Markov Chains under Combinatorial Constraints: Analysis and Synthesis

by

Jane Breen

A thesis submitted to the Faculty of Graduate Studies of

The University of Manitoba

in partial fulfilment of the requirements of the degree of

DOCTOR OF PHILOSOPHY

Department of Mathematics

University of Manitoba

Winnipeg

Abstract

A finite, discrete-time, time-homogeneous Markov chain is a type of mathematical model used to describe dynamical systems which transition between a finite number of possible states in discrete time increments. A Markov chain model may be used in a wide range of applications, such as urban road traffic, computational drug design, and the spread of disease. In many such applications, there are existing constraints on the structure of the underlying network dictating which transitions are possible, and which are not. In this thesis, the influence of these combinatorial constraints on the behaviour of a Markov chain is explored.

A Markov chain may be completely described by a stochastic matrix $T = [t_{i,j}]$, where $t_{i,j}$ represents the probability of the chain transitioning from the i^{th} state to the j^{th} state in a single time-step. Given a directed graph D, which represents the underlying network, we define the set $\mathcal{S}_D$ as the set of all stochastic matrices T for which $t_{i,j} > 0$ only if there is an arc in D from the i^{th} to the j^{th} vertex of D. That is, $\mathcal{S}_D$ represents the set of transition matrices of Markov chains respecting the network given by D.

To determine the influence of a combinatorial constraint, we first consider and characterise the set of all possible stationary distributions (long-term behaviours) of irreducible matrices T in $\mathcal{S}_D$. We then consider the range of mean first passage times for a Markov chain with transition matrix $T \in \mathcal{S}_D$, and determine a lower bound on the maximum mean first passage time of any Markov chain, and determine some directed graphs for which equality holds in this lower bound. This provides an indication of how the network influences the short-term behaviour of a Markov chain. We consider the question of how to detect clustering behaviour in a Markov chain using the eigenvalues

of T. Finally, we examine Kemeny's constant $\mathcal{K}(T)$—which is a measure of how well-connected the states of the Markov chain are—and produce a condition number for $\mathcal{K}(T)$. This provides a measure of how sensitive the calculation of $\mathcal{K}(T)$ is to errors or perturbations of the entries of T. We also consider the sensitivity of $\mathcal{K}(T)$ where T is the transition matrix for the random walk on certain classes of graphs, again indicating how a combinatorial constraint can influence the behaviour of a Markov chain.

Acknowledgements

I would like to thank the staff and faculty in the Department of Mathematics at the University of Manitoba, and also in the Hamilton Institute at Maynooth University, where I began this thesis. I am grateful for the financial support provided by the Department of Mathematics and the Faculty of Graduate Studies at the University of Manitoba, as well as the National Sciences and Engineering Research Council and Science Foundation Ireland.

I would like to thank my family, who have been supportive throughout—even after I moved across the ocean to pursue my studies. I am thankful for friends, new and old, for all the good times throughout my studies. I am also extremely grateful to my partner Jason for his help and support, and I wouldn't have made it this far without him.

Most of all, I would like to thank my supervisor, Dr. Steve Kirkland, who has gone above and beyond what is expected of a supervisor, with his generosity, his advice, and his encouragement.

Post-Defence Acknowledgement:

I would like to thank Drs. Judith McDonald, Xikui Wang, Michael Doob, and Robert Craigen for their questions, comments, and suggestions which helped to improve this thesis.

To Jason.

Contributions of Authors

Chapter 3 is a version of a journal article co-authored with Steve Kirkland which has been published in [5]. I am the primary author.

Chapter 4 is a version of a journal article co-authored with Steve Kirkland which has been published in [6]. I am the primary author.

Chapter 5 is a version of a journal article which has been submitted for publication and is under review. This article is co-authored by Emanuele Crisostomi, Mahsa Faizrahnemoon, Steve Kirkland, and Robert Shorten. A preliminary version of the results also appears in [28]. I am the primary author of the submitted article.

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O	a zero matrix
J	an all-ones matrix
$\mathbb{1}$	a column vector of all-ones
e_i	the i^{th} standard basis vector
$u^\top$, $A^\top$	the transpose of a vector/matrix
A_{dg}	the diagonal matrix formed from the square matrix A by setting all off-diagonal entries of A to zero
$\text{diag}(u)$	the diagonal matrix with diagonal entries given by the vector u
$A_{(j)}$	the j^{th} principal submatrix of A; the matrix formed from the square matrix A by deleting the j^{th} row and column of A
$A^\#$	the group inverse of A
$\rho(A)$	the spectral radius of A
$\mathcal{K}(T)$	Kemeny's constant for a Markov chain with transition matrix T
$\mathfrak{c}(T)$	a condition number for the stationary vector of T
$\mathcal{D}(A)$	the directed graph of the matrix A
A_D	the adjacency matrix of the directed graph D
$\mathcal{B}(A)$	the bipartite graph of the matrix A
$\mathcal{S}_D$	the set of all stochastic matrices respecting the directed graph D

Chapter 1

Introduction

A *finite, discrete, time-homogeneous Markov chain* refers to a mathematical model of a system which, at any given time, occupies one of a finite number of states $\{s_1, \ldots, s_n\}$, and transitions between states in discrete time-steps, according to prescribed transition probabilities. In particular, for any pair of states s_i and s_j, there is a specified probability $t_{i,j}$ that the system moves to state s_j in one time-step, given that it is currently in state s_i. A Markov chain is *memoryless*, meaning that the movement of the system in the next time-step depends only on the current state the system occupies. A Markov chain can be represented by a row-stochastic matrix $T = [t_{i,j}]$—that is, a matrix in which each row sums to 1—referred to as the *probability transition matrix* of the chain.

The applications of Markov chains are diverse, including their use as a model of traffic in road networks (see [20]), of web traffic on the world wide web (see [64]), and in molecular conformational dynamics in drug design (see [25]). The advantages of modelling such systems with Markov chains are broad; given only a transition matrix, many features of the real-world system can be determined with techniques in linear algebra. Under mild hypotheses, the long-term behaviour of the system is encapsulated

in the *stationary distribution vector*, which is simply a left eigenvector of T corresponding to the eigenvalue 1. The short-term behaviour can be examined using the mean first passage time from the i^{th} state to the j^{th} state, $m_{i,j}$—i.e. the expected time it will take to reach state s_j for the first time if the system begins in state s_i. An interesting quantifying feature of a Markov chain which has been the recent subject of extensive study is *Kemeny's constant*, denoted $\mathcal{K}(T)$, which is interpreted in terms of the 'expected time to mixing' in the system (see [44, 57]), and gives an overall measure of how well-connected the system is, due to its interpretation in terms of the expected length of a trip from a randomly-selected initial state to a randomly-selected destination state (see [64]).

In many applications of Markov chains, the underlying network of possible transitions between states is specified in advance. For example, the transition matrix of a Markov chain modelling vehicle traffic is constrained by the given road network, which determines the transitions between states (road segments) that are possible in one time-step. Hence it is of interest to consider the range of certain Markov chain properties (such as those listed above) over the class of stochastic matrices representing a Markov chain on that network. In particular, we wish to investigate the influence of the underlying directed graph, and the extent to which it dictates the behaviour of the system. This is the principal aim of this thesis. The remainder of the document is arranged as follows.

In Chapter 2, we present the necessary mathematical preliminaries, and review the literature in order to ground this work in context.

In Chapter 3, we consider the question of how the stationary vector is limited by a specified directed graph. In particular, an algorithm is presented by which necessary and sufficient conditions can be derived from a given directed graph in order for a given probability vector w to be the stationary distribution vector for some Markov chain

respecting that directed graph.

In Chapter 4, the range of possible values of mean first passage times between states is discussed, and how this range is affected by the underlying directed graph. After some preliminary observations, a lower bound is given for the maximum mean first passage time between distinct states in terms of the stationary distribution. We determine directed graphs for which equality holds in this lower bound, again highlighting the influence of the directed graph on the properties of the Markov chain.

In Chapter 5, we discuss the manifestation of clustering behaviour in a Markov chain, and how it can be measured using the mean first passage times and the transition probabilities. We investigate how the eigenvectors of the transition matrix of a Markov chain can be used to determine clusters of states that the chain is unlikely to leave, or in which the chain spends a long time before transitioning to a different cluster. This is given through lower bounds on the spectral radius of a principal submatrix corresponding to the subset of states in the cluster.

In Chapter 6, attention is turned to Kemeny's constant, which has recently been a subject of great attention and interest. We consider the sensitivity of Kemeny's constant to perturbations in the transition matrix—that is, we develop a condition number for Kemeny's constant, which provides a measure of confidence in the computed value of Kemeny's constant in a numerical setting.

This thesis concludes in Chapter 7 with discussions of future directions.

Any MATLAB code used in this thesis is given in Appendix A for the interested reader.

Chapter 2

Markov chains and directed graphs

In this chapter, we introduce the theory of Markov chains and of directed graphs, their interconnections, and previous research on which we build in this thesis.

2.1 Introduction to probability

A *random variable* X is a variable whose possible values represent outcomes of a random phenomenon. A discrete random variable is one for which there are countably many outcomes. The *probability distribution* of a discrete random variable can be thought of as a list of probabilities that are associated with each of its possible outcomes. We write $\mathbb{P}[X = x]$ to denote the probability that the random variable X takes on the value or outcome x. The *expected value* of a discrete random variable X is the probability-weighted average of all outcomes; that is, the expected value of X is given by $\mathbb{E}(X) = \sum x \cdot \mathbb{P}[X = x]$. Intuitively, this can be thought of as the average outcome if we sample X many times.

If X and Y are two random variables, we write $\mathbb{P}[\, Y = y \mid X = x \,]$ to denote the *conditional probability* that Y takes on the value y, if it is known that X takes the

value x.

2.2 Introduction to Markov chains

Definition 2.2.1. A sequence of random variables $X_0, X_1, X_2, \ldots, X_k, \ldots$ taking values $x_0, x_1, x_2, \ldots, x_k, \ldots$ is called a *Markov chain* if it satisfies the property that

$$\mathbb{P}[\, X_{k+1} = x_{k+1} \mid X_k = x_k, X_{k-1} = x_{k-1}, \ldots, X_0 = x_0 \,] = \mathbb{P}[\, X_{k+1} = x_{k+1} \mid X_k = x_k \,]. \tag{2.1}$$

The possible values of the random variables X_i form a countable set $\mathcal{S} = \{s_1, s_2, \ldots\}$, which is called the *state space* of the chain, and $x_k \in \mathcal{S}$ for all k. The elements s_i are referred to as the *states* of the chain.

We think of a Markov chain as a model for a system which transitions between states in discrete time-steps, with the sequence $X_0, X_1, \ldots$ thought of as being indexed by time, with X_0 the initial state of the system. The property (2.1) is known as the *Markov property*, and we can interpret this to mean that the behaviour of the system in the next time increment depends only on the current state of the system; i.e. past behaviour is irrelevant. Given a Markov chain $X_0, X_1, \ldots$, the probability

$$\mathbb{P}[\, X_{m+1} = s_j \mid X_m = s_i \,]$$

is the *transition probability* from state i to state j at time m. The chain is called *time-homogeneous* if the transition probabilities at time m are equal for all $m \in \mathbb{N}$, and we denote the transition probability from s_i to s_j by $t_{i,j}$.

Given a time-homogeneous Markov chain on a finite state space $\{s_1, s_2, \ldots, s_n\}$ and transition probabilities $t_{i,j}$, $i, j \in \{1, \ldots, n\}$, we form the *one-step probability transition*

matrix (or simply the *transition matrix*) of the chain:

$$T = \begin{bmatrix} t_{1,1} & t_{1,2} & \cdots & t_{1,n} \\ t_{2,1} & t_{2,2} & \cdots & t_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ t_{n,1} & t_{n,2} & \cdots & t_{n,n} \end{bmatrix}.$$

This matrix is *stochastic* (i.e. nonnegative, and all rows sum to one) since for any i:

$$\begin{aligned} \sum_{j=1}^{n} t_{i,j} &= \sum_{j=1}^{n} \mathbb{P}[X_1 = s_j \mid X_0 = s_i] \\ &= \mathbb{P}[X_1 \in \mathcal{S} \mid X_0 = s_i] \\ &= 1. \end{aligned}$$

Letting $\mathbb{1}$ represent a column vector of all ones, this can be written as $T\mathbb{1} = \mathbb{1}$. Here and elsewhere in this document, the size of $\mathbb{1}$ will be clear from the context.

In this thesis we will only discuss finite, time-homogeneous Markov chains. For such a Markov chain, this probability transition matrix T completely describes the behaviour of the system over time. First of all, it can be shown that the behaviour of the system after m time-steps is given by the entries $t_{i,j}^{(m)}$ of the m^{th} power of the transition matrix T.

Theorem 2.2.2. *Let $T = [t_{i,j}]$ be the transition matrix of a time-homogeneous Markov chain with state space $\mathcal{S} = \{s_1, s_2, \ldots, s_n\}$. Then for all $i, j \in \{1, \ldots, n\}$, the probability of transitioning from s_i to s_j in exactly m steps is given by the $(i,j)^{th}$ entry of T^m; that is,*

$$\mathbb{P}[\, X_m = s_j \mid X_0 = s_i \,] = t_{i,j}^{(m)}. \tag{2.2}$$

Proof. Fix i, j; we prove the result using induction on m. The case $m = 1$ is trivial;

now assume (2.2) holds for all $l < m$, for some fixed $m \geq 1$. We condition on X_1:

$$\begin{aligned}
\mathbb{P}[X_m = s_j \mid X_0 = s_i] &= \sum_{k=1}^{n} \mathbb{P}[X_m = s_j \mid X_1 = s_k, X_0 = s_i] \cdot \mathbb{P}[X_1 = s_k \mid X_0 = s_i] \\
&= \sum_{k=1}^{n} \mathbb{P}[X_m = s_j \mid X_1 = s_k] \cdot \mathbb{P}[X_1 = s_k \mid X_0 = s_i] \\
&\qquad \text{(by the Markov property)} \\
&= \sum_{k=1}^{n} \mathbb{P}[X_{m-1} = s_j \mid X_0 = s_k] \cdot \mathbb{P}[X_1 = s_k \mid X_0 = s_i] \\
&\qquad \text{(by time-homogeneity)} \\
&= \sum_{k=1}^{n} t_{i,k} t_{k,j}^{(m-1)} \\
&\qquad \text{(by the induction hypothesis)} \\
&= t_{i,j}^{(m)}.
\end{aligned}$$

Hence, by induction, (2.2) holds for all $m \in \mathbb{N}$. □

Let e_i denote the i^{th} standard basis vector in $\mathbb{R}^n$. It is clear that

$$e_i^\top T = \begin{bmatrix} t_{i,1} & t_{i,2} & \cdots & t_{i,n} \end{bmatrix};$$

i.e. $e_i^\top T$ produces the probability distribution of the Markov chain after a single time-step, given that the chain starts in state s_i. Furthermore, $e_i^\top T^m$ produces the probability distribution of the Markov chain after m time-steps, given that the chain starts in state s_i. The vector $e_i^\top$ can be thought of as an initial probability distribution for the chain; i.e. a probability distribution for the random variable X_0. Moreover for any initial distribution of the Markov chain $u = \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix}^\top$ (for which $u \geq 0$, entrywise, and $u_1 + \cdots + u_n = 1$), $u^\top T^m$ returns the probability distribution of X_m; i.e. the probability distribution of the Markov chain after m steps.

Classification of states

Suppose a finite, time-homogeneous Markov chain has state space $\mathcal{S} = \{s_1, \ldots, s_n\}$ and transition matrix $T = [t_{i,j}]$. We say that s_j is *accessible* from s_i (and denote it as $s_i \rightsquigarrow s_j$) if there exists $m \geq 1$ such that $t_{i,j}^{(m)} > 0$; that is, there is a nonzero probability that the chain reaches s_j from s_i in m steps. The states s_i and s_j are said to *communicate* if $s_i \rightsquigarrow s_j$ and $s_j \rightsquigarrow s_i$.

The states in $\mathcal{S}$ can be classified as follows: for a state $s_i \in \mathcal{S}$, if there exists $s_j \in \mathcal{S}$ such that $s_i \rightsquigarrow s_j$ but $s_j \not\rightsquigarrow s_i$, then s_i is called an *inessential state*. Otherwise, s_i is called an *essential state*. Considering 'communication' as an equivalence relation on $\mathcal{S}$, we see by the equivalence classes of this relation that all essential states can be grouped into *essential classes*, in which every state communicates with those in its own class, but no state outside the class is accessible from a state inside the class. All inessential states may also be divided into inessential classes in the same way, although the Markov chain may transition from one inessential state to a state in a different class. An inessential state s_i is also called a *transient* state, since as time passes, eventually the Markov chain will never return to s_i. An essential state which forms an essential class on its own is called *absorbing*; that is, s_i is absorbing if $t_{i,i} = 1$ and $t_{i,j} = 0$ for $j \neq i$. In this situation, once the Markov chain transitions to the state s_i, it never leaves.

A Markov chain is said to be *irreducible* (or *ergodic*) if every state is accessible from every other state. Otherwise, the Markov chain is said to be *reducible*. In an irreducible Markov chain, the states form a single essential class, and there are no transient states. Since the transition matrix completely represents the Markov chain, unsurprisingly there is a matrix-theoretic condition by which one may determine if the Markov chain is reducible or irreducible.

