TQ}(N-k)$. Thus

$$\begin{aligned}
\bar{\mathcal{A}}_{k+1,k} &= (N-k)f_{QT}(k), \\
\bar{\mathcal{A}}_{k-1,k} &= kf_{TQ}(N-k)
\end{aligned}$$

and

$$\bar{\mathcal{A}}_{k,k} = -(N-k)f_{QT}(k) - kf_{TQ}(N-k).$$

So the equations are

$$\begin{aligned}
\dot{Y}^k &= (k+1)f_{TQ}(N-k-1)Y^{k+1} + (N-k+1)f_{QT}(k-1)Y^{k-1} \\
&\quad - ((N-k)f_{QT}(k) + kf_{TQ}(N-k))Y^k.
\end{aligned}$$

For variables Y^N and Y^0 , some terms on the right-hand side become zero, and we arrive at the equations claimed. \square

Lumping for the star network

Consider a star-like network with $N > 2$ nodes. In this network, a single central node is connected to all other nodes with no further connections, as in Fig. 2.10a. Let the first node be the centre of the star. Thus, for example $TQQ \cdots Q$ denotes the state when the central node is of status T and the other nodes are of status Q . We will show that in the case of a star network, the 2^N -dimensional system as defined by equation (2.6) can be lumped to a $2N$ -dimensional system for an arbitrary binary dynamics. The automorphism group of the star graph is the permutation group \mathbf{S}_{N-1} : an automorphism must leave the central node unchanged but can permute the remaining $N-1$ nodes in an arbitrary way. Therefore, two states are equivalent via an automorphism if and only if the centre is of the same status and the number of non-central nodes of status T is the same. Hence, for $l = 1, 2, \dots, N-1$, class \mathcal{C}^l of states of the graph, such that there are l nodes of status T , can be lumped into two classes: in the first class, the central node is T and there are $l-1$ non-central T nodes; in the second class, the central node is Q and there are l non-central T nodes.

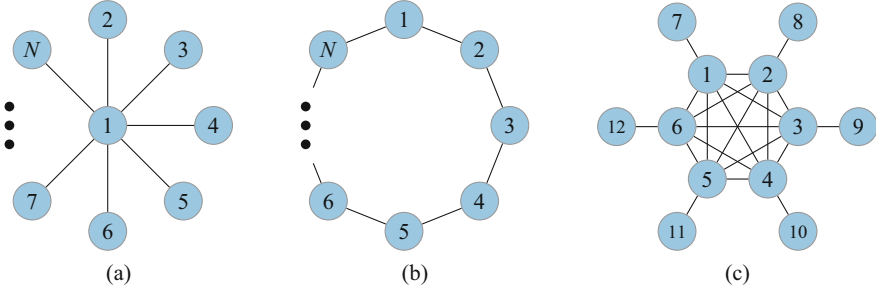


Fig. 2.10: (a) General star and (b) general cycle networks with N nodes. (c) Household network with 12 nodes (6 households).

In the case $l = 0$ and $l = N$, there is obviously only one class. This means that altogether there are $2 + 2(N - 1) = 2N$ lumping classes: $\mathcal{C}^0 = \{S^0\}$, $\mathcal{C}^N = \{S^N\}$, and for $k \in \{1, 2, \dots, N - 1\}$, we have $\mathcal{C}_1^k = \{S_j^k : S_j^k(1) = T\}$, $\mathcal{C}_2^k = \{S_j^k : S_j^k(1) = Q\}$. So for $1 \leq k \leq N - 1$, a subscript of 1 denotes that the central node has status T and a subscript of 2 denotes status Q . We use L_1^k and L_2^k to denote the induced partitions of $\{1, \dots, c_k\}$ corresponding to \mathcal{C}_1^k and \mathcal{C}_2^k . Thus, the lumped variables can be introduced as

$$Y^0 = X^0, \quad Y^N = X^N, \quad Y_1^k = \sum_{i \in L_1^k} X_i^k, \quad Y_2^k = \sum_{i \in L_2^k} X_i^k,$$

for $k = 1, \dots, N - 1$. Similarly to Proposition 2.3, we can prove:

Proposition 2.4 *Let G be a star graph of N nodes, with the central node labelled 1. Then*

$$\begin{aligned} \dot{Y}^0 &= f_{TQ}(N-1)Y_1^1 + f_{TQ}(1)Y_2^1 - Nf_{QT}(0)Y^0, \\ \dot{Y}^N &= f_{QT}(1)Y_1^{N-1} + f_{QT}(N-1)Y_2^{N-1} - Nf_{TQ}(0)Y^N \end{aligned}$$

and, for $k = 1, 2, \dots, N - 1$,

$$\begin{aligned} \dot{Y}_1^k &= (N-k+1)f_{QT}(1)Y_1^{k-1} + f_{QT}(k-1)Y_2^{k-1} + kf_{TQ}(0)Y_1^{k+1} \\ &\quad - ((N-k)f_{QT}(1) + (k-1)f_{TQ}(0) + f_{TQ}(N-k))Y_1^k, \\ \dot{Y}_2^k &= (N-k)f_{QT}(0)Y_2^{k-1} + f_{TQ}(N-k-1)Y_1^{k+1} + f_{TQ}(1)(k+1)Y_2^{k+1} \\ &\quad - (f_{QT}(k) + (N-k-1)f_{QT}(0) + kf_{TQ}(1))Y_2^k. \end{aligned}$$

Proof. We first address Y_1^k for $1 \leq k \leq N - 1$. Taking $S_l \in \mathcal{C}_1^k$, the central node has status T , and $(N - k)$ of the peripheral nodes have status Q . The remaining $k - 1$

peripheral nodes have status T . The rate at which the central node changes status is $f_{TQ}(N-k)$, yielding a state in \mathcal{C}_2^{k-1} . The rate at which each of the $N-k$ status Q peripheral node changes status is $f_{QT}(1)$, yielding a state in \mathcal{C}_1^{k+1} . The rate at which the remaining $k-1$ status T peripheral nodes change status is $f_{TQ}(0)$, yielding a state in \mathcal{C}_1^{k-1} . So the total rate of flow of probability from \mathcal{C}_1^k to \mathcal{C}_2^{k-1} is $f_{TQ}(N-k)Y_1^k$, to \mathcal{C}_1^{k+1} is $(N-k)f_{QT}(1)Y_1^k$ and to \mathcal{C}_1^{k-1} is $(k-1)f_{TQ}(0)$.

We now consider \mathcal{S}_2^k , where the central node has status Q and there are k status T peripheral nodes and $(N-k-1)$ status Q peripheral nodes. Similar analysis gives that the total rate of flow of probability to \mathcal{C}_1^{k+1} is $f_{QT}(1)$, to \mathcal{C}_2^{k+1} is $(N-k-1)f_{TQ}(0)$ and to \mathcal{C}_2^{k-1} is $kf_{TQ}(1)$. Similar analysis applies to \mathcal{C}^0 and \mathcal{C}^N . Combining these results together yields the claimed equations. \square

Lumping for the household network

Consider the simplest network with a so-called household structure of Fig. 2.10c. It consists of two types of nodes, inner and outer nodes. Outer nodes have only within-household connections, while inner nodes have both within-household connections, and connections to other households. We consider the simplest case where each household has two nodes, an inner and an outer node. The inner nodes of all households form a complete graph with $N/2$ nodes (N is an even number), and every outer node is connected to an inner node. Thus, the degree of all inner nodes is $\frac{N}{2}$ and the degree of all outer nodes is 1, as in Fig. 2.10c. It is possible to prove that for this household-type network, the 2^N -dimensional system given by (2.6) can be lumped to an $\binom{N/2+3}{3}$ -dimensional system.

The automorphism group of this graph is the permutation group $S_{N/2}$: an automorphism can permute the inner nodes in an arbitrary way, and once the automorphism is given on the inner nodes, its effect on the outer nodes is determined uniquely. In order to determine the lumping classes, note first that there may be four different types of households in this graph: QT households, in which the inner node is Q and the outer node is T , TQ households, QQ households, and TT households. Therefore, two states of the whole graph are equivalent through an automorphism if and only if the number of QT -, TQ -, QQ - and TT -type households is the same in the two states. Hence, to obtain all different states we have to choose (with repetition) $N/2$ households out of the four different types. Thus, using the formula for the number of combinations with repetitions, the number of different states is $\binom{4+N/2-1}{N/2} = \binom{N/2+3}{3}$. Hence, states with the same number of QQ -, QT -, TQ - and TT -type households can be lumped into one newly defined lumped variable.