Definition 2.2.3. A matrix A is *reducible* if there is some simultaneous permutation of the rows and columns of A that produces a block-triangular matrix; that is, if there is some permutation matrix P such that

$$PAP^{\top} = \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline O & A_{22} \end{array}\right].$$

A matrix which is not reducible is said to be *irreducible*. Note that any 1×1 matrix is irreducible.

Using the above, one can say that a Markov chain is irreducible (respectively, reducible) if and only if its transition matrix T is irreducible (resp., reducible). This is easily seen by considering T^m; if T is reducible, there is at least one entry pair of indices i, j, $i \neq j$, such that for every value of $m \geq 1$, $t_{i,j}^{(m)} = 0$. Hence s_j is not accessible from s_i. Conversely, suppose that a Markov chain with transition matrix T is reducible. Then there is at least one essential class which is not equal to the entire state space. Ordering the states so that this collection of states appear at the end, the transition matrix T will take the form

$$\left[\begin{array}{c|c} T_{11} & T_{12} \\ \hline O & T_{22} \end{array}\right]$$

where T_{22} represents transitions within that essential class, with no transitions from this collection of states to states outside of that class. In fact, the states of a reducible

Markov chain can be ordered appropriately so that T takes the form

$$\left[\begin{array}{c|c|c|c|c} T_{11} & T_{12} & T_{13} & \cdots & T_{1k} \\ \hline O & T_{22} & T_{23} & \cdots & T_{2k} \\ \hline O & O & T_{33} & \cdots & T_{3k} \\ \hline \vdots & \vdots & \vdots & \ddots & \vdots \\ \hline O & O & O & \cdots & T_{kk} \end{array}\right] \tag{2.3}$$

where each T_{ii} is square and irreducible. This is called *Frobenius normal form*, and more details can be found for general matrices (i.e. not stochastic) in [9, Sec. 3.2]. In the context of Markov chains, this form corresponds to an ordering of the states based on their equivalence classes under the 'communicating' equivalence relation, and the transitions from states in one class to another. For more details, see [76, Sec. 1.2].

Irreducible Markov chains can be further subclassified into *periodic* Markov chains and *aperiodic* or *regular* Markov chains. A state s_i of a Markov chain is called *periodic* if the length of time it takes to return to s_i is always a multiple of some $p \geq 2$. Formally, the *period* of the state s_i is given by

$$p_i := \gcd\{m \geq 0 \mid t_{i,i}^{(m)} > 0\},$$

and s_i is called periodic if $p_i \geq 2$, and aperiodic if $p_i = 1$. A Markov chain is called *periodic* if it is irreducible and every state is periodic. The *period* of a periodic Markov chain is the greatest common divisor of the periods p_i, $i = 1, \ldots n$. A Markov chain is called *aperiodic* if it is irreducible and every state is aperiodic. It is well-known that if one state of an irreducible Markov chain has period one, then every state is aperiodic.

Again, these properties of the Markov chain (periodicity/aperiodicity) may be determined via the transition matrix T.

Definition 2.2.4. A nonnegative matrix A is called *primitive* if there exists some $m \geq 1$ for which A^m is a positive matrix.

A Markov chain is regular if and only if its transition matrix T is primitive. Furthermore, a periodic Markov chain with a transition matrix T that is irreducible but imprimitive can be written in *periodic normal form* (see [76, Sec. 1.3]); that is, there is a permutation matrix P such that

$$PTP^\top = \left[\begin{array}{c|c|c|c|c} O & T_1 & O & \cdots & O \\ \hline O & O & T_2 & \cdots & O \\ \hline \vdots & \vdots & \ddots & \ddots & \vdots \\ \hline O & O & \cdots & O & T_{d-1} \\ \hline T_d & O & \cdots & O & O \end{array}\right], \tag{2.4}$$

where T has period d. Note that the zero diagonal blocks are square; the off-diagonal blocks need not be square. Observe that each of the cyclic products

$$T_1T_2\cdots T_d, \qquad T_2\cdots T_dT_1, \qquad \cdots \qquad T_dT_1\cdots T_{d-1}$$

is a square stochastic matrix. Further, it can be shown that each cyclic product is primitive (see [9, Theorem 3.4.5]).

2.3 Limiting behaviour of an irreducible Markov chain

As with any model of a dynamical system, one of the primary considerations is how one can describe the long-term behaviour of the system. As discussed, the behaviour of a Markov chain after m time-steps is determined by T^m and some information about

the initial distribution. The limiting behaviour of the Markov chain refers to the range of possible behaviours of the system as $m \to \infty$.

For irreducible Markov chains (both regular and periodic) the limiting behaviour of the chain is determined using a well-known theorem from nonnegative matrix theory; see [76, Sec. 1.1] for a proof.

Theorem 2.3.1 (The Perron-Frobenius theorem for primitive matrices)**.** *Suppose that A is an $n \times n$ nonnegative primitive matrix. Then there exists an eigenvalue r such that:*

(a) r is real and positive;

(b) with r can be associated strictly positive left and right eigenvectors;

(c) if $\lambda \neq r$ is an eigenvalue of A, then $|\lambda| < r$;

(d) the eigenvectors associated with r are unique to constant multiples;

(e) If $O \leq B \leq A$ and β is an eigenvalue of B, then $\beta \leq r$. Moreover, $|\beta| = r$ implies $B = A$.

(f) r is a simple root of the characteristic equation of A.

Note that for an irreducible, imprimitive, nonnegative matrix A, (a)–(f) also hold, but with (c) replaced by the weaker statement that for λ an eigenvalue of A, $|\lambda| \leq r$. The eigenvalue r here represents the *spectral radius of* A, which we denote by $\rho(A)$. For an arbitrary matrix A, $\rho(A)$ is defined to be the largest modulus of an eigenvalue of A. In the case of a nonnegative matrix where $\rho(A)$ is an eigenvalue of A, it is referred to as the *Perron value* of A, and the corresponding eigenvectors are *Perron vectors*.

Corollary 2.3.2. *Let A be a primitive nonnegative matrix, with right and left Perron vectors u and v (respectively), normalised so that $v^\top u = 1$. Then*

$$\lim_{m\to\infty} \frac{1}{\rho(A)^m} A^m = uv^\top.$$

Since the transition matrix T for an irreducible Markov chain is row-stochastic, we have $T\mathbb{1} = \mathbb{1}$, and so $\mathbb{1}$ is a right Perron vector corresponding to the Perron value $\rho(T) = 1$. The corresponding positive left Perron vector—that is, the vector w for which $w^\top T = w^\top$ and $w^\top \mathbb{1} = 1$—has special significance in Markov chain theory. In particular, for a regular Markov chain, Corollary 2.3.2 shows that the limiting behaviour of the chain is given by this vector w, in that

$$\lim_{m\to\infty} T^m = \mathbb{1}w^\top = \begin{bmatrix} w_1 & w_2 & \cdots & w_n \\ w_1 & w_2 & \cdots & w_n \\ \vdots & \vdots & \ddots & \vdots \\ w_1 & w_2 & \cdots & w_n \end{bmatrix}.$$

That is, regardless of the starting state, the probability the chain is in s_i in the long term is given by the i^{th} entry w_i of the vector w. Furthermore, given any initial probability distribution u,

$$\lim_{m\to\infty} u^\top T^m = u^\top \mathbb{1} w^\top = w^\top,$$

since $u^\top \mathbb{1} = 1$.

For a periodic Markov chain, the limiting behaviour is slightly different. Suppose

T is a transition matrix for a Markov chain with period d, and that

$$T = \left[\begin{array}{c|c|c|c|c} O & T_1 & O & \cdots & O \\ \hline O & O & T_2 & \cdots & O \\ \hline \vdots & \vdots & \ddots & \ddots & \vdots \\ \hline O & O & \cdots & O & T_{d-1} \\ \hline T_d & O & \cdots & O & O \end{array}\right],$$

as in (2.4). Letting w_i be the left Perron vector of the i^{th} cyclic product $S_i := T_i \cdots T_d T_1 \cdots T_{i-1}$, normalised so that $w_i^\top \mathbb{1} = 1$, we have that T has left Perron vector

$$w = \frac{1}{d}\left[\begin{array}{c} w_1 \\ \hline w_2 \\ \hline \vdots \\ \hline w_d \end{array}\right],$$

and $w^\top \mathbb{1} = 1$. Furthermore, note that $w_i^\top = w_1^\top T_1 T_2 \cdots T_{i-1}$.

We have the following result for the limiting behaviour of a periodic Markov chain.

Theorem 2.3.3. *Let T be an irreducible stochastic matrix representing a periodic Markov chain with period d, and let $\mathbb{1}$ and w be its right and left Perron vectors respectively, with $w^\top \mathbb{1} = 1$. Then*

$$\lim_{m\to\infty} \frac{1}{d} \sum_{j=m}^{m+d-1} T^j = \mathbb{1} w^\top.$$

Proof. Consider first that for any positive integer m, we can write $m = kd + r$, for

$r \in \{0, 1, \ldots, d-1\}$. We also have

$$T^{kd} = \left[\begin{array}{c|c|c|c} S_1^k & O & \cdots & O \\ \hline O & S_2^k & \cdots & O \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline O & O & \cdots & S_d^k \end{array}\right]$$

and since S_i is primitive with left and right Perron vectors w_i and $\mathbb{1}$ respectively, by Corollary 2.3.2 we have

$$\lim_{k\to\infty} T^{kd} = \left[\begin{array}{c|c|c|c} \mathbb{1}w_1^\top & O & \cdots & O \\ \hline O & \mathbb{1}w_2^\top & \cdots & O \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline O & O & \cdots & \mathbb{1}w_d^\top \end{array}\right].$$

Next, consider that

$$\sum_{j=0}^{d-1} T^j = \left[\begin{array}{c|c|c|c|c|c} I & T_1 & T_1T_2 & T_1T_2T_3 & \cdots & T_1T_2\cdots T_{d-1} \\ \hline T_2T_3\cdots T_d & I & T_2 & T_2T_3 & \cdots & T_2T_3\cdots T_{d-1} \\ \hline T_3\cdots T_d & T_3\cdots T_dT_1 & I & T_3 & \cdots & T_3T_4\cdots T_{d-1} \\ \hline \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ \hline \vdots & \vdots & \vdots & \ddots & I & T_{d-1} \\ \hline T_d & T_dT_1 & T_dT_1T_2 & \cdots & T_dT_1\cdots T_{d-2} & I \end{array}\right].$$

From this, and the fact that $w_i^\top = w_1^\top T_1 T_2 \cdots T_{i-1}$, we have

$$\begin{aligned}\frac{1}{d}\left(\lim_{k\to\infty} T^{kd}\right)\sum_{j=0}^{d-1} T^j &= \frac{1}{d}\left[\begin{array}{c|c|c|c} \mathbb{1}w_1^\top & \mathbb{1}w_1^\top & \cdots & \mathbb{1}w_1^\top \\ \hline \mathbb{1}w_2^\top & \mathbb{1}w_2^\top & \cdots & \mathbb{1}w_2^\top \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline \mathbb{1}w_d^\top & \mathbb{1}w_d^\top & \cdots & \mathbb{1}w_d^\top \end{array}\right] \\ &= \mathbb{1}w^\top.\end{aligned}$$

Finally, considering the limiting behaviour of T^{kd+r} as $k \to \infty$, we have that for any fixed r,

$$\begin{aligned}\lim_{k\to\infty} \frac{1}{d} \sum_{j=kd+r}^{(kd+r)+d-1} T^j &= \frac{1}{d}\lim_{k\to\infty} T^{kd+r}\sum_{j=0}^{d-1} T^j \\ &= T^r \frac{1}{d}\lim_{k\to\infty} T^{kd}\sum_{j=0}^{d-1} T^j \\ &= T^r \mathbb{1}w^\top \\ &= \mathbb{1}w^\top,\end{aligned}$$

since T is stochastic. Hence

$$\lim_{m\to\infty} \frac{1}{d} \sum_{j=m}^{m+d-1} T^j = \mathbb{1}w^\top.$$

□

From this, we can conclude that the i^{th} entry of the normalised left Perron vector w of a transition matrix T can be interpreted for periodic Markov chains to represent the *proportion* of time spent in the i^{th} state in the long term.

Definition 2.3.4. Let T be an irreducible stochastic matrix representing a Markov

chain. The *stationary distribution vector* (or *stationary vector*) of T is the left eigenvector w corresponding to the eigenvalue 1 of T, normalised so that the entries sum to 1.

Since the long-term behaviour of an irreducible Markov chain is catalogued by the entries of the stationary distribution vector in this way, it is a key quantity of interest in this thesis.

We note that the stationary vector for a given Markov chain with transition matrix T can be found using a divide-and-conquer approach known as *stochastic complementation*. We will make use of this in later chapters; hence we present a brief discussion here (see [66] for a more in-depth discussion and rigorous proofs).

Suppose that we have an irreducible stochastic matrix T with

$$T = \left[\begin{array}{c|c} T_{11} & T_{12} \\ \hline T_{21} & T_{22} \end{array}\right].$$

Define

$$\begin{aligned} S_1 &:= T_{11} + T_{12}(I - T_{22})^{-1}T_{21}; \\ S_2 &:= T_{22} + T_{21}(I - T_{11})^{-1}T_{12}, \end{aligned}$$

where $I - T_{ii}$ is invertible since T_{ii} is substochastic, so $\rho(T_{ii}) < 1$. These stochastic complements S_1 and S_2 are irreducible and stochastic. Let w_i be the stationary distribution of S_i; then the stationary distribution of T is

$$w = \left[\begin{array}{c} a_1 w_1 \\ \hline a_2 w_2 \end{array}\right]$$

where $[a_1\, a_2]$ is the stationary vector of the 2×2 matrix

$$\left[\begin{array}{c|c} w_1^\top T_{11}\mathbb{1} & w_1^\top T_{12}\mathbb{1} \\ \hline w_2^\top T_{21}\mathbb{1} & w_2^\top T_{22}\mathbb{1} \end{array}\right]. \tag{2.5}$$

2.4 Mean first passage times

While the stationary distribution vector w describes the long-term behaviour of a regular Markov chain, the short-term behaviour is examined via first passage times (sometimes called hitting times).

Definition 2.4.1. Consider a finite time-homogeneous irreducible Markov chain with state space $\{s_1, s_2, \ldots, s_n\}$ The *first passage time* from s_i to s_j is a random variable $f_{i,j}$ representing the number of time-steps elapsed (≥ 1) before the chain reaches s_j for the first time, given that it begins in s_i. The *mean first passage time* from s_i to s_j, denoted $m_{i,j}$, is the expected value of this random variable.

To derive an expression for $m_{i,j}$ in terms of the transition matrix T for a Markov chain, suppose that the chain is initially in s_i, and condition on the state of the Markov chain after one time-step. That is,

$$\begin{aligned} m_{i,j} &= t_{i,j} + \sum_{k \neq j} t_{i,k}(m_{k,j} + 1) \\ &= \sum_{k \neq j} t_{i,k} m_{k,j} + 1. \end{aligned} \tag{2.6}$$

Let $M = [m_{i,j}]$ denote the matrix of mean first passage times, or the *mean first passage matrix* of the chain, and let M_{dg} denote a diagonal matrix consisting of just the diagonal entries of M and zeros elsewhere. Let $J = \mathbb{1}\mathbb{1}^\top$; i.e. an $n \times n$ matrix of all ones. Then

(2.6) can be rewritten so that M is the unique solution to the matrix equation

$$M = T(M - M_{dg}) + J. \tag{2.7}$$

This equation provides the starting point for deriving expressions for $m_{i,j}$, for a given i and j. First, consider multiplying (2.7) on the left by $w^\top$, the stationary vector of T. Then

$$\begin{aligned} w^\top M &= w^\top T(M - M_{dg}) + w^\top J \\ \Rightarrow w^\top M &= w^\top M - w^\top M_{dg} + \mathbb{1}^\top \\ \Rightarrow w^\top M_{dg} &= \mathbb{1}^\top \\ \Rightarrow w_i m_{i,i} &= 1, \quad \text{for each } i, \end{aligned}$$

and hence the *mean first return time*, $m_{i,i}$, is given by $\frac{1}{w_i}$.

Proposition 2.4.2. *Let T be an $n \times n$ irreducible stochastic matrix. For $i, j \in \{1, 2, \ldots, n\}$, $i \neq j$, the mean first passage time from i to j is given by*

$$m_{i,j} = \begin{cases} e_i^\top (I - T_{(j)})^{-1} \mathbb{1}, & \text{if } i < j; \\ e_{i-1}^\top (I - T_{(j)})^{-1} \mathbb{1}, & \text{if } i > j; \end{cases}$$

where $T_{(j)}$ denotes the j^{th} principal submatrix of T.

Proof. Without loss of generality, let $j = n$. Partition off the n^{th} row and column of T, so that

$$T = \left[\begin{array}{c|c} T_{(n)} & (I - T_{(n)})\mathbb{1} \\ \hline r^\top & t_{n,n} \end{array}\right],$$

where $r = [t_{n,1}\ t_{n,2}\ \cdots\ t_{n,n-1}]^\top$. Now suppose the mean first passage matrix M is

partitioned conformally, so that

$$M = \left[\begin{array}{c|c} M_{(n)} & y \\ \hline s^\top & m_{n,n} \end{array}\right],$$

where $y = [m_{1,n}\ m_{2,n}\ \cdots\ m_{n-1,n}]^\top$ and $s = [m_{n,1}\ m_{n,2}\ \cdots\ m_{n,n-1}]^\top$. Examining the matrix equation (2.7) in this partitioned form, we have

$$\left[\begin{array}{c|c} M_{(n)} & y \\ \hline s^\top & m_{n,n} \end{array}\right] = \left[\begin{array}{c|c} T_{(n)} & (I - T_{(n)})\mathbb{1} \\ \hline r^\top & t_{n,n} \end{array}\right] \left[\begin{array}{c|c} (M - M_{dg})_{(n)} & y \\ \hline s^\top & 0 \end{array}\right] + \left[\begin{array}{c|c} J & \mathbb{1} \\ \hline \mathbb{1}^\top & 1 \end{array}\right]$$

which produces $y = T_{(n)}y + \mathbb{1}$. Hence $y = (I - T_{(n)})^{-1}\mathbb{1}$; i.e.

$$(I - T_{(n)})^{-1}\mathbb{1} = \begin{bmatrix} m_{1,n} \\ m_{2,n} \\ \vdots \\ m_{n-1,n} \end{bmatrix}.$$

Hence $m_{i,n} = e_i^\top (I - T_{(n)})^{-1}\mathbb{1}$, for $i = 1, \ldots, n$.

The same techniques of partitioning may be applied after an appropriate permutation of the rows and columns of T and M to produce the given expressions for $m_{i,j}$. $\square$

Note that a slightly different expression in Proposition 2.4.2 arises when $j < i$ because the mean first passage time $m_{i,j}$ is the row sum of $(I - T_{(j)})^{-1}$ corresponding to the i^{th} state. However, if $j < i$ then we have deleted a row and column before i in the index ordering, and the row of $(I - T_{(j)})^{-1}$ corresponding to state s_i is now row $i - 1$.

2.5 The group inverse of a singular matrix

An instrumental tool in Markov chain theory is a certain generalised matrix inverse called the *group inverse*. Indeed, in [68], Carl Meyer Jr. states that "if $Q = I - T$, it will be shown that once the group inverse $Q^{\#}$ of Q is known, then the answer to every important question concerning the chain can be obtained from $Q^{\#}$."

Definition 2.5.1. Let A be an $n \times n$ complex singular matrix such that the geometric and algebraic multiplicities of the eigenvalue 0 of A coincide (i.e. 0 is a *semisimple eigenvalue*). Then the *group inverse* of A, denoted $A^{\#}$, exists and is given by the unique matrix X satisfying

$$AXA = A; \qquad XAX = X; \qquad AX = XA. \tag{2.8}$$

To find the group inverse of a given singular matrix A with 0 as a semisimple eigenvalue, consider the Jordan form of A and note that there exists some invertible matrix P such that

$$A = P \left[\begin{array}{c|c} B & O \\ \hline O & O \end{array}\right] P^{-1}$$

such that B is invertible. Then the matrix

$$X = P \left[\begin{array}{c|c} B^{-1} & O \\ \hline O & O \end{array}\right] P^{-1}$$

can readily be seen to satisfy the three equations in (2.8). To show uniqueness of this solution, we must consider the range and null space of X and of A, where X is a solution to (2.8); see [52, Section 2.1] for more details.

We note here some properties of $A^{\#}$ which will be useful.

Theorem 2.5.2. *Let A be a singular complex $n \times n$ matrix with 0 as a semisimple eigenvalue, and let $A^{\#}$ be the group inverse of A. Then $A^{\#}$ has the following spectral properties:*

(a) $A^{\#}$ has 0 as a semisimple eigenvalue, and its multiplicity is equal to the multiplicity of 0 as an eigenvalue of A.

(b) For a vector v, $Av = 0$ if and only if $A^{\#}v = 0$. Similarly, $v^{\top}A = 0$ if and only if $v^{\top}A^{\#} = 0$.

(c) $\lambda \neq 0$ is an eigenvalue of A of multiplicity m if and only if $\frac{1}{\lambda}$ is an eigenvalue of $A^{\#}$ of multiplicity m.

(d) $Av = \lambda v$ if and only if $A^{\#}v = \frac{1}{\lambda}v$. Similarly, $v^{\top}A = \lambda v^{\top}$ if and only if $v^{\top}A^{\#} = \frac{1}{\lambda}v^{\top}$.

(e) The matrix $I - AA^{\#}$ is the eigenprojection of A onto the eigenspace of A corresponding to the eigenvalue 0. In particular, if 0 is a simple eigenvalue of A (having multiplicity 1), with right and left null vectors v and $u^{\top}$ respectively, normalised so that $u^{\top}v = 1$, then $AA^{\#} = A^{\#}A = I - vu^{\top}$.

The group inverse of $I - T$ can be used to produce an expression for the mean first passage matrix M from (2.7). The following was first proven in [68].

Theorem 2.5.3. *Let T be an irreducible stochastic matrix with stationary vector w. Let $Q = I - T$, and let M be the mean first passage matrix of T. Let $W = \operatorname{diag}(w)$, the diagonal matrix with the entries of w on the diagonal, and let $Q^{\#}_{dg}$ denote the diagonal matrix consisting of the diagonal entries of $Q^{\#}$ and zeros elsewhere. Then*

$$M = (I - Q^{\#} + JQ^{\#}_{dg})W^{-1}. \tag{2.9}$$

Proof. Since the mean first return time is given by $m_{i,i} = \frac{1}{w_i}$, (2.7) can be rewritten as $M = TM - TW^{-1} + J$. Hence $QM = -TW^{-1} + J$, and multiplying by $Q^{\#}$ on the left yields

$$(I - \mathbb{1}w^{\top})M = -Q^{\#}TW^{-1} + Q^{\#}J = -Q^{\#}TW^{-1}.$$

Now, $-Q^{\#}T = I - \mathbb{1}w^{\top} - Q^{\#}$, and it follows that there must be some suitable vector v such that $M = (I + \mathbb{1}v^{\top} - Q^{\#})W^{-1}$. Since we know that $m_{i,i} = \frac{1}{w_i}$, examining this leads us to conclude that the entries of v must be the diagonal entries of $Q^{\#}$; i.e. $v = Q^{\#}_{dg}\mathbb{1}$. The result follows. □

The use of generalised matrix inverses in Markov chain theory did not begin in [68] with the group inverse; the original introduction of a 'fundamental matrix' from which the main quantities of interest could be derived appeared in [47], where

$$Z = (I - (T - \mathbb{1}w^{\top}))^{-1}$$

was shown to be central to the computation of key characteristics of the Markov chain. Decell and Odell also attempted in [22] to apply the Moore-Penrose inverse of $I - T$ to the problem; however, it was the foundational paper [68] by Meyer that cemented the group inverse to be the generalised matrix inverse of choice when discussing finite homogeneous Markov chains, and this theory is developed further in [11]. There has been great development of literature on the group inverse since then, particularly relating to the class of matrices known as M-matrices (of which the singular matrix $I - T$ is a member), and the recent book [52] by Kirkland and Neumann serves as another great reference text for the diverse collection of results which may be applied to finite Markov chains.

Note that some authors choose to develop results in terms of arbitrary generalised matrix inverses—in particular, Hunter has several results (see [42, 45]) characterising

expressions for stationary vectors and mean first passage times in terms of *any* generalised inverse of $I-T$, which are divided into classes determined by the number of the five key properties a generalised inverse (or g-inverse) may satisfy. Supposing X is a g-inverse of a given complex matrix A, the five properties (of which X must satisfy at least the first) are:

$$1.\ AXA = A; \qquad 2.\ XAX = X; \qquad 3.\ (AX)^* = AX;$$

$$4.\ (XA)^* = XA; \qquad 5.\ AX = XA.$$

For example, the group inverse is referred to as a (1, 2, 5) g-inverse, as it satisfies properties 1, 2, and 5, and the Moore-Penrose inverse is a (1, 2, 3, 4) g-inverse. Kemeny and Snell's fundamental matrix Z is a (1, 5) g-inverse. Although this approach constructs more general expressions, there is little lost in choosing a specific generalised inverse such as the group inverse, and making use of the expressions known for that type. In particular, note that since Kemeny and Snell's fundamental matrix Z requires first the computation of the stationary vector and then a matrix inversion, the robustness of this calculation is called into question in [68] when the stationary vector of T is poorly conditioned—compared to the computation of $(I-T)^{\#}$, which does not require the stationary vector. Because of this, and since more theory has been developed about the group inverse because of its prominence in Markov chain theory literature (see [11, 52]), this is the approach we will take in this thesis.

2.6 Kemeny's constant

Consider an irreducible Markov chain with mean first passage times $m_{i,j}$ and stationary distribution w. Fix an index i, and set

$$\kappa_i := \sum_{\substack{j=1 \\ j \neq i}}^{n} m_{i,j} w_j.$$

This quantity represents the expected time it takes the chain to get to a randomly-chosen destination state, given that it starts in s_i. This was first introduced in [47] and remarkably, it can be shown to be independent of the initial state s_i!

Theorem 2.6.1. *Let T be the transition matrix for an irreducible Markov chain, let w be the stationary vector for T, and $M = [m_{i,j}]$ the matrix of mean first passage times. Let $1, \lambda_2, \ldots, \lambda_n$ denote the eigenvalues of T. Then*

$$\kappa_i = \sum_{j=2}^{n} \frac{1}{1-\lambda_j}.$$

Proof. Let $W = \text{diag}(w)$, the diagonal matrix with the entries of w on the diagonal, and consider that w can be written $W\mathbb{1}$. Taking $M = (I - Q^{\#} + JQ_{dg}^{\#})W^{-1}$ from (2.9), it follows that

$$\begin{aligned} Mw &= (I - Q^{\#} + JQ_{dg}^{\#})W^{-1}W\mathbb{1} \\ &= \mathbb{1} - Q^{\#}\mathbb{1} + \mathbb{1}\mathbb{1}^{\top}Q_{dg}^{\#}\mathbb{1} \\ &= \mathbb{1} + \text{trace}(Q^{\#})\mathbb{1}. \end{aligned}$$

Now, if $\lambda \neq 1$ is an eigenvalue of T, $\frac{1}{1-\lambda}$ is an eigenvalue of $Q^{\#}$ by Theorem 2.5.2(c).

Hence

$$Mw = \left(1 + \sum_{j=2}^{n} \frac{1}{1-\lambda_j}\right) \mathbb{1}.$$

Then

$$\kappa_i + 1 \;=\; \sum_{\substack{j=1 \\ j\neq i}}^{n} m_{i,j} w_j + 1 \;=\; \sum_{j=1}^{n} m_{i,j} w_j \;=\; 1 + \sum_{j=2}^{n} \frac{1}{1-\lambda_j}.$$

□

Definition 2.6.2. Let T be the transition matrix for a Markov chain, with stationary vector w and mean first passage times $m_{i,j}$, $i, j = 1, \ldots n$. For any i, the quantity $\sum_{j\neq i} m_{i,j} w_j$ is called *Kemeny's constant*, and is denoted $\mathcal{K}(T)$.

As previously stated, for a transition matrix T, $\mathcal{K}(T)$ can be interpreted as the expected length of (i.e. number of steps in) a random trip in the Markov chain that originates at a fixed state s_i. In [64], it was observed that

$$\mathcal{K}(T) + 1 = \sum_{i=1}^{n} \sum_{j=1}^{n} w_i m_{i,j} w_j, \tag{2.10}$$

which admits the interpretation of Kemeny's constant in terms of the expected length of a trip from a randomly-chosen initial state to a randomly-chosen destination state in the chain. Finally, a description of Kemeny's constant is given in [44] as the *expected time to mixing* for the Markov chain. This concept may be summarised as follows: let Y be a random variable whose probability distribution is given by $w^\top$. Sample Y, and suppose that $Y = j$; we then start the Markov chain $\{X_m\}$ in initial state $X_0 = i$, and define the *time to mixing* to be the smallest $k \geq 1$ for which $X_k = j$. It follows that the expected value of k is given by $\mathcal{K}(T) + 1$.

Because of these practical interpretations, Kemeny's constant can be used to represent a kind of global connectivity of a Markov chain—a measure which quantifies how easily the system moves between states, in that low values of $\mathcal{K}(T)$ represent a

"well-connected" system. Note also that Kemeny's constant arises in the conditioning of a Markov chain (discussed later) and the stationary vector of a system with large $\mathcal{K}(T)$ will be very sensitive to perturbations of the transition probabilities.

2.7 Directed graphs

A *directed graph* D (or digraph) is a pair (V, E) consisting of a set of vertices $V = \{v_1, v_2, \ldots, v_n\}$ along with a collection of *arcs* or *directed edges* $E = \{(v_i, v_j) \mid \text{some } i, j \in \{1, \ldots, n\}\} \subseteq V \times V$. For an arc (v_i, v_j), v_i is called the initial vertex of the arc, and v_j the terminal vertex of the arc. We will sometimes denote an arc from v_i to v_j as $v_i \to v_j$. We say that v_i and v_j are *adjacent* to each other, and that v_i and v_j are *incident* to the arc (v_i, v_j). An arc (v_i, v_i) is referred to as a *loop* at v_i. The *indegree* (respectively, *outdegree*) of a vertex v is equal to the number of arcs in D of which v is the terminal vertex (respectively, initial vertex) of the arc.

A *subgraph* or *subdigraph* of a directed graph D is a directed graph $D_1 = (V_1, E_1)$ where $V_1 \subseteq V$ and E_1 is a subset of the arcs in D incident with vertices in V_1. If $V_1 = V$, then D_1 is called a *spanning subdigraph* of D.

A *walk* from v_i to v_j in a directed graph D is a collection of vertices and arcs

$$v_i = v_{i_1} \to v_{i_2} \to \cdots \to v_{i_l} = v_j.$$

If there are no repeated vertices, the walk is called a *path*. A walk from v_i to v_i is called a *closed walk* and a closed walk from v_i to v_i in which the only repeated vertex is v_i is called a *cycle*. A loop is trivially a cycle. The *length* of a walk, path, or cycle refers to the number of arcs therein. The distance from v_i to v_j, denoted $\text{dist}(v_i, v_j)$, is the length of the shortest path from v_i to v_j in D.

A directed graph D is called *strongly connected* if for every pair of vertices $v_i \neq v_j$,

there is a walk from v_i to v_j in D, and a walk from v_j to v_i. A *strongly connected component* of D is a maximal strongly connected subdigraph of D.

Directed graphs and matrices

Given a directed graph D on vertices $\{v_1, v_2, \ldots v_n\}$, the *adjacency matrix* of D, denoted A_D, is the $n \times n$ matrix where the $(i,j)^{th}$ entry is equal to 1, if $v_i \to v_j$ in D, and 0 otherwise.

The adjacency matrix can be used to determine many properties of the directed graph. For example, the $(i,j)^{th}$ entry of A_D^k counts the number of walks in D of length k from v_i to v_j. Thus D is strongly connected if and only if A_D is irreducible. Furthermore, given a $n \times n$ matrix $A = [a_{i,j}]$, we can associate to it a directed graph $\mathcal{D}(A)$ consisting of vertex set $\{v_1, \ldots v_n\}$, and an arc $v_i \to v_j$ if and only if $a_{i,j} \neq 0$. Then properties of the matrix A can be determined from its directed graph. Any nonnegative matrix A is irreducible only if $\mathcal{D}(A)$ is strongly connected, and primitive only if $\mathcal{D}(A)$ is strongly connected and the greatest common divisor of the lengths of all cycles in $\mathcal{D}(A)$ is equal to 1. The combinatorial structure of the matrix A is sometimes discussed in terms of the *zero pattern* of A, i.e. the set of entries of the matrix A which are zero. This is essentially the same as considering the directed graph, since the locations of the nonzero entries of A determine the arcs of $\mathcal{D}(A)$.

For a Markov chain with transition matrix T, the directed graph $D = \mathcal{D}(T)$ provides an easy visualisation of the system. That is, the vertices $v_1, \ldots, v_n$ of D represent the states $s_1, \ldots, s_n$, with an arc $v_i \to v_j$ whenever $t_{i,j} > 0$, thus displaying the transitions which are possible in a single time-step. We may also imagine these arcs to be *weighted* with the transition probability $t_{i,j}$.

Undirected graphs

An *undirected graph* $\mathcal{G}$ is a pair $(V, E_{\mathcal{G}})$ consisting as before of a set of vertices V and edges $E_{\mathcal{G}}$, where in this case, the edges are unordered pairs of vertices, so that $\{v_i, v_j\}$ represents a connection between vertices v_i and v_j, with no direction assigned. Analogous definitions for a subgraph, spanning subgraph, walk, path, circuit or cycle follow. The *degree* of a vertex v, denoted $\deg(v)$, is the number of edges incident with v. A vertex of degree 1 is called a *pendent vertex*. A graph in which for every pair v_i, v_j there exists a walk from v_i to v_j is simply called *connected*. A *connected component* is a maximal connected subgraph of $\mathcal{G}$. A graph containing no cycles is called *acyclic*, and is also known as a *forest*. A connected acyclic graph is called a *tree*. A graph $\mathcal{G}$ is *bipartite* if there exists a partition of the vertex set $V = V_1 \dot{\cup} V_2$ such that every edge in $\mathcal{G}$ is incident to one vertex in V_1 and one vertex in V_2.

2.8 Applications of Markov chains

There is an extensive range of applications to which a Markov chain may be put to use, from the standard classroom example of a weather system, to earthquake sequencing, computational drug design, ranking webpages on the world wide web, and the spread of infectious disease. We refer the interested reader to, respectively, [47],[16], [24, 25], [64], and [1]. In general, many complex dynamical systems can be difficult to analyse, but a Markov chain approach to analysing such a system is both simple and powerful; see [34] for an introduction to modelling complex dynamical systems using a Markov chain. We discuss one application here in more detail in order to motivate the proposed research.