Lumping for the cycle network: non-trivial lumping

For completely connected and star networks, lumping can be carried out intuitively. However, intuition alone is prone to error, and thus, it is desirable to use the automorphism group to work out lumping classes rigorously. Even for a relatively simple

network such as the cycle graph (C_N), where N nodes are connected in a close chain such that each node connects to the two nearest neighbours only, as in Fig. 2.10b, we can encounter surprises. For illustration, consider the $N = 5$ case.

The automorphisms of the cycle network is known as the *dihedral group* D_N , and can be given in terms of all possible *rotations* and *reflections* of the network (see, for example, the case $N = 5$ in the table in Fig. 2.6). There are N rotations and N reflections, so $|D_N| = 2N$. Here, D_5 is made up of five rotations (including the identity) and five reflections. We now look for the lumping classes \mathcal{C}_i^k for $i \in \{1, 2, \dots, c_k\}$, with c_k yet to be determined.

Each \mathcal{C}_i^k is a subset of \mathcal{C}^k , so in particular for $k = 0$, the first lumping class is trivial $\mathcal{C}_1^0 = \{(QQQQQ)\}$. Now consider

$$\mathcal{C}^1 = \{(QQQQT), (QQQTQ), (QQTQQ), (QTQQQ), (TQQQQ)\}.$$

We can see that the orbit of the first element ($QQQQT$) is

$$D_5((QQQQT)) = \{\Phi((QQQQT)) : \Phi \in D_5\} = \mathcal{C}^1.$$

Hence, $\mathcal{C}_1^1 = \mathcal{C}^1$. The situation changes when \mathcal{C}^2 is considered

$$\begin{aligned} \mathcal{C}^2 = \{ & (QQQTT), (QQTQT), (QTQQT), (TQQQT), (QQTTQ), \\ & (QTQTQ), (TQQTQ), (QTTQQ), (TQTQQ), (TTQQQ) \}. \end{aligned}$$

The orbit of the first element ($QQQTT$) $\in S^2$ is

$$\begin{aligned} D_5((QQQTT)) &= \{\Phi((QQQTT)) : \Phi \in D_5\} = \\ & \{(QQQTT), (TQQQT), (QQTTQ), (QTTQQ), (TTQQQ)\} = \mathcal{C}_1^2. \end{aligned}$$

The orbit of ($QQQTT$) only captures 5 out of the 10 possible states in \mathcal{C}^2 . The rotations and reflections map ($QQQTT$) onto identical configurations. This increases the number of lumping classes, so the dimensionality reduction of the system is less significant. The remaining five elements form another lumping class

$$\mathcal{C}_2^2 = \{(QQTQT), (QTQQT), (QTQTQ), (TQQTQ), (TQTQQ)\}.$$

Continuing, four more lumping classes can be identified. This means that the original system with $2^5 = 32$ equations can be reduced to a system with only 8 equations. Using similar arguments, for $N = 6$ and $N = 7$, the exact systems can be lumped from 64 and 128 to 18 and 30 equations, respectively. Given that for the cycle graph $2^N > |\text{Aut}(G)| = 2N$, the argument presented in Section 2.4.4 can be used to show that the number of lumping classes for the cycle graph is bounded from below by $\frac{2^N}{2N} = \frac{2^{N-1}}{N}$. This indicates that the number of equations in the lumped system is much larger than polynomial in N . It is interesting to note that in the case when the number of nodes is a prime number, $N = p$, then it can be shown that the number of lumping classes is $(2^{p-1} - 1)/p + 2^{(p-1)/2} + 1$. A similar formula is not known in the general case of an arbitrary value of N .

2.6 Conclusions and outlook

In this chapter, we have investigated network processes for which the status of a node can change in response to the status of its neighbours. These processes are relevant to understanding a number of important phenomena such as epidemic propagation, firing in neuronal networks, the voter model in social sciences or the Ising model in statistical physics. Such processes are controlled by the structure of the graph. We have provided a unified framework for arbitrary networks and arbitrary dynamics. The system of master equations serves as a theoretical basis for deriving and developing further exact and approximate models, e.g. the pair approximation model. Moreover, approximating models can be validated by comparing them to these exact models. The exact model also enables us to test simulation results. In Fig. 2.11, we show that for the fully connected and star networks and SIS dynamics, the lumped system is identical to results based on stochastic simulation. The lumped systems are obtained from Propositions 2.3 and 2.4 with node statuses $Q = S$ and $T = I$, and by substituting the actual transition rates as follows: $f_{SI} = \tau n$, where n denotes the number of infected neighbours and $f_{IS} = \gamma$. This not only confirms that lumping is correct, but provides strong evidence that the simulations are correctly implemented.