A Markov chain model of the movement of vehicles in road networks was developed in [20], where states correspond to road segments, and transitions between states repre-

sent turning probabilities that may be observed, say, from traffic cameras. The entries of the stationary vector for this transition matrix, then, represent the traffic congestion on the corresponding road segments. Mean first passage times play a primary role in determining travel times between locations, while Kemeny's constant represents the length of an average trip on the road network. This model was then adapted to model pollution levels on the network (see [71, 21]), where these quantities can inform strategies on reducing emissions.

In many of these real-world applications of Markov chains, the systems are governed by an underlying directed graph that dictates which transitions are permitted. In this road traffic example, the existing road network dictates which transitions between states (road segments) are possible. However, the values of the different transition probabilities may vary to some degree by altering the timing of traffic lights, etc.

Given a directed graph D with vertex set $\{v_1, \dots v_n\}$, we define a set $\mathcal{S}_D$ to be the family of $n \times n$ stochastic matrices T for which $t_{i,j} > 0$ only if (v_i, v_j) is an arc in D. That is, $\mathcal{S}_D$ is the set of all stochastic matrices whose directed graphs $\mathcal{D}(T)$ are subordinate to the given digraph D. There is an existing body of recent research in the area of finite Markov chain theory that aims to determine the range of properties matrices in $\mathcal{S}_D$ can have, in order to determine how the combinatorial influence of the directed graph restricts the behaviour of the system; see [49, 50, 57, 58, 59].

2.9 Literature review

The results presented in this thesis will centre around these three key concepts; the stationary vector, the mean first passage times, and Kemeny's constant for a given Markov chain. These are quantifiers of the performance of the system modelled by the Markov chain, and as such, a better understanding is desired of how they are related

to one another, and how they are restricted by the underlying combinatorial structure of the Markov chain. In this section, we discuss some known results to motivate and contextualise the results of this thesis.

While Kemeny's constant was first introduced in [47] in 1960, it has only more recently become the subject of extensive research. The eigenvalue characterisation of Kemeny's constant in Theorem 2.6.1 was derived in [64], along with its intuitive interpretation as the expected length of a random trip in the Markov chain as described by the expression (2.10), in the context of a random surfer clicking links on a web graph. Hunter then investigated $\mathcal{K}(T)$ independently in [44] as the expected time to mixing of a Markov chain, found it to be independent of i, and determined some bounds on the effect of perturbations of the transition probabilities on the stationary vector which used $\mathcal{K}(T)$. More recently, the research regarding Kemeny's constant is centred around determining bounds on $\mathcal{K}(T)$. In particular, in [57], the directed graphs are characterised for which $\mathcal{K}(T)$ is bounded from above for every $T \in \mathcal{S}_D$. In [15], conditions are determined on the directed graph D for which $\mathcal{K}(T)$ does not depend on T at all. In [60], the following lower bound is given in terms of the entries of the stationary vector w of T, where it is assumed that $w_1 \leq \cdots \leq w_n$:

$$\mathcal{K}(T) \geq \sum_{j=1}^{n} (j-1)w_j.$$

The matrices T for which equality is attained in this lower bound are also characterised. This is comparable to an earlier result in [44], where it was shown that $\mathcal{K}(T) \geq \frac{n-1}{2}$, with equality when T is the adjacency matrix of the directed cycle on n vertices; in [57] this was determined to be the sole instance of equality attained for this lower bound on $\mathcal{K}(T)$.

Finally, we note that Kemeny's constant has been examined recently as a kind of

graph invariant for simple undirected graphs, by considering Kemeny's constant for the random walk on the graph. Due to the eigenvalue characterisation of Theorem 2.6.1, there are many connections with other graph invariants, such as the effective graph resistance or Kirchhoff index (see [80]), the Estrada index (see [77]), and others. The value of $\mathcal{K}(T)$ has been considered for various classes of graphs, including trees (see [61]), and the Erdős–Rényi random graphs (see [65]).

Although the stationary distribution vector is well-established, it is still a subject of great interest simply because it represents the long-term behaviour of the system modelled by the Markov chain, and analysis of future behaviour is the principal aim of many mathematical models applied to dynamical systems (take stability analysis of solutions to ordinary differential equations, for example). Conditioning is one of the most extensive research areas involving the stationary vector, where condition numbers (usually denoted as some function of T, $\mathfrak{c}(T)$) measure the change in the stationary vector relative to the size of some perturbation of T. In this way, the condition numbers determine the level of confidence we can have in the stationary vector for our Markov chain, since the transition matrix T may be subject to errors, depending on how the transition probabilities for the system are computed. There are many different known methods of formulating a condition number; most of them appear in the survey paper [18] from 2001, which gives a review and comparison of the main ones at that time. Note that mean first passage times can be used to provide a perturbation bound on the entries of the stationary distribution vector, as can Kemeny's constant (see [17, 44], respectively). Several other approaches have been taken towards conditioning, such as conditioning on a single entry of the stationary vector (see [53, 49]), determining the influence of the directed graph D on the conditioning properties of $T \in \mathcal{S}_D$ (see [49, 50]), as well as determining lower bounds for certain condition num-

bers (see [48]) and characterising transition matrices which attain equality in these lower bounds—i.e. representing well-conditioned Markov chains (see [51]). We will discuss the conditioning of stationary vectors further in Chapter 6.

While conditioning of stationary vectors is valuable in the consideration of Markov chain applications, a different theoretical approach is to ask about a wider range of stationary vectors that a Markov chain—with certain constraints—can attain, rather than just the effect of small perturbations on the existing stationary vector. This was first examined in [58] where it was sought to minimise the value of $||w||_\infty = \max_i\{w_i\}$ over all irreducible $T \in \mathcal{S}_D$, for a given directed graph D. That is, the author wanted to find the transition matrix for which the maximum entry of the stationary vector was as small as possible, characterising it as a 'load-balancing problem' for the system.

The final approach we mention regarding the analysis of the stationary distribution of a Markov chain is that of the Markov chain matrix tree theorem stated in [32], which provides solutions to the entries of the stationary distribution vector in terms of properties of the directed graph, again indicating the significant influence of the underlying directed graph on the Markov chain.

Mean first passage times usually appear in the literature as a useful tool for direct use in an applied setting. For this reason, most of the research devoted to mean first passage times revolves around different or improved methods of computation, either individually or via the matrix M as a whole. The earliest in-depth discussion appears in [47], giving an expression for the mean first passage matrix in terms of the fundamental matrix Z. Meyer then produced an article [68] in 1975 giving a more efficient expression in terms of the group inverse of $I - T$. Further research includes a divide-and-conquer approach to computing the mean first passage matrix using the theory of stochastic complementation (see [54]). An interesting offshoot is to consider the *variances* of first

passage times (see [11, 46, 47]). More recently, some work has been undertaken in [70] to investigate the conditions under which a given nonnegative matrix is the mean first passage matrix for some Markov chain; this is known as the inverse mean first passage matrix problem. Finally, the uses of mean first passage times other than the direct interpretation in an applied setting are that they can be used to compute conditioning properties of a stochastic matrix (see [17]), and they can also play a role in determining clustering behaviour in a system modelled by a Markov chain, since mean first passage times between two clusters will be large, indicating that the chain takes a long time to reach one group of states from the other. This is quantified in [20, Theorem A.1], and will be discussed again in Chapter 5.

Chapter 3

Stationary vectors of a Markov chain under combinatorial constraints

In this chapter, we discuss the following problem: given a strongly connected directed graph D, let $\mathcal{S}_D$ denote the set of all stochastic matrices whose directed graphs are spanning subdigraphs of D; that is,

$$\mathcal{S}_D = \{T \in \mathbb{R}^{n\times n} \mid T \geq 0,\, T\mathbb{1} = \mathbb{1},\, \text{and } \mathcal{D}(T) \subseteq D\}.$$

Can we describe the set of all possible stationary vectors of irreducible matrices in $\mathcal{S}_D$? Furthermore, supposing that w is some admissible stationary vector of an irreducible matrix in $\mathcal{S}_D$, we aim to characterise the set of matrices in $\mathcal{S}_D$ possessing w as a stationary vector. A solution to this problem will lend itself to the design of a Markov chain which simultaneously respects this given directed graph, and achieves some desirable stationary distribution. This, then, provides an indication of how to control or

influence the modelled system so that it has some desirable long-term behaviour.

Our principal achievement in this chapter is the provision of a theoretical characterisation given in Theorem 3.2.10 of the set of all admissible stationary vectors for irreducible matrices in $\mathcal{S}_D$, while an exploration of possible implementations is carried out in Section 3.4. Though we indicate that these methods can be computationally costly for large or dense directed graphs, the example discussed in Section 3.5 emphasises the fact that there are many small-scale cases of practical interest that can be analysed using the results in this chapter. We use our results to examine the sustainability of the North Atlantic right whale population, further demonstrating that there are applications of these results outside the realm of stochastic matrices and Markov chains. The content of this chapter has been published and appears in [5].

3.1 Introduction

Let $T \in \mathcal{S}_D$, and suppose that $x^\top T = x^\top$, for some $x \in \mathbb{R}^n_+$, such that $x^\top \mathbb{1} = 1$. Set $X := \operatorname{diag}(x)$, the diagonal matrix with the entries of x along the diagonal, and consider the matrix $S := XT$. Notice that

$$S\mathbb{1} = x \quad \text{and} \quad \mathbb{1}^\top S = x^\top. \tag{3.1}$$

In this way, we see that a positive probability vector x is admissible as a stationary vector for an irreducible $T \in \mathcal{S}_D$ if and only if there exists a nonnegative irreducible matrix S respecting the directed graph D such that (3.1) holds.

Our approach will be to assume that $x = [x_1 \cdots x_n]^\top$ is some admissible vector (i.e. that there exists some fixed $T \in \mathcal{S}_D$ such that $x^\top T = x^\top$) and to consider the equations in (3.1) as a linear system in the nonzero entries of S. The positions of these are known from the zero pattern of the matrix T, and we note that $s_{i,j} > 0$ only if

(i, j) is an arc in D. We will show that in the case that the *bipartite graph of* S is acyclic, solutions may be found to these 'variables' in terms of the entries of x – i.e. each $s_{i,j}$ may be written as an expression in $x_1, \ldots, x_n$. Then, since $s_{i,j} > 0$, we achieve an inequality condition on x which must be satisfied in order for x to be admissible. Notice that this approach also allows us to construct the matrix S satisfying (3.1) for our chosen x, and hence a matrix $T \in \mathcal{S}_D$ possessing x as a stationary vector.

It is evident from (3.1) that the matrix S is a member of the *symmetric transportation polytope* $\mathfrak{S}_n(x)$—defined as the set of $n \times n$ nonnegative matrices whose row and column sum vectors are both equal to x.

A *convex polytope* of $n \times n$ matrices is, formally, the bounded intersection of a finite number of closed halfspaces in $\mathbb{R}^{n \times n}$. It is sufficient here to think of it as a compact, convex set of matrices such that every matrix in the set is a convex combination of a finite number of *extreme points*; that is, matrices $A_1, A_2, \ldots, A_m$ such that for any matrix A in the set, there exist nonnegative constants $c_1, \ldots c_m$ such that $A = c_1 A_1 + c_2 A_2 + \cdots + c_m A_m$, where $\sum_i c_i = 1$. See [36] for further definitions and results regarding convex polytopes. The symmetric transportation polytope $\mathfrak{S}_n(x)$ described above is an example of a convex polytope. Note that the action $T \to XT$ was observed in [37] to act as a bijection between the convex set

$$\mathfrak{T}_n(x) := \{T \in \mathbb{R}^{n \times n} \mid T \geq 0, T\mathbb{1} = \mathbb{1}, \text{ and } x^\top T = x^\top\}$$

and $\mathfrak{S}_n(x)$, when $x \in \mathbb{R}^n_+$. We will use techniques from the areas of convex sets and transportation polytopes to generalise our approach beyond matrices whose bipartite graphs are acyclic. Note also that similar techniques were used in [35] to determine the class of stochastic matrices having a common left fixed vector.

Due to the preliminary description of our approach as determining information

about the class of matrices with a given row and column sum vector x, it is not surprising that some of the results in the next section are similar to those in the literature on transportation problems. However, we emphasise that our question, as stated, is motivated in the opposite way to those problems discussed in this linear programming context. In particular, the traditional approach has been to choose certain row and column sum vectors, and attempt to describe the combinatorial properties of the class of matrices with those sum vectors. Our aim, however, is to investigate how a combinatorial property of a matrix (in particular, the zero pattern, or associated directed graph) affects the range of possible vectors that can be both the row and column sum vector. While very different in spirit, some of the mechanics of dealing with these questions at the small scale remain the same, and we refer the interested reader to [4] and [19].

Remark 3.1.1. We note that in the definition of $\mathfrak{T}_n(x)$ above, we have not excluded the possibility that a matrix T satisfying $x^\top T = x^\top$ may be reducible. In general, since our set $\mathcal{S}_D$ contains both reducible and irreducible matrices, we will make no distinction between x being a stationary vector of a matrix T, or simply a left fixed vector, which will allow the possibility that T is reducible. Relaxing the constraint in this way will allow us to compute the conditions that are required for x to be the left fixed vector of any matrix in $\mathcal{S}_D$, and in Section 3.3 we discuss the stricter conditions under which this matrix will be irreducible.

3.2 The role of the bipartite graph

Let $T \in \mathcal{S}_D$ and let x be some positive probability vector, and suppose that $x^\top T = x^\top$. As before, set $X := \mathrm{diag}(x)$ and $S := XT$. In this section we describe the role of the bipartite graph of S in examining the linear system in (3.1).

Definition 3.2.1. Let $A = [a_{i,j}]$ be an $n \times n$ matrix. The *bipartite graph of* A, denoted $\mathcal{B}(A)$, is the undirected graph with vertex set $\{r_1, \ldots, r_n\} \cup \{c_1, \ldots, c_n\}$, where r_i is adjacent to c_j if and only if $a_{i,j} \neq 0$. The r_i are called the *row vertices* and the c_j the *column vertices*. For a directed graph D, we let $\mathcal{B}(D)$ denote the bipartite graph of the adjacency matrix of D.

Definition 3.2.2. Let $\mathcal{G}$ be an undirected graph with vertices $v_1, \ldots, v_n$ and edges $e_1, \ldots, e_m$. The *vertex-edge incidence matrix* of $\mathcal{G}$ is the $n \times m$ matrix N such that

$$n_{i,j} = \begin{cases} 1, & \text{if } v_i \text{ is incident to } e_j; \\ 0, & \text{otherwise.} \end{cases}$$

Consider the bipartite graph $\mathcal{B}(S)$ (which is equal to $\mathcal{B}(T)$) with row vertices $r_1, \ldots, r_n$ and column vertices $c_1, \ldots, c_n$. Let $\omega(\cdot)$ denote the *weight* of an edge or a vertex, and set

$$\omega(r_i c_j) := s_{i,j}.$$

Suppose we also weight the row vertices so that $\omega(r_i) := x_i$, for $i = 1, \ldots, n$. Then the row sums of S (given by $S\mathbb{1} = x$) are evident from the bipartite graph in that each equation in $S\mathbb{1} = x$

$$x_i = \sum_{j=1}^{n} s_{i,j},$$

is given by

$$\omega(r_i) = \sum_{j=1}^{n} \omega(r_i c_j).$$

By similarly weighting the column vertices, the column sums $\mathbb{1}^\top S = x^\top$ are also immediately evident from the bipartite graph. This results in the following proposition.

Proposition 3.2.3. *Let S be an $n \times n$ matrix with bipartite graph $\mathcal{B}(S)$, and let $x \in \mathbb{R}^n_+$.*

The coefficient matrix of the linear system obtained from the equations

$$S\mathbb{1} = x, \quad \mathbb{1}^\top S = x^\top$$

is equal to the vertex-edge incidence matrix of $\mathcal{B}(S)$.

This correspondence will be used to determine the conditions on x that ensure x is admissible as a left fixed vector of some matrix $T \in \mathcal{S}_D$. We will also see that it is useful when the bipartite graph $\mathcal{B}(T)$ is a forest (that is, acyclic); in particular, the incidence matrix has full column rank when $\mathcal{B}(T)$ is a forest with no isolated vertices, while this is not true in general. However, we show first that it is in fact enough to consider only cases in which the bipartite graph is a forest with no isolated vertices.

Proposition 3.2.4. *Suppose that* $x \in \mathbb{R}^n_+$ *and* $x^\top T = x^\top$ *for some* $T \in \mathcal{S}_D$. *Then there exists* $\tilde{T} \in \mathcal{S}_D$ *such that* $x^\top \tilde{T} = x^\top$, *and the bipartite graph of* $\tilde{T}$ *is a forest with no isolated vertices.*

Proof. Let $x \in \mathbb{R}^n_+$, and suppose $T \in \mathcal{S}_D$ such that $x^\top T = x^\top$. Then $T \in \mathfrak{T}_n(x)$ (defined in Section 3.1), which is a convex polytope, and thus T may be written as a convex combination of the extreme points of $\mathfrak{T}_n(x)$:

$$T = c_1 T_1 + c_2 T_2 + \cdots + c_m T_m, \quad \text{some } m,$$

where $c_i > 0$ and $\sum_i c_i = 1$. Of course, $x^\top T_i = x^\top$ for each i, and $\mathcal{B}(T_i) \subseteq \mathcal{B}(T)$, so $T_i \in \mathcal{S}_D$ for each i.

It is proven in [62] that a matrix $A \in \mathfrak{S}_n(x)$ is an extreme point if and only if the

bipartite graph of A is a forest with no isolated vertices. Since the bijection

$$\begin{aligned} \mathfrak{T}_n(x) &\longleftrightarrow \mathfrak{S}_n(x) \\ T &\longleftrightarrow XT \end{aligned}$$

described in [37] (and referenced above) preserves the extreme points of the polytope and does not affect the bipartite graph, we conclude that $\mathcal{B}(T_i)$ is a forest with no isolated vertices, for each i. □

Remark 3.2.5. For the remainder of this section, we operate under the assumption that the bipartite graph $\mathcal{B}(D)$ is a forest. If not, then it follows from the above that we may consider each spanning subgraph $\mathcal{F}$ of $\mathcal{B}(D)$ which is a forest, and find the corresponding conditions that ensure x is a left fixed vector of some matrix $\widehat{T} \in \mathcal{S}_D$ whose bipartite graph is this $\mathcal{F}$. Then for any $T \in \mathcal{S}_D$ written as a convex combination

$$T = c_1 T_1 + \cdots + c_m T_m, \tag{3.2}$$

where $\mathcal{B}(T_i) = \mathcal{F}_i$, some spanning forest $\mathcal{F}_i \subset \mathcal{B}(D)$, we have $x^\top T = x^\top$ if and only if x satisfies the conditions of *each* $\mathcal{F}_i$.

Note that with regard to the characterisation of the set of matrices possessing a given x as a left fixed vector, this result implies that for every forest $\mathcal{F}_i \subset \mathcal{B}(D)$ of which x satisfies the conditions, we can construct the unique matrix T_i such that $x^\top T_i = x^\top$, and $\mathcal{B}(T_i) = \mathcal{F}_i$. These matrices T_i are then the extreme points of the convex polytope of matrices possessing x as a left fixed vector, and every such matrix is of the form (3.2).

We now consider the rank of the linear system (3.1) through the correspondence with the incidence matrix of the bipartite graph.

Proposition 3.2.6. *Given a tree $\mathcal{T}$ on at least two vertices, there exists an ordering of the vertices and edges of $\mathcal{T}$ such that when the vertex-edge incidence matrix N is obtained with respect to this order, $n_{i,j} = 0$ whenever $j > i$, and $n_{i,j} = 1$ for $i = j$. In particular, N has full column rank.*

Proof. We use induction on the order of $\mathcal{T}$. For the base case, suppose that $|\mathcal{T}| = 2$. The reader may readily verify that the hypothesis holds for the incidence matrix of such a tree.

Suppose now that the induction hypothesis holds for all trees $\mathcal{T}$, $|\mathcal{T}| < m$, and consider a tree $\mathcal{T}$ with m vertices, of which k are pendent vertices. Label the k pendent vertices as $v_1, \ldots, v_k$ in any order, and let $e(i)$ denote the pendent edge incident to v_i, so that these vertices and edges appear first in the ordering. Then delete these edges and vertices. By induction there exists some method of ordering the remaining vertices so that according to this order, the vertex-edge incidence matrix is

$$N = \left[\begin{array}{c|c} I_k & O \\ \hline N_{21} & N' \end{array}\right]$$

where N_{21} is some $(0,1)$-matrix and O is the zero matrix, both of appropriate dimension, while I_k is the $k \times k$ identity matrix, and N' is an $(m-k) \times (m-k-1)$ incidence matrix of the smaller tree $\mathcal{T}'$ obtained by the removal of the pendent vertices and edges from $\mathcal{T}$. By induction N' satisfies the condition stated in the proposition and thus the proposition holds for all trees. □

Corollary 3.2.7. *The vertex-edge incidence matrix of a forest $\mathcal{F}$ with no isolated vertices has full column rank.*

Proof. For a forest with r components, each of which is a tree, we may order the vertices and edges of each component according to Proposition 3.2.6, and list these

sequentially so that the incidence matrix N of $\mathcal{F}$ is a block matrix with rectangular blocks representing the components of $\mathcal{F}$, and zeros elsewhere; i.e.

$$N = \left[\begin{array}{c|c|c|c} C_1 & O & \cdots & O \\ \hline O & C_2 & \cdots & O \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline O & O & \cdots & C_r \end{array}\right]. \tag{3.3}$$

Since each submatrix C_i has full column rank by Proposition 3.2.6, it follows that N has full column rank. □

Note that Proposition 3.2.6 and Corollary 3.2.7 are well-known results in the literature; see for example, [2, Lemma 2.17]. These results, coupled with Proposition 3.2.4, demonstrate that when $\mathcal{B}(S)$ is a forest, there are unique solutions for the weights $s_{i,j}$ in terms of the vector entries x_k, assuming (as we may) that the linear system is consistent. In order to find these solutions, and the conditions required on x that give a nonnegative solution to the linear system, we bring the augmented matrix for the linear system to row echelon form. The entries in the augmented column will then be linear combinations of $x_1, \ldots, x_n$, while there will be some nonzero rows and some zero rows in the coefficient matrix of the system. The augmented entries corresponding to the nonzero rows will determine the inequality conditions described before, and the entries in the augmented column that correspond to zero rows produce extra conditions on x. There will be one zero row in each rectangular block of the matrix (3.3), indicating that these extra conditions are derived from the component structure of $\mathcal{B}(T)$. The following proposition describes these conditions, which we will refer to as *component conditions*.

Proposition 3.2.8. *Given a directed graph D, let $T \in \mathcal{S}_D$ and let $x \in \mathbb{R}^n_+$ such that*

$x^\top T = x^\top$. *For each component* $\mathcal{C}$ *of* $\mathcal{B}(T)$,

$$\sum_{r_i \in \mathcal{C}} x_i = \sum_{c_j \in \mathcal{C}} x_j. \tag{3.4}$$

Proof. It is easily seen that if u is a left null vector of an incidence matrix N, then if vertex i is adjacent to vertex j,

$$u_i + u_j = 0.$$

From this, it is not difficult to show that the left null space of N is spanned by vectors $u_{\mathcal{C}}$, where, for each component $\mathcal{C}$ of the graph represented by N, the j^{th} entry of $u_{\mathcal{C}}$ is given by

$$u_{\mathcal{C}}(j) = \begin{cases} 1, & \text{if } j \text{ corresponds to a row vertex in } \mathcal{C}; \\ -1, & \text{if } j \text{ corresponds to a column vertex in } \mathcal{C}; \\ 0, & \text{otherwise.} \end{cases}$$

Letting N be the incidence matrix of $\mathcal{B}(D)$ and considering the vectors $u_{\mathcal{C}}$ which span its null space, we have, for each component $\mathcal{C}$

$$u_{\mathcal{C}}^\top \hat{x} = 0$$

where $\hat{x}$ is a vector of vertex weights x_i in the appropriate order. The component conditions (3.4) follow. □

We now consider a method for finding the unique solutions for the unknown matrix entries $s_{i,j}$.

From the linear system in (3.1), we have that

$$x_i = \sum_j s_{i,j} \quad \text{and} \quad x_i = \sum_k s_{k,i}.$$

Suppose we are looking for the weight $s_{i,j}$ of a particular edge $r_i c_j$ in terms of the x_i. Then

$$\begin{aligned} s_{i,j} &= x_i - \sum_{k \neq j} s_{i,k} \\ &= x_j - \sum_{k \neq i} s_{k,j}. \end{aligned} \tag{3.5}$$

Thus an expression can be given of the weight $\omega(e)$ of an edge e in terms of the x_i when the expressions of the weights of all of the other edges incident to either the row vertex or the column vertex of e are known.

Now, the weight of a pendent edge, say $r_i c_j$, is immediately determined by the pendent vertex to which it is incident; that is, $s_{i,j} = x_i$ if $\deg(r_i) = 1$ (similarly, $s_{i,j} = x_j$ if $\deg(c_j) = 1$). Referring to the edge ordering in Proposition 3.2.6, note that the weight of the edge $e(k)$ may be written in terms of the edges $e(i)$, where $i < k$. Thus using (3.5) we may solve inductively for the weights of all edges in $\mathcal{F}$.

We can also give a formula for computing the weight of any edge $r_i c_j$ in $\mathcal{F}$.

Proposition 3.2.9. *Let $\mathcal{F}$ be a forest, $x \in \mathbb{R}^n_+$, and suppose that S is an $n \times n$ matrix such that $\mathcal{B}(S) = \mathcal{F}$ and $S\mathbb{1} = x$, $\mathbb{1}^\top S = x^\top$. Then the weight $s_{i,j} := \omega(r_i c_j)$ may be determined directly from $\mathcal{F}$ as follows:*

Let $\mathcal{C}_r$ denote the component of $\mathcal{F} \setminus \{r_i c_j\}$ containing r_i, and $\mathcal{C}_c$ the component of $\mathcal{F} \setminus \{r_i c_j\}$ containing c_j, and let $V(\mathcal{C}_r), V(\mathcal{C}_c)$ denote the vertex sets of $\mathcal{C}_r$ and $\mathcal{C}_c$, respectively. Then

$$\omega(r_i c_j) = \sum_{r_k \in V(\mathcal{C}_r)} x_k - \sum_{c_l \in V(\mathcal{C}_r)} x_l, \tag{3.6}$$

or, equivalently,

$$\omega(r_i c_j) = \sum_{c_k \in V(\mathcal{C}_c)} x_k - \sum_{r_l \in V(\mathcal{C}_c)} x_l. \tag{3.7}$$

Proof. First of all, note that the equivalence of these two expressions follows from

Proposition 3.2.8, since $V(\mathcal{C}_r) \cup V(\mathcal{C}_c)$ determines a single component of $\mathcal{F}$ (the one containing the edge $r_i c_j$), and equating these expressions gives us the corresponding component condition as in (3.4).

To prove these solutions, we will use the induction alluded to above. For the base case, suppose that $r_i c_j$ is a pendent edge, and, without loss of generality, suppose that r_i is the pendent vertex. Then $V(\mathcal{C}_r) = \{r_i\}$, and $\omega(r_i c_j) = x_i$, and the hypothesis holds.

Now fix $r_i c_j \in \mathcal{F}$. We assume that the weight of every other edge incident to r_i is known, and is computed according to the induction hypothesis. That is, let $r_i c_{j_1}, r_i c_{j_2}, \ldots, r_i c_{j_s}$ denote the relevant edges, and let $\mathcal{C}_\alpha$ denote the component of $\mathcal{F} \setminus \{r_i c_{j_\alpha}\}$ that contains c_{j_α}, for each $\alpha = 1, \ldots, s$. Then we have assumed that

$$\omega(r_i c_{j_\alpha}) = \sum_{c_k \in V(\mathcal{C}_\alpha)} x_k - \sum_{r_l \in V(\mathcal{C}_\alpha)} x_l.$$

Notice that the vertex set of the component $\mathcal{C}_r$ of $\mathcal{F} \setminus \{r_i c_j\}$ that contains r_i is equal to

$$V(\mathcal{C}_1) \cup V(\mathcal{C}_2) \cup \cdots \cup V(\mathcal{C}_s) \cup \{r_i\}.$$

From (3.5),

$$\begin{aligned}
\omega(r_i c_j) &= x_i - \sum_{k \neq j} s_{i,k} \\
&= x_i - \sum_{\alpha=1}^{s} \omega(r_i c_{j_\alpha}) \\
&= x_i - \sum_{\alpha=1}^{s} \left(\sum_{c_k \in V(\mathcal{C}_\alpha)} x_k - \sum_{r_l \in V(\mathcal{C}_\alpha)} x_l \right) \\
&= \sum_{r_l \in V(\mathcal{C}_r)} x_l - \sum_{c_k \in V(\mathcal{C}_r)} x_k.
\end{aligned}$$

□

We note that the inductive method is more straightforward for finding the weights of every edge in the bipartite graph, while Proposition 3.2.9 gives a concise formula which may be more appropriate when the weight of a single edge is required.

We summarise the results of this section with the following theorem:

Theorem 3.2.10. *Let D be a strongly connected directed graph, $\mathcal{B}(D)$ its bipartite graph, and let $x \in \mathbb{R}^n_+$. Then x is a left fixed vector of some $T \in \mathcal{S}_D$ if and only if there is a spanning forest $\mathcal{F}$ of $\mathcal{B}(D)$ with no isolated vertices, such that:*

(a) the component condition (3.4) holds for each component $\mathcal{C}$ of $\mathcal{F}$;

(b) for each edge r_ic_j of F, the weight $w(r_ic_j)$ as computed in (3.6) and (3.7) is positive.

Remark 3.2.11. We emphasise that in the statement of the above theorem, we say that *any* vector in $\mathbb{R}^n$ (not necessarily positive) that satisfies the conditions in Propositions 3.2.8 and 3.2.9 must then be a positive left fixed vector of a matrix in $\mathcal{S}_D$. This is a consequence of the inductive method of determining the weights: if the weight of a pendent edge is positive, this ensures the positivity of a single entry of x, and using (3.5), positivity of the whole vector follows.

If we are only interested in probability vectors, then we must include the condition that $x_1 + x_2 + \cdots + x_n = 1$.

Remark 3.2.12. An alternative formulation of the conditions in Theorem 3.2.10 can be found in a paper of Brualdi [8], which discusses the more general set $\mathfrak{P}(x, y)$ of matrices with a given zero pattern $\mathfrak{P}$, row sum vector x, and column sum vector y. What we have named component conditions in this special case are accounted for in the author's assumption of *nondecomposability*, and our edge-weight conditions can be seen to be equivalent to the author's characterisation of a necessary and sufficient

condition for $\mathfrak{P}(x, y)$ to be nonempty [8, Theorem 2.1], when $\mathfrak{P}$ is the zero pattern of a matrix whose bipartite graph is a forest.

Notable differences between the approaches include Brualdi's investigation of the more general transportation polytope, while we focus on the symmetric case (i.e. $x = y$) since the basis of our discussion is concerned with stationary vectors of stochastic matrices. We observe that the strength of our approach rests on Remark 3.2.5, as we succeed in completely characterising the set of all matrices with a given row and column sum vector, while [8] gives only a construction of one matrix in the class on the condition that the row and column sums are rational, along with a method for constructing a new matrix in the class from one that is known. Additionally, by focusing only on matrices in the class whose bipartite graphs are forests, we reduce the complexity of the directed graph before performing the analysis, so that we can present fewer, and more explicit conditions.

Finally, we note that Brualdi's result gives a condition for the existence of a matrix with precisely the given directed graph and desired row/column sums, while our approach allows for solutions with edges of the original directed graph being absent. The difference in intention is key here; our problem is posed because of the applications of Markov chain theory, and such an approach is a natural consideration in some of these settings, e.g. to allow the closure of some roads in a road network-type example.

Example 3.2.13. Consider the bipartite graph $\mathcal{B}(D)$ shown in Figure 3.1. We first note that it is a forest of two components, imposing the condition

$$x_1 + x_3 + x_4 = x_2 + x_5 \tag{3.8}$$

on any left fixed vector x of a matrix in $\mathcal{S}_D$. We refer to the component with darker edges in Fig. 3.1 as Component 1, and the other as Component 2.

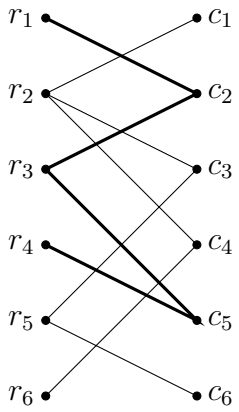


Figure 3.1: The bipartite graph $\mathcal{B}(D)$ considered in Example 3.2.13.

The conditions derived as the weights of the edges are as follows:

- Component 1:

$$\begin{aligned}
\omega(r_1c_2) &= x_1 \\
\omega(r_4c_5) &= x_4 \\
\omega(r_3c_2) &= x_2 - x_1 \\
\omega(r_3c_5) &= x_5 - x_4
\end{aligned}$$

- Component 2:

$$\begin{aligned}
\omega(r_2c_1) &= x_1 \\
\omega(r_5c_6) &= x_6 \\
\omega(r_6c_4) &= x_6 \\
\omega(r_5c_3) &= x_5 - x_6 \\
\omega(r_2c_4) &= x_4 - x_6 \\
\omega(r_2c_3) &= x_2 - x_4 + x_6 - x_1
\end{aligned}$$

We have presented these in the order described in Proposition 3.2.6, so that the reader may see more clearly the inductive method described above. For example, the weight of r_2c_3 is determined by assuming that those before it in the order are known, as follows:

$$\begin{aligned} & \omega(r_2) &=& \omega(r_2c_1) + \omega(r_2c_3) + \omega(r_2c_4) \\ \Rightarrow \quad & \omega(r_2c_3) &=& \omega(r_2) - \omega(r_2c_1) - \omega(r_2c_4) \\ & &=& x_2 - x_1 - (x_4 - x_6). \end{aligned} \tag{3.9}$$

To illustrate the equivalence of the expressions in Proposition 3.2.9, suppose we remove r_2c_3 from $\mathcal{B}(D)$. The corresponding row component $\mathcal{C}_r$ is the induced subgraph with vertex set $\{r_2, r_6, c_1, c_4\}$, and the column component $\mathcal{C}_c$ is induced by the vertex set $\{r_5, c_3, c_6\}$. Thus

$$\begin{aligned} & \omega(r_2c_3) &=& x_2 + x_6 - x_1 - x_4 \\ \text{or} \quad & \omega(r_2c_3) &=& x_3 + x_6 - x_5 \end{aligned}$$

which are equivalent to each other by (3.8), and also to the expression obtained in (3.9).