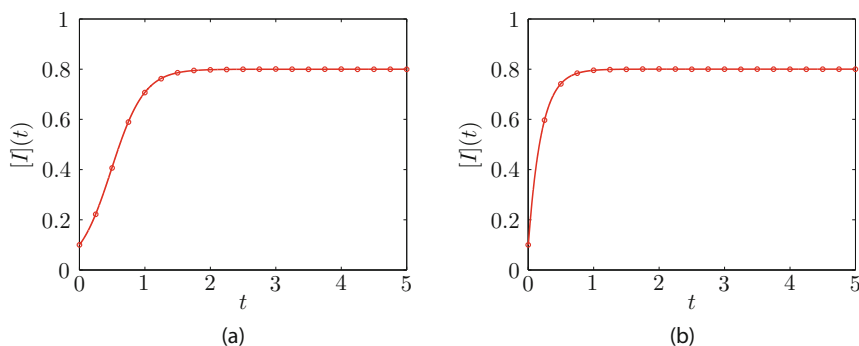


Fig. 2.11: Illustration of the perfect agreement between the lumped systems (solid lines) and stochastic simulations (\circ) for the (a) full and (b) star networks with $N = 1000$ and $\gamma = 1$, and with (a) $\tau = 0.005$ and (b) $\tau = 4.0$.

The master equations allow us to determine the time dependence of the probability of an arbitrary state, e.g. QTQ in a network with three nodes, meaning that nodes 1 and 3 are in status Q and node 2 is in status T . As a consequence, marginal probabilities (e.g. the probability of a node having a given status or the expected number of nodes with a given status) can be obtained, for example, the probability node 1 has status Q is $X_{QQQ} + X_{QQT} + X_{QTQ} + X_{QTT}$.

Spectral investigation of the transition matrix gives information about the long-term behaviour of the system [230, 312]. The transition matrix P , given in (2.3), has a zero eigenvalue, because the sum of the entries in each column is zero. The entries in the diagonal are negative and other entries are non-negative; hence, Gershgorin's theorem [109, 119] yields that all eigenvalues have real parts at most zero. The spectrum of the transition matrix has been studied in more detail in the case of SIS dynamics. For a complete graph, the system can be lumped to a tractable size. The spectrum of the resulting $(N + 1) \times (N + 1)$ matrix was studied in [230] in order to understand the quasi-steady state behaviour. Picard [252] proved that the matrix has a single zero eigenvalue (with eigenvector corresponding to the disease-free fully susceptible state) and all other eigenvalues are real and negative. We note that this is true for a more general class of tridiagonal matrices (see Theorem 8.2.6 in [99]).

Numerical investigation shows that one negative eigenvalue (denoted λ_1 and called the small eigenvalue) is very close to zero and the remaining negative eigenvalues (called large eigenvalues) are far from zero. As N or the infection rate increases, the small eigenvalue λ_1 converges rapidly to zero and the large eigenvalues decrease further; the spectral gap increases. This explains the appearance of a quasi-steady state, since the small eigenvalue dominates according to $\exp(\lambda_1 t)$. Thus, the time to extinction is of order $-1/\lambda_1$. Lumping enables us to determine λ_1 as a function of the infection rate τ even for relatively large graphs with a few hundred nodes. (In [312], graphs with at most $N = 13$ nodes are investigated.) In Fig. 2.12, $-1/\lambda_1$ is plotted for a range of τ values for a graph with $N = 500$ nodes and for recovery rate $\gamma = 1$.

It is well known that the threshold for the existence of the endemic equilibrium in the mean-field approximation for a complete graph is given by $N\tau = \gamma$; hence, for these parameter values the mean-field yields $\tau_c = 1/N\gamma = 0.002$ as a threshold value. In Fig. 2.12, one can see the well-known fact that the continuous-time Markov chain does not give a threshold value; on the other hand, $-1/\lambda_1$ depends on τ in a strongly nonlinear way when $\tau > \tau_c$. The inset with a logarithmic scale shows that in this range the time to extinction increases faster than exponentially, and becomes soon of order 10^6 . Practically, this means that the quasi-steady state is almost equivalent to a steady state in the classical sense. In Fig. 2.12, one can see that around $\tau = 0.0027$ there is a threshold-like abrupt change in the value of the time to extinction. We emphasise again that these plots are based on using the exact master equations and exploit the possibility of lumping.