Consider

$$x^\top = \begin{bmatrix} 0.1 & 0.2 & 0.225 & 0.125 & 0.25 & 0.1 \end{bmatrix}.$$

It may be verified that x satisfies the conditions derived from $\mathcal{B}(D)$, and thus there exists $T \in \mathcal{S}_D$ such that $x^\top T = x^\top$. But since $s_{i,j} = \omega(r_ic_j)$, we can compute the

matrix S to be

$$S = \begin{bmatrix} 0 & 0.1 & 0 & 0 & 0 & 0 \\ 0.1 & 0 & 0.075 & 0.025 & 0 & 0 \\ 0 & 0.1 & 0 & 0 & 0.125 & 0 \\ 0 & 0 & 0 & 0 & 0.125 & 0 \\ 0 & 0 & 0.15 & 0 & 0 & 0.1 \\ 0 & 0 & 0 & 0.1 & 0 & 0 \end{bmatrix}$$

and thus

$$\begin{aligned} T &= X^{-1}S \\ &= \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0.375 & 0.125 & 0 & 0 \\ 0 & 0.\dot{4} & 0 & 0 & 0.\dot{5} & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0.6 & 0 & 0 & 0.4 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}. \end{aligned}$$

Remark 3.2.14. While Proposition 3.2.9 is an interesting result, and reinforces the importance of the bipartite graph in this problem, there are certainly computationally simpler methods by which the edge-weight conditions may be found. In particular, we may do the following: the incidence matrix of the bipartite graph (or coefficient matrix

	r_1c_2	r_4c_5	r_3c_2	r_3c_5	r_2c_1	r_5c_6	r_6c_4	r_5c_3	r_2c_4	r_2c_3
r_1	1	0	0	0						
r_4	0	1	0	0						
c_2	1	0	1	0						
c_5	0	1	0	1						
r_3	0	0	1	1						
c_1					1	0	0	0	0	0
c_6					0	1	0	0	0	0
r_6					0	0	1	0	0	0
r_5					0	1	0	1	0	0
c_4					0	0	1	0	1	0
c_3					0	0	0	1	0	1
r_2					1	0	0	0	1	1

(a) The incidence matrix N of $\mathcal{B}(D)$ from Example 3.2.13.

	r_1	r_4	c_2	c_5	c_1	c_6	r_6	r_5	c_4	c_3
r_1c_2	1	0	0	0						
r_4c_5	0	1	0	0						
r_3c_2	−1	0	1	0						
r_3c_5	0	−1	0	1						
r_2c_1					1	0	0	0	0	0
r_5c_6					0	1	0	0	0	0
r_6c_4					0	0	1	0	0	0
r_5c_3					0	−1	0	1	0	0
r_2c_4					0	0	−1	0	1	0
r_2c_3					0	1	0	−1	0	1

(b) The inverse of the truncated incidence matrix, $\widehat{N}^{-1}$.

$$\left[\begin{array}{cccc|cccccc} 1 & 0 & 0 & 0 & & & & & & \\ 0 & 1 & 0 & 0 & & & & & & \\ -1 & 0 & 1 & 0 & & & & & & \\ 0 & -1 & 0 & 1 & & & & & & \\ \hline & & & & 1 & 0 & 0 & 0 & 0 & 0 \\ & & & & 0 & 1 & 0 & 0 & 0 & 0 \\ & & & & 0 & 0 & 1 & 0 & 0 & 0 \\ & & & & 0 & -1 & 0 & 1 & 0 & 0 \\ & & & & 0 & 0 & -1 & 0 & 1 & 0 \\ & & & & 0 & 1 & 0 & -1 & 0 & 1 \end{array}\right] \left[\begin{array}{c} x_1 \\ x_4 \\ x_2 \\ x_5 \\ \hline x_1 \\ x_6 \\ x_6 \\ x_5 \\ x_4 \\ x_3 \end{array}\right] = \left[\begin{array}{c} x_1 \\ x_4 \\ x_2 - x_1 \\ x_5 - x_4 \\ \hline x_1 \\ x_6 \\ x_6 \\ x_5 - x_6 \\ x_4 - x_6 \\ x_3 - x_5 + x_6 \end{array}\right] = \left[\begin{array}{c} \omega(r_1c_2) \\ \omega(r_4c_5) \\ \omega(r_3c_2) \\ \omega(r_3c_5) \\ \hline \omega(r_2c_1) \\ \omega(r_5c_6) \\ \omega(r_6c_4) \\ \omega(r_5c_3) \\ \omega(r_2c_4) \\ \omega(r_2c_3) \end{array}\right]$$

(c) The vector $\widehat{N}^{-1}\hat{x}$ displaying the edge-weight conditions as they would be produced using Prop. 3.2.9.

Figure 3.2: Application of Remark 3.2.14 to Example 3.2.13

of the system) may be decomposed according to the components of $\mathcal{B}(S)$, so that

$$N = \left[\begin{array}{c|c|c|c} C_1 & O & \cdots & O \\ \hline O & C_2 & \cdots & O \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline O & O & \cdots & C_k \end{array}\right].$$

As observed earlier, this matrix in row echelon form has k zero rows, while the rest are nonzero. Deleting those zero rows results in an invertible matrix, $\widehat{N}$, since N has full column rank. Suppose a new vector $\hat{x}$ of length $2n-k$ is constructed from x so that the weights x_i appear in an order corresponding to the vertex order with respect to which N is written, and entries that correspond to deleted rows are also deleted from $\hat{x}$. It is evident that the product of the i^{th} row of $\widehat{N}^{-1}$ with $\hat{x}$ is the weight of the i^{th} edge. Thus the inverse matrix $\widehat{N}^{-1}$ is all that is necessary to determine the weights of the edges, $s_{i,j}$.

Let us illustrate using Example 3.2.13. The incidence matrix for the bipartite graph in Fig. 3.1, written with respect to the order described in Prop. 3.2.6, is the one shown in Fig. 3.2a (where the blank entries in the off-diagonal blocks are zero). If we delete the rows corresponding to the vertices r_3 and r_2 (one from each component), and invert the resulting matrix, we obtain the matrix $\widehat{N}^{-1}$ shown in Fig. 3.2b. Constructing the vector $\hat{x}$ according to our description above and multiplying by $\widehat{N}^{-1}$ results in the vector of edge-weight conditions displayed in Fig. 3.2c, which is identical to the set of conditions derived from the bipartite graph $\mathcal{B}(D)$ shown in Fig. 3.1.

We remark that this example also demonstrates that when computing the edge weights it is sufficient to consider each component (and its vertex-edge incidence matrix) individually—an observation we will use when discussing the implementation of our results in Section 3.4.

Remark 3.2.15. We note with regard to Example 3.2.13 that once the weight of each edge in $\mathcal{B}(D)$ was found, the set of conditions derived from each spanning forest $\mathcal{F} \subset \mathcal{B}(D)$ would be easily achieved, since if $e \in \mathcal{B}(D)$ is not an edge of $\mathcal{F}$, we simply have $\omega(e) = 0$. Although we observed early in this section that when $\mathcal{B}(D)$ is not acyclic it is enough to find conditions from any spanning forest of $\mathcal{B}(D)$, we now conclude that we may consider only *edge-maximal* forests, and relax the positivity constraint of the edge weights, insisting only that for each i, there exists some j such that $\omega(r_i c_j) > 0$. This is to ensure that the bipartite graph has no isolated vertices, and hence the resulting matrix – of which x is a left fixed vector – has no zero rows or columns.

3.3 Determining stationary vectors of irreducible matrices

Thus far, we have derived conditions by which we may determine all left fixed vectors of matrices in $\mathcal{S}_D$, although some of these matrices may be reducible. In this section we determine the conditions under which a left fixed vector x is in fact the stationary vector of an irreducible matrix in $\mathcal{S}_D$, and the conditions under which it is a left fixed vector of only reducible members of $\mathcal{S}_D$. First, we determine a relationship between a reducible matrix and its bipartite graph.

Definition 3.3.1. Let $\mathcal{G}$ be a bipartite graph with vertex set $\{r_1, \ldots, r_n\} \cup \{c_1, \ldots, c_n\}$, and let $\widehat{\mathcal{G}}$ be an induced subgraph of $\mathcal{G}$. We say that $\widehat{\mathcal{G}}$ is a *balanced subgraph* of $\mathcal{G}$ if $\widehat{\mathcal{G}}$ has no isolated vertices, and $r_i \in \widehat{\mathcal{G}} \Leftrightarrow c_i \in \widehat{\mathcal{G}}$.

We now observe the following relationship between certain edges in the bipartite graph, or certain entries of the matrix $S = XT$.

Proposition 3.3.2. *Let S be an $n \times n$ matrix and $x \in \mathbb{R}^n_+$ such that $\mathbb{1}^\top S = x^\top$ and $S\mathbb{1} = x$. If for some permutation matrix P,*

$$PSP^\top = \left[\begin{array}{c|c} S_{11} & S_{12} \\ \hline S_{21} & S_{22} \end{array}\right]$$

where S_{11}, S_{22} are square, then the sum of the entries in the submatrix S_{12} is equal to the sum of entries in S_{21}.

Proof. Suppose that S_{11} is a $k \times k$ submatrix. Since the sum of the first k rows and the sum of the first k columns of $PSP^\top$ are equal, it follows that the sums of the entries in S_{12} and the entries in S_{21} must be equal. □

Corollary 3.3.3. *Given a directed graph D, let x be a positive vector such that $x^\top T = x^\top$ for some $T \in \mathcal{S}_D$. Then T is reducible if and only if there exists a permutation matrix P such that*

$$PTP^\top = \left[\begin{array}{c|c} T_{11} & O \\ \hline O & T_{22} \end{array}\right].$$

Equivalently, T is reducible if and only if $\mathcal{B}(T)$ is the disjoint union of two balanced subgraphs of $\mathcal{B}(D)$.

In this way, we have established that a positive vector x is the left fixed vector of a reducible matrix in $\mathcal{S}_D$ if and only if it satisfies the component and edge-weight conditions derived from a spanning forest of $\mathcal{B}(D)$ that is a disjoint union of two balanced subgraphs.

Example 3.3.4. The bipartite graph $\mathcal{B}(D)$ of Example 3.2.13 (see Fig. 3.1) admits the two subgraphs shown in Fig. 3.3, each of which is a disjoint union of two balanced subgraphs. We note that $\mathcal{B}(D)$ does not admit any other such subgraphs – i.e. any

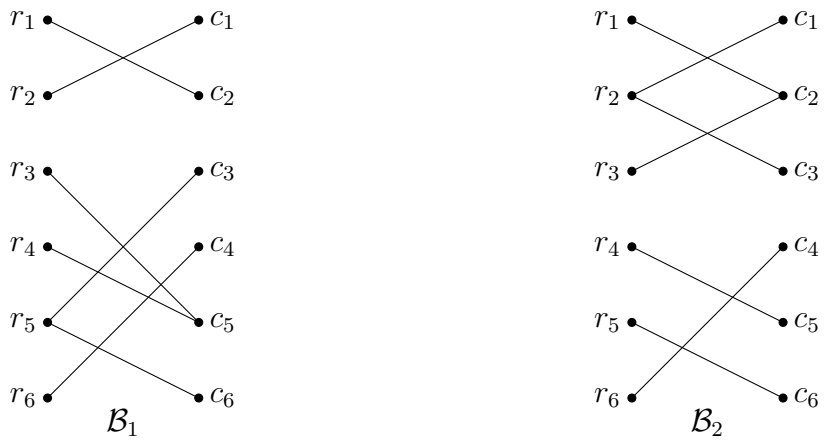


Figure 3.3: Two spanning subgraphs of the bipartite graph $\mathcal{B}(D)$ in Fig. 3.1 representing reducible matrices in $\mathcal{S}_D$

reducible matrix in $\mathcal{S}_D$ with a positive left fixed vector must have one of these graphs in Fig. 3.3 as its bipartite graph.

In the case of $\mathcal{B}_1$, reducibility is achieved when r_2c_3, r_2c_4 and r_3c_2 are absent from the graph of $\mathcal{B}(D)$ – i.e. $\omega(r_2c_3) = \omega(r_2c_4) = \omega(r_3c_2) = 0$. Similarly, a matrix $T \in \mathcal{S}_D$ with left fixed vector x has bipartite graph $\mathcal{B}_2$ if and only if $\omega(r_2c_4) = \omega(r_3c_5) = \omega(r_5c_3) = 0$.

Suppose now that $x \in \mathbb{R}^n_+$ is a left fixed vector of some matrix $T \in \mathcal{S}_D$. Then T is reducible if and only if x satisfies each of

$$\begin{aligned} x_2 - x_1 &= 0 \\ x_3 - x_5 + x_6 &= 0 \\ x_4 - x_6 &= 0 \end{aligned}$$

or each of

$$\begin{aligned} x_4 - x_6 &= 0 \\ x_5 - x_4 &= 0 \\ x_5 - x_6 &= 0. \end{aligned}$$

Given a directed graph D such that $\mathcal{B}(D)$ is as in Fig. 3.1 on page 49, and some x that is a left fixed vector of a matrix in $\mathcal{S}_D$ (i.e. x is known to satisfy the conditions of Theorem 3.2.10), we can say that x is in fact a stationary vector if and only if at least one expression from each group above is positive. Alternatively (in this case), x is a stationary vector if the forest whose conditions are satisfied by x as per Theorem 3.2.10 is $\mathcal{B}(D)$ itself, since every spanning subgraph of $\mathcal{B}(D)$ with no isolated vertices is equivalent to those shown in Fig. 3.3 (via Proposition 3.3.2).

As the preceding example suggests, a precise description of the set of positive vectors that serve as the stationary vectors for some irreducible member of $\mathcal{S}_D$ will, in general, be quite involved, particularly when $\mathcal{B}(D)$ is not acyclic. Consequently, we will not pursue that problem further here. However, as the following result shows, any stationary vector associated with an irreducible member of $\mathcal{S}_D$ can be approximated arbitrarily closely by vectors satisfying the conditions of Theorem 3.2.10.

Proposition 3.3.5. *Given a strongly connected directed graph D, the set of all positive left fixed vectors of matrices in $\mathcal{S}_D$ is the topological closure of the set of stationary distributions of irreducible members of $\mathcal{S}_D$.*

Proof. Let $T \in \mathcal{S}_D$ be reducible, and suppose, without loss of generality, that

$$T = \left[\begin{array}{c|c} T_{11} & O \\ \hline O & T_{22} \end{array}\right], \tag{3.10}$$

with T_{11}, T_{22} irreducible, and that T has a positive left fixed probability vector

$$x^\top = [\beta_1 w_1^\top \mid \beta_2 w_2^\top],$$

where w_1, w_2 are the stationary vectors of T_{11}, T_{22} respectively, and $0 < \beta_1, \beta_2 < 1$, $\beta_1 + \beta_2 = 1$.

Consider the family of matrices defined as follows:

$$T'(\varepsilon, \delta) = \left[\begin{array}{c|c} T_{11} - \varepsilon e_i e_j^\top & \varepsilon e_i e_k^\top \\ \hline \delta e_r e_s^\top & T_{22} - \delta e_r e_t^\top \end{array}\right], \tag{3.11}$$

where $\varepsilon, \delta > 0$, and where indices i, j, k, r, s, t are chosen appropriately; that is, in such a way that the (i, j) entry of T_{11} and the (r, t) entry of T_{22} are both nonzero, and the (i, k) or the (r, s) entry of the relevant off-diagonal block is one that corresponds to an edge in D. In other words, this family of matrices $T'(\varepsilon, \delta)$ represent perturbations of the matrix T that result in an irreducible matrix in $\mathcal{S}_D$.

We will show that there exists a sequence of matrices $T'(\varepsilon, \delta)$ such that the stationary vectors converge to the left fixed vector x of T as $\varepsilon \to 0$. To do this, we will describe the stationary vector of a matrix of the form (3.11) using stochastic complementation (see Section 2.3), and then express δ in terms of ε in such a way as to achieve the

result. Consider the stochastic complement of T_{11}:

$$\begin{aligned} S_1 &= (T_{11} - \varepsilon e_i e_j^\top) + \varepsilon e_i e_k^\top (I - T_{22} + \delta e_r e_t^\top)^{-1} \delta e_r e_s^\top \\ &= T_{11} - \varepsilon e_i e_j^\top + \varepsilon e_i e_s^\top, \end{aligned}$$

since S_1 must be stochastic. We denote the stationary vector of S_1 by z_1. Similarly, we compute the stochastic complement of T_{22},

$$S_2 = T_{22} - \delta e_r e_t^\top + \delta e_r e_k^\top,$$

and denote its stationary vector by z_2. Note that $z_1 \to w_1$ as $\varepsilon \to 0$, and $z_2 \to w_2$ as $\delta \to 0$, since T_{11} and T_{22} are both irreducible.

Now, the stationary vector of $T'(\varepsilon, \delta)$ may be written as

$$z(\varepsilon, \delta)^\top = [\alpha_1 z_1^\top \mid \alpha_2 z_2^\top]$$

where $[\alpha_1 \, \alpha_2]$ is the stationary vector of the 2×2 matrix computed as in (2.5); that is,

$$\begin{aligned} \alpha_1 &= \frac{\delta z_2(r)}{\varepsilon z_1(i) + \delta z_2(r)}; \\ \alpha_2 &= \frac{\varepsilon z_1(i)}{\varepsilon z_1(i) + \delta z_2(r)}, \end{aligned}$$

where $z_j(k)$ denotes the k^{th} entry of the vector z_j. Choosing

$$\delta := \frac{\varepsilon \beta_1 w_1(i)}{\beta_2 w_2(r)}$$

ensures that $\alpha_1 \to \beta_1$ and $\alpha_2 \to \beta_2$ as $\varepsilon \to 0$, and also that $z_2 \to w_2$ as $\varepsilon \to 0$.

Thus given some reducible matrix $T \in \mathcal{S}_D$ of the form (3.10), there exists an

irreducible $T' \in \mathcal{S}_D$, dependent on some $\varepsilon > 0$, such that the stationary vector of T' converges to the left fixed vector of T as $\varepsilon \to 0$.

Now suppose that T has k strongly connected components, i.e.

$$T = \left[\begin{array}{c|c|c|c} T_{11} & O & \cdots & O \\ \hline O & T_{22} & \cdots & O \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline O & O & \cdots & T_{kk} \end{array}\right], \qquad \text{some } k.$$

The argument presented above may be used as a technique to show that if x is a left fixed vector of the matrix T with k strong components, then given $\varepsilon > 0$, there is a matrix $\widehat{T} \in \mathcal{S}_D$ having $k-1$ strong components and a left fixed vector $\hat{x}$ such that $||x - \hat{x}|| < \varepsilon$. Iterating this argument yields an irreducible matrix $T' \in \mathcal{S}_D$ having stationary vector y, such that

$$||x - y|| < (k-1)\varepsilon.$$

Thus the set of all left fixed probability vectors of matrices in $\mathcal{S}_D$ is the topological closure of the set of all stationary vectors of irreducible matrices in $\mathcal{S}_D$.

□

3.4 Implementation

In this section, we describe our algorithm for implementing our results, and discuss its *computational complexity*. The computational complexity refers to a classification of how long a process will take, based on the size of the input. If an input has size n, the time a process will take can be expressed as a function of n, say $f(n)$. Typically,

one is not interested in the exact function, but rather the order of magnitude of the function. We say that $f(n) = \mathcal{O}(g(n))$ if there exists some $c \in \mathbb{R}$, and $N_0 \in \mathbb{N}$ such that $f(n) \leq c \cdot g(n)$ for all $n > N_0$.

Given a directed graph D, our implementation centres around finding the edge-maximal subforests of $\mathcal{B}(D)$ and the corresponding conditions described in Propositions 3.2.8 and 3.2.9. Both tasks require extensive time to do by hand, and so it is preferable to use mathematical programming software such as MATLAB instead. Since graphs can be more difficult to deal with in such software, we rely on the linear algebraic approach outlined in Remark 3.2.14, where it was observed that the edge-weight conditions can be found by inverting the truncated incidence matrices of the maximal subforests.

The edge-maximal acyclic subgraphs of a connected component $\mathcal{C}$ of $\mathcal{B}(D)$ are found by removing a single edge from each cycle in $\mathcal{C}$. Any two trees obtained in this way will differ from each other only in the choice of edge removed from each cycle. This suggests that a possible update scheme may be useful, which deduces the edge-weight conditions of one tree from a similar one.

An algorithm is provided in [78] that returns all spanning trees of a connected graph. It achieves this by giving a 'root tree' and a series of edge exchanges, and the results are ordered so that two adjacent trees in the sequence differ by the exchange of exactly one edge. We can then use a formula found in [41] to compute the inverse incidence matrix of one tree from that of another, when they differ by one edge. In particular, for trees $\mathcal{T}_1, \mathcal{T}_2$ on the same set of vertices with N_1, N_2 denoting the truncated incidence matrices (obtained with respect to the same ordering), we can write

$$N_2 = N_1 + ye_k^\top,$$

where y is equal to the k^{th} column of $N_2 - N_1$. This amounts to replacing the k^{th} edge of T_1 by some other edge. By [41, Section 0.7.4], if $1 + e_k^\top N_1^{-1} y \neq 0$, then

$$N_2^{-1} = N_1^{-1} - \frac{1}{1 + e_k^\top N_1^{-1} y} N_1^{-1} y e_k^\top N_1^{-1}. \tag{3.12}$$

Observation 3.4.1. We claim that the denominator of this fraction in (3.12), $1 + e_k^\top N_1^{-1} y$, is equal to either ± 1, simplifying the above expression. Our reasoning for this is as follows:

- Each of N_1, N_2 can, by an appropriate permutation of rows and columns, be brought to lower triangular form with 1s on the diagonal. Hence $\det(N_1)$ is either $+1$ or -1 (depending on the signs of the row and and column permutations that bring it to triangular form), and similarly $\det(N_2)$ is either $+1$ or -1.

- It is clear that $\det(N_1^{-1} N_2)$ is also either $+1$ or -1, and we have $N_1^{-1} N_2 = I + N_1^{-1} y e_k^\top$.

- It's a straightforward exercise to show that if $u, v \in \mathbb{R}^n$, then $\det(I + uv^\top) = 1 + v^\top u$. Hence $\det(I + N_1^{-1} y e_k^\top) = 1 + e_k^\top N_1^{-1} y$.

- Consequently we have

$$\begin{aligned} 1 + e_k^\top N_1^{-1} y &= \det(I + N_1^{-1} y e_k^\top) \\ &= \det(N_1^{-1} N_2) \\ &= \pm 1. \end{aligned}$$

In this way, (3.12) may be simplified to read:

$$N_2^{-1} = N_1^{-1} \pm N_1^{-1} y e_k^\top N_1^{-1}. \tag{3.13}$$

We may determine the circumstances under which we get $+1$ or -1 by determining the signs of the row and column permutations that bring N_1 and N_2 to lower triangular form. Without loss of generality, assume that N_1 is in lower triangular form, and that N_2 is formed by removing a column of N_1 and replacing it with some new column vector that represents the new edge. Assuming the resulting matrix is no longer in lower triangular form, we know that it can be achieved by permuting the rows and columns in such a way that the corresponding vertices and edges of $\mathcal{T}_2$ have been re-ordered appropriately.

Recall, however, that a row (corresponding to some vertex v) has been deleted from each of N_1 and N_2. For this reason, we describe a new method of ordering the vertices and edges of $\mathcal{T}_2$, dependent on v, so that v arrives last in the vertex order and the resulting incidence matrix satisfies the conditions of Proposition 3.2.6. This is easily extended from the inductive method described in the proof of Proposition 3.2.6 by simply passing over v at each inductive step; i.e. if at some stage v is a pendent vertex of $\mathcal{T}_2$, we do not label it among the others that we add to the order and then delete. The edge order is deduced from the vertex order by setting v as the *source vertex*, and orienting (assigning direction to) each edge so that it points away from v. Then $e(i)$ is defined to be the edge pointing towards the i^{th} vertex in the vertex order.

To determine the signs of the row and column permutations required to bring N_2 to lower triangular form, we determine the number of edges in $\mathcal{T}_2$ that have a different orientation than in $\mathcal{T}_1$. If no edges change orientation, then a simultaneous permutation of rows and columns is required to bring N_2 to lower triangular form, which has sign $+1$. If some edges change orientation, then we perform a simultaneous permutation of the rows and columns so that the vertex order is achieved, and we then require some further re-ordering of the columns to achieve the edge order.

Suppose the new edge e' added to create $\mathcal{T}_2$ becomes oriented to some vertex v_{i_1}.

Then the edge $e(i_1)$ that was oriented to v_{i_1} in $\mathcal{T}_1$ has had its position in the ordering usurped by e', and we must swap these two columns of N_2. Now, $e(i_1)$ must now be oriented to some other vertex v_{i_2}, and so this enforces another exchange, of the columns representing $e(i_1)$ and $e(i_2)$. This process will continue until it reaches the vertex v_{i_k} to which the removed edge e was oriented. It is clear, then, that the permutation of the columns is a product of transpositions, the number of which is equal to the number of edges in the path from v_{i_1} to v_{i_k}. However, note that if e and e' are oriented in the same direction (i.e. right-to-left or left-to-right) then the number must be even, as v_{i_1} and v_{i_k} are both row or both column vertices. If e and e' are oriented in opposite directions, the number of transpositions will be odd. Hence the sign in the update formula (3.13) will be -1 if we exchange an edge for one oriented in the same direction, and $+1$ for one oriented in the opposite direction.

We illustrate the process with an example.

Example 3.4.2. We refer back to the bipartite graph shown in Fig. 3.1 on page 49, and examined in Example 3.2.13 and Remark 3.2.14. Suppose that we want to find the edge-weight conditions of the bipartite graph obtained from $\mathcal{B}(D)$ by exchanging the edge r_2c_3 for r_6c_6. The conditions derived from Component 1 will not be affected, so we examine only Component 2, which will be our $\mathcal{T}_1$. The last vertex in the ordering of Component 2 is r_2, and we show the orientation of the edges in Fig. 3.4a, along with the truncated incidence matrix N_1, labelled with the vertex and edge orderings of $\mathcal{T}_1$.

Fig. 3.4b displays the bipartite graph obtained by removing r_2c_3 and adding the edge r_6c_6, along with the matrix obtained from N_1 by replacing the column corresponding to r_2c_3 by one representing r_6c_6, and then performing a simultaneous permutation so that the rows are ordered according to the new vertex order of $\mathcal{T}_2$. Evidently, further re-ordering of the columns is necessary to bring it to lower triangular form. To further re-order the columns in N_2, we see that we must swap r_6c_6 in the order for the edge

previously oriented to c_6, r_5c_6, which is now oriented to r_5. We then swap r_5c_6 for r_5c_3, which is now oriented to c_3, the vertex to which r_2c_3 was oriented. Thus the permutation that brings N_2 to lower triangular form has sign $+1$, and so to find the edge-weight conditions for $\mathcal{T}_2$, we compute N_2^{-1} using the update formula (3.13) with a -1 as opposed to a $+1$. This could be inferred immediately by comparing the orientation of r_6c_6 in $\mathcal{T}_2$ with the orientation of r_2c_3 in $\mathcal{T}_1$: since they are oriented the same way, this implies the permutation will have sign $+1$, and the update formula (3.13) will use a -1.

Suppose instead that we were to exchange r_2c_4 for r_6c_6, as shown in Fig. 3.4c. Since these edges have opposite orientation to each other, this means we would use the update formula with a $+1$.

Remark 3.4.3. We have described the process of determining the sign in the update formula using the properties of the bipartite graph, which, as we have observed, are more difficult to deal with in the software we wish to use to implement our solutions. For this reason, we give the following alternative method for determining the sign in (3.13).

We have defined $y := (N_2 - N_1)e_k$, and from (3.13) we deduce that

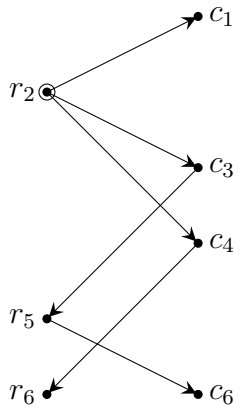
$$N_1 - N_2 = \pm N_2 N_1^{-1} y e_k^\top$$

and hence

$$-y = \pm N_2(N_1^{-1}y).$$

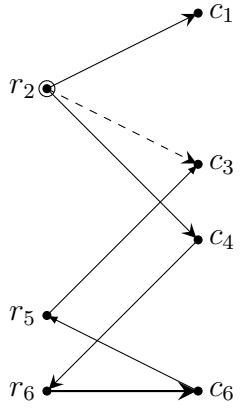
Compute $N_1^{-1}y$ (in $\mathcal{O}(n)$ operations), and then select a nonzero entry of y, say y_a. We can determine the sign from the equation

$$-y_a = \pm e_a^\top N_2 N_1^{-1} y$$



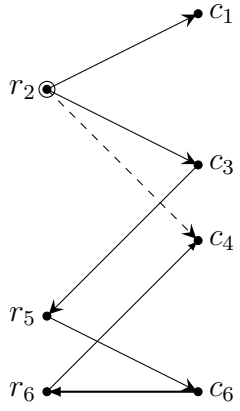
$$\begin{array}{c} \\ c_1 \\ c_6 \\ r_6 \\ r_5 \\ c_4 \\ c_3 \end{array} \begin{array}{c} \begin{array}{cccccc} r_2c_1 & r_5c_6 & r_6c_4 & r_5c_3 & r_2c_4 & r_2c_3 \end{array} \\ \left[\begin{array}{cccccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \end{array}\right] \end{array}$$

(a) $\mathcal{T}_1$ and the truncated incidence matrix N_1



$$\begin{array}{c} \\ c_1 \\ c_3 \\ r_5 \\ c_6 \\ r_6 \\ c_4 \end{array} \begin{array}{c} \begin{array}{cccccc} r_2c_1 & \mathbf{r_6c_6} & r_5c_3 & r_5c_6 & r_6c_4 & r_2c_4 \end{array} \\ \left[\begin{array}{cccccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{array}\right] \end{array}$$

(b) $\mathcal{T}_2$ and the permuted incidence matrix N_2, before the edge re-ordering



$$\begin{array}{c} \\ c_1 \\ c_4 \\ r_6 \\ c_6 \\ r_5 \\ c_3 \end{array} \begin{array}{c} \begin{array}{cccccc} r_2c_1 & \mathbf{r_6c_6} & r_6c_4 & r_5c_6 & r_5c_3 & r_2c_3 \end{array} \\ \left[\begin{array}{cccccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{array}\right] \end{array}$$

(c) $\mathcal{T}_3$ and the permuted incidence matrix N_3, before the edge re-ordering

Figure 3.4: An illustration of Observation 3.4.1 using Example 3.2.13.

in another $\mathcal{O}(n)$ operations.

Both the algorithm in [78] and the process of obtaining the inverse incidence matrices may be implemented by applying the methods to the connected components of $\mathcal{B}(D)$. We note, however, that the time complexity of the algorithm in [78] is $\mathcal{O}(V + E + m)$, where V is the number of vertices, E the number of edges, and m the number of spanning trees of the graph, and that this is optimal. This implementation of our results suffers, then, for large or particularly dense graphs.

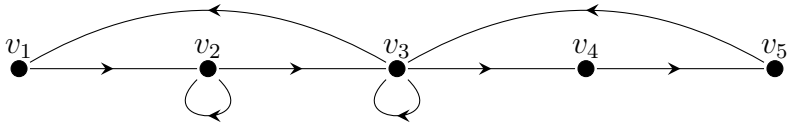
Despite the issues with time complexity, we note that there are many applications involving systems that are governed by relatively small or sparse directed graphs. We present the following example to demonstrate the usefulness of our results in such cases.

3.5 Example: North Atlantic right whale population dynamics

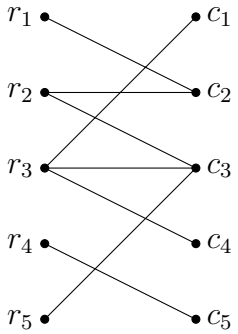
We observe that to any nonnegative irreducible matrix A we may associate an irreducible stochastic matrix as follows: Let $\rho(A)$ denote the Perron value of A, and let u and v be right and left Perron vectors of A, respectively, normalised so that $v^\top u = 1$. Letting U denote a diagonal matrix whose i^{th} diagonal entry is u_i, we see that

$$T := \frac{1}{\rho(A)} U^{-1} A U$$

is both irreducible and stochastic, and, most importantly for us in this chapter, the directed graphs of T and A coincide. Furthermore, the stationary vector w of T is equal to Uv, so that $w_i = u_i v_i$, for $i = 1, \ldots, n$. It is known (see, for example, [52, Sec. 3.2]) that for each i, $u_i v_i$ is the derivative of $\rho(A)$ with respect to the i^{th} diagonal entry of A.



(a) The directed graph D indicating population contributions between life stages of the whale



(b) The bipartite graph $\mathcal{B}(D)$

Figure 3.5: Life cycle graph for the North American right whale (female) and the corresponding bipartite graph

We can apply this approach to the population projection matrix of a stage-classified matrix model of a population (detailed in [13, Ch. 4]). Since the Perron value of this projection matrix represents the asymptotic growth rate of the population, information regarding the stationary vector of the corresponding stochastic matrix T will provide some insight into the sensitivity of this growth rate. This could indicate better strategies for managing a population, a common aim in examining these models.

To demonstrate how our results in this chapter may be useful in such a situation, we consider the specific example of the female North Atlantic right whale population. The projection matrix for this population has directed graph indicated in Fig. 3.5, according to [14] - which is also referred to as a life cycle graph. Each vertex represents a stage in the life cycle of the female whale (calf, immature, mature, mother, post-breeding), while arcs indicate a contribution by one class to another within a single projection interval (one year, in this case), either via reproduction or by leaving one stage and entering another. Note that the loops at each vertex in the graph represent

the proportion of the population in a single class that survive and remain in the same class after the interval has passed.