The lumped system also enables us to derive an explicit formula for the approximation of the quasi-steady state. Namely, the quasi-steady state can be obtained starting from the tridiagonal transition matrix by omitting its first row and column and changing the upper-left entry in such a way that the sum of the first column becomes zero. Then, the remaining $N \times N$ matrix does not have an absorbing state and its stationary state is the quasi-steady state of the original system. This stationary state is given by the eigenvector corresponding to the zero eigenvalue. For a tridiagonal matrix, this can be given explicitly. Carrying out this calculation, the quasi-steady state is

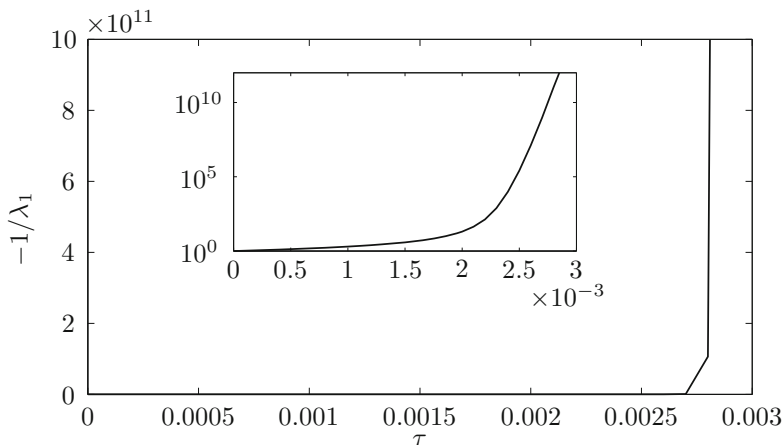


Fig. 2.12: Dependence of the time to extinction (that is of order $-1/\lambda_1$) on the per-edge infection rate τ for SIS dynamics on a complete graph with $N = 500$ and $\gamma = 1$ with a lin-log plot in the inset.

$$[I]^e = \sum_{k=0}^{N-1} (k+1)A_k \bigg/ \sum_{k=0}^{N-1} A_k, \quad (2.18)$$

where $A_0 = 1$ and

$$A_k = \frac{\tau^k (N-1)(N-2)\cdots(N-k)}{\gamma^k (k+1)}, \quad k = 1, 2, \dots, N-1.$$

This formula will be used later in Chapter 4 to test the accuracy of mean-field approximations.

Unfortunately, the number of equations required for an exact description of the probabilities of each state grows exponentially with the size of the network. Automorphisms of the graph can be exploited to reduce the number of equations through lumping. We have identified the precise link between the lumpability of the equations resulting from network processes and the symmetries of the network as specified by the automorphism group of the network. In Table 2.1, we display a number of networks for which lumping can be carried out with success (i.e. the full system can be reduced to a more tractable system, which is still exact, and can be evaluated numerically.)

It is worth noting that lumping in general relies on the identification of the automorphism group of a network, which in itself is a formidable task. However, as seen from our example, it is not necessary to have the complete group in order to obtain a significant reduction. It is also feasible to consider the possibility of a procedure that would not be exact, but rather an approximate lumping.

In general, this top-down technique and lumping work best and are ideal for networks of small size or networks with many symmetries. In many instances, the long-

term behaviour is of interest. Using this approach, dynamics with a single absorbing state (like the SIS) are difficult to analyse. For dynamics with more absorbing states (like the voter model or SIR), the final ratio of probabilities of the different absorbing states can be studied.

It is relatively straightforward to generalise this approach to transition rates which may depend on the density of different statuses in the immediate neighbourhood or beyond. This could include dependence on global properties, e.g. the total number of infected nodes, or modelling population-wide effects. This method applies similarly to hypergraphs [38, 111, 193] when classic edges are replaced by hyperedges. For this or for the former case, transition rates may depend non-linearly on the number of nodes of different statuses in the immediate neighbourhood or in the hyperedge.

	Network	Full system	Lumped system
SIS	2 line	4	3
	3 line	8	6
	4 line	16	10
	4 cycle	16	6
	Lollipop	16	12
	Toast	16	9
	Fully connected N	2^N	$N + 1$
	Star N	2^N	$2N$
SIR	2 line	9	6
	3 line	27	18
	Fully connected 3	27	10
	Fully connected N	3^N	$(N + 1)(N + 2)/2$
	Star N	3^N	$3N(N + 1)/2$

Table 2.1: The reduction in number of equations from the full to the lumped system for SIS and SIR epidemics and for a number of networks.

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