Letting D denote the directed graph in Fig. 3.5a, we consider the bipartite graph $\mathcal{B}(D)$, also shown in Fig. 3.5b. The component condition given by this graph is

$$x_4 - x_5 = 0,$$

and the edge-weights are:

$$\begin{aligned}
\omega(r_1c_2) &= x_1 \\
\omega(r_3c_1) &= x_1 \\
\omega(r_3c_4) &= x_4 \\
\omega(r_5c_3) &= x_5 \\
\omega(r_2c_2) &= x_2 - x_1 \\
\omega(r_3c_3) &= x_3 - x_1 - x_4 \\
\omega(r_2c_3) &= x_1 \\
\omega(r_4c_5) &= x_4.
\end{aligned}$$

Thus the only non-trivial conditions on the stationary vector x of a stochastic matrix with this bipartite graph are as follows:

$$\begin{aligned}
x_4 &= x_5, \\
x_2 &\geq x_1, \\
x_3 &\geq x_1 + x_4.
\end{aligned} \tag{3.14}$$

From this, we see that the given directed graph D dictates some unexpected relation-

ships between the derivatives of the Perron value with respect to the diagonal entries of the transition matrix. In this example, we have determined that the derivative of $\rho(A)$ with respect to either the second or third diagonal entry of A is the largest, regardless of how the projection matrix A might vary. In particular, this may be interpreted to mean that the growth rate of the population is most sensitive to increases in the proportion of members of the immature or mature (fertile) classes that survive and remain in the class within one projection interval. Though one may intuitively expect this, we note that these conditions (3.14) produce quantitative conclusions as well as the above qualitative conclusion - for example, x_3 is not only larger than x_1 and x_4, it is larger than the sum of these quantities. In general, these relationships may help to inform conservation techniques for a population modelled in this way.

Chapter 4

Minimising the largest mean first passage time of a Markov chain

The stationary vector (discussed in the previous chapter) describes the long-term behaviour of the system modelled by a Markov chain. The short-term behaviour, however, is described by the mean first passage times. In this chapter, we explore how the mean first passage times are influenced by the combinatorial restriction of a given directed graph. In particular, given a strongly connected directed graph D and considering the set $\mathcal{S}_D$ of all stochastic matrices respecting that directed graph, can we describe the range of possible values of the mean first passage time $m_{i,j}$ from s_i to s_j?

We begin by considering the range of values of $m_{i,j}$, and determine conditions on D under which the supremum is bounded. We then consider the separate problem of the range of mean first passage times for a transition matrix T with a given stationary distribution vector. A lower bound for the maximum mean first passage time is found in terms of the stationary distribution vector of T in Proposition 4.2.1 and its corollary, and some matrices for which equality is attained are produced. The main objective in this chapter is to characterise the directed graphs D for which any stochastic matrix

$T \in \mathcal{S}_D$ attains equality in this lower bound, producing a class of Markov chains with optimal short-term behaviour, and further indicating the influence of the directed graph. We obtain a partial characterisation, stated in Corollary 4.3.10, and discuss methods for extending to a full characterisation in Section 4.3.2. The results of this chapter are published and appear in [6], with the exception of Propositions 4.1.2, 4.1.3 and 4.1.4 in Section 4.1, which are original to this thesis.

4.1 Introduction

It is clear that mean first passage times and Kemeny's constant are related concepts, although the mean first passage times encompass a larger quantity of information, while $\mathcal{K}(T)$ is a single-valued parameter of a Markov chain. Regardless, in similar questions asked of the range of values of $\mathcal{K}(T)$ for all $T \in \mathcal{S}_D$ where D is a given directed graph (see [15, 57]), the cycle structure of D played an important role. Indeed, we will see a similar theme arising in the characterisation of digraphs D for which mean first passage times $m_{i,j}$ are bounded for all $T \in \mathcal{S}_D$. This is not unexpected, as the structure of D is already known to influence the mean first passage times of transition matrices in the family $\mathcal{S}_D$. We recall the following result:

Proposition 4.1.1 ([43, 52])**.** *For a strongly connected directed graph D with vertices $\{v_1, \ldots, v_n\}$ and for some irreducible $T \in \mathcal{S}_D$ with mean first passage times denoted by $m_{i,j}$, for any triple of indices i, j, k,*

$$m_{i,j} \leq m_{i,k} + m_{k,j}, \tag{4.1}$$

with equality if and only if k is distinct from i and j and every path in $\mathcal{D}(T)$ from v_i to v_j passes through v_k.

This inequality was proven in [43] and a separate proof is given in [52, Theorem 6.2.1] which allows for the characterisation of equality, demonstrating the influence the directed graph can have on mean first passage times between states of any Markov chain on that digraph; i.e. regardless of the transition probabilities. We will make use of this inequality several times in the sequel.

We begin by establishing the range of values of a specific $m_{i,j}$ (some $i \neq j$) over all possible transition matrices T respecting a given directed graph D on n vertices.

Proposition 4.1.2. *Let D be a strongly connected directed graph on n vertices, and let $i, j \in \{1, \ldots, n\}$ be fixed with $i \neq j$. Then*

$$\inf_{\substack{T \in \mathcal{S}_D \\ \textit{irreducible}}} \{m_{i,j}\} = \operatorname{dist}(v_i, v_j).$$

Proof. Let $f_{i,j}$ denote the random variable representing the first passage time from s_i to s_j. Since D is strongly connected, there is a shortest path from v_i to v_j of length $\operatorname{dist}(v_i, v_j)$, say:

$$v_i = v_{i_1} \to v_{i_2} \to \cdots \to v_{i_p} = v_j$$

where $p = \operatorname{dist}(v_i, v_j) + 1$. Certainly $f_{i,j} \geq p - 1$, as the (i, j) entry of T^k is 0 for all $k < \operatorname{dist}(v_i, v_j)$. Hence $m_{i,j} \geq \operatorname{dist}(v_i, v_j)$ also.

Without loss of generality assume that $i_k = k$, for $k = 1, \ldots, p$, so that we are considering the mean first passage time $m_{1,p}$. Then there exists a stochastic matrix

$T \in \mathcal{S}_D$ such that

$$T = \left[\begin{array}{ccccc|c} 0 & 1 & 0 & \cdots & 0 & \\ 0 & 0 & 1 & \cdots & 0 & \\ \vdots & \vdots & \ddots & \ddots & \vdots & O \\ 0 & 0 & 0 & \cdots & 1 & \\ 0 & 0 & 0 & \cdots & 0 & \\ \hline & & & & & \\ & & T_{21} & & & T_{22} \\ & & & & & \end{array}\right] + e_p e_l^\top,$$

where l is such that (v_p, v_l) is an arc in D.

Now, the mean first passage time $m_{1,p}$ for the chain represented by this transition

matrix is

$$
\begin{aligned}
e_1^\top (I - T_{(p)})^{-1} \mathbb{1} &= e_1^\top \left[\begin{array}{ccccc|c} 1 & -1 & 0 & \cdots & 0 & \\ 0 & 1 & -1 & \cdots & 0 & \\ \vdots & \vdots & \vdots & \ddots & \vdots & O \\ 0 & 0 & 0 & \cdots & -1 & \\ 0 & 0 & 0 & \cdots & 1 & \\ \hline & & -\hat{T}_{21} & & & I - T_{22} \end{array}\right]^{-1} \mathbb{1} \\
&= \hat{e}_1^\top \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} \mathbb{1} \\
&= p - 1 \\
&= \operatorname{dist}(v_1, v_p).
\end{aligned}
$$

Note that T might not be irreducible; however, since mean first passage times are continuous functions of the entries in the transition matrix, we can always choose some irreducible $\tilde{T} \in \mathcal{S}_D$ such that the mean first passage time from s_1 to s_p is within ε of $\operatorname{dist}(v_1, v_p)$, for any $\varepsilon > 0$. Hence the statement of the result holds as an infimum over all irreducible members of $\mathcal{S}_D$. □

Proposition 4.1.3. *Let D be a strongly connected directed graph on n vertices, and let $i, j \in \{1, \ldots, n\}$ be fixed such that $i \neq j$. Then $\sup_{T \in \mathcal{S}_D}\{m_{i,j}\}$ is unbounded (over irreducible matrices T) if there is a cycle in D containing v_i which does not contain v_j.*

Proof. Without loss of generality, we consider $\sup_{T\in\mathcal{S}_D}\{m_{1,n}\}$.

Suppose there is a cycle in D passing through v_1 which does not pass through v_n. Then there exists a stochastic matrix $T \in \mathcal{S}_D$ such that, without loss of generality on the ordering of the vertices,

$$T = \left[\begin{array}{c|c} C & E \\ \hline T_{21} & T_{22} \end{array}\right],$$

where

$$C = \begin{bmatrix} 0 & 1 & 0 & & \cdots & 0 \\ 0 & 0 & 1 & & \cdots & 0 \\ & & & \ddots & & \\ \vdots & \vdots & \vdots & & 1-\varepsilon & \vdots \\ & & & & & \vdots \\ 0 & 0 & 0 & & \cdots & 1 \\ 1 & 0 & 0 & & \cdots & 0 \end{bmatrix}$$

i.e. C is essentially the transition matrix for a random walk on a directed cycle, with one transition probability reduced by ε, some $\varepsilon > 0$. We assume E is some matrix with one entry equal to ε in the appropriate row, and T_{21} and T_{22} are such that T is stochastic and respects the directed graph D.

Then the mean first passage time from s_1 to s_n is

$$\begin{aligned} m_{1,n} &= e_1^\top (I - T_{(n)})^{-1} \mathbb{1} \\ &\geq \hat{e}_1^\top (I - C)^{-1} \mathbb{1} \\ &= \hat{e}_1^\top \left(\sum_{k=0}^{\infty} C^k \right) \mathbb{1} \\ &\geq \sum_{k=0}^{\infty} (1-\varepsilon)^k \\ &= \frac{1}{\varepsilon}. \end{aligned}$$

Again, although T may be reducible, since $m_{1,n}$ is a continuous function in the entries of the transition matrix there is certainly an irreducible $\tilde{T} \in \mathcal{S}_D$ with $\tilde{m}_{1,n}$ arbitrarily close to $m_{1,n}$. Hence for any $N > 0$ we can find an irreducible $T \in \mathcal{S}_D$ such that the mean first passage time from s_1 to s_n in the Markov chain with transition matrix T is greater than N; i.e. $\sup_{T \in \mathcal{S}_D}\{m_{1,n}\}$ is unbounded. □

Proposition 4.1.4. *Let D be a strongly connected directed graph on n vertices, and fix $i, j \in \{1, \ldots, n\}$, $i \neq j$. Let*

$$\hat{V} = \{v_i\} \cup \{v_k \in V \mid \textit{there is a walk in } D \textit{ from } v_i \textit{ to } v_k \textit{ which does not pass through } v_j\},$$

and let $\hat{D}$ be the induced subdigraph on $\hat{V}$. Then $\sup_{T \in \mathcal{S}_D} m_{i,j}$ is bounded if and only if $\hat{D}$ is acyclic. If $\hat{D}$ is acyclic, then $\sup_{T \in \mathcal{S}_D} m_{i,j}$ is equal to the length of the longest path from v_i to v_j in D.

Proof. Suppose first that $\hat{D}$ contains a cycle. Then there is a cycle in D containing some $v_k \in \hat{V}$ which does not contain v_j; hence $m_{k,j}$ is unbounded over $\mathcal{S}_D$. Furthermore, since there is a walk from v_i to v_k in D, there is a (possibly reducible) $T \in \mathcal{S}_D$ for which every walk from v_i to v_j in $\mathcal{D}(T)$ passes through v_k, and for which $m_{k,j}$ is as large as we like. Hence by the equality case of (4.1), $m_{i,j} = m_{i,k} + m_{k,j}$. So $m_{i,j} > m_{k,j}$, and hence $m_{i,j}$ is also unbounded over $T \in \mathcal{S}_D$. Therefore $\sup_{T \in \mathcal{S}_D} m_{i,j}$ is bounded only if $\hat{D}$ is acyclic.

Next suppose that $\hat{D}$ is acyclic. We will show that $m_{i,j}$ is bounded. Without loss of generality, let $j = n$. For any $T \in \mathcal{S}_D$, $m_{i,n} = e_i^\top (I - T_{(n)})^{-1} \mathbb{1}$.

The principal submatrix $T_{(n)}$ may be converted to Frobenius normal form as in

(2.3), so that without loss of generality on ordering,

$$T_{(n)} = \left[\begin{array}{c|c|c|c|c} T_{11} & T_{12} & T_{13} & \cdots & T_{1m} \\ \hline O & T_{22} & T_{23} & \cdots & T_{2m} \\ \hline O & O & T_{33} & \cdots & T_{3m} \\ \hline \vdots & \vdots & \vdots & \ddots & \vdots \\ \hline O & O & O & \cdots & T_{mm} \end{array}\right].$$

Suppose that it is the k^{th} block above which corresponds to the i^{th} row of $T_{(n)}$. Then

$$e_i^\top (I - T_{(n)})^{-1} \mathbb{1} = e_1^\top (I - \hat{T})^{-1} \mathbb{1}$$

where

$$\hat{T} = \left[\begin{array}{c|c|c|c} T_{kk} & T_{k,k+1} & \cdots & T_{km} \\ \hline O & T_{k+1,k+1} & \cdots & T_{k+1,m} \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline O & O & \cdots & T_{mm} \end{array}\right]$$

and it is assumed that the i^{th} row of $T_{(n)}$ corresponds to the first row of $\hat{T}$, again without loss of generality. Note that the states represented by $\hat{T}$ correspond to vertices in $\hat{D}$ defined above.

If $\hat{D}$ is acyclic, then necessarily the diagonal blocks $T_{kk}, \ldots, T_{mm}$ are 1×1 zero matrices. Hence $\hat{T}$ is nilpotent, since it is strictly upper triangular, and so $\hat{T}^d$ is the

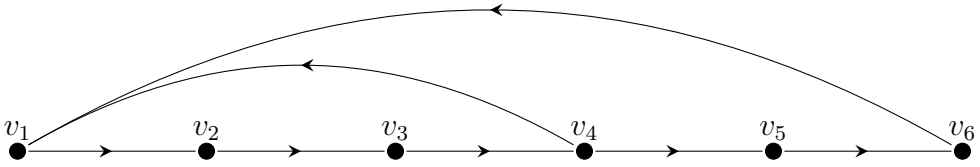


Figure 4.1: An example of a directed graph D for which $\sup_{T\in\mathcal{S}_D}\{m_{1,6}\}$ is unbounded.

zero matrix, for some positive integer d. Now

$$\begin{aligned} m_{i,n} &= e_1^\top (I-\hat{T})^{-1}\mathbb{1} \\ &= e_1^\top \left(\sum_{r=0}^{\infty}\hat{T}^r\right)\mathbb{1} \\ &= e_1^\top \left(\sum_{r=0}^{d-1}\hat{T}^r\mathbb{1}\right) \\ &\leq d; \end{aligned}$$

i.e. $m_{i,n}$ is bounded. Clearly if $\hat{D}$ is acyclic, $m_{i,n}$ is less than the length of the longest path from v_i to v_n in D. To show that this is achievable as a supremum, suppose that the longest path is

$$v_i = v_{i_1} \to v_{i_2} \to \cdots \to v_{i_l} \to v_{i_{l+1}} = v_n.$$

Then choose any $T \in \mathcal{S}_D$ such that $t_{i_k,j} = 0$ if $j \neq i_{k+1}$ and $t_{i_k,i_{k+1}} = 1$. Then the submatrix $\hat{T}$ is a (0, 1)-matrix and $\hat{T}^l = O$, so

$$m_{i,n} = e_1^\top \left(\sum_{r=0}^{\infty}\hat{T}^r\right)\mathbb{1} = e_1^\top \left(\sum_{r=0}^{l-1}\hat{T}^r\right)\mathbb{1} = l.$$

Although T as chosen may be reducible, there is some irreducible $\tilde{T} \in \mathcal{S}_D$ with $\tilde{m}_{i,n}$ arbitrarily close to $m_{i,n}$. □

We now provide an example to illustrate the above.

Example 4.1.5. Let D be the directed graph as shown in Figure 4.1. Then an example of a transition matrix T respecting this directed graph is

$$T = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1-\varepsilon & 0 & 0 & 0 & \varepsilon & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Note that there is a cycle containing v_1 which does not contain v_6, so by Proposition 4.1.3, $m_{1,6}$ should be unbounded.

The mean first passage matrix is

$$M = \begin{bmatrix} 4+2\varepsilon & 1 & 2 & 3 & \frac{4}{\varepsilon} & 1+\frac{4}{\varepsilon} \\ 3+2\varepsilon & 4+2\varepsilon & 1 & 2 & \frac{4}{\varepsilon}-1 & \frac{4}{\varepsilon} \\ 2+2\varepsilon & 3+2\varepsilon & 4+2\varepsilon & 3 & \frac{4}{\varepsilon}-2 & \frac{4}{\varepsilon}-1 \\ 1+2\varepsilon & 2+2\varepsilon & 3+2\varepsilon & 4+2\varepsilon & \frac{4}{\varepsilon}-3 & \frac{4}{\varepsilon}-2 \\ 2 & 3 & 4 & 5 & 2+\frac{4}{\varepsilon} & 1 \\ 1 & 2 & 3 & 4 & \frac{4}{\varepsilon} & 2+\frac{4}{\varepsilon} \end{bmatrix}.$$

It is easily seen that by choosing ε small enough, $m_{1,6}$ can be made as large as we like. Furthermore, note that $m_{6,5}$ is also unbounded as expected from Proposition 4.1.4, because although every cycle containing v_6 also contains v_5, the set $\hat{D}$ constructed as in Proposition 4.1.4 is not acyclic.

Essentially, by choosing $T \in \mathcal{S}_D$ in this way, the probabilities are weighted so that the chain gets 'stuck' in the cycle $v_1 \to v_2 \to v_3 \to v_4 \to v_1$ for a long time.

Note that the stationary vector of T in Example 4.1.5 is given by

$$w^\top = \frac{1}{4+2\varepsilon}\begin{bmatrix}1 & 1 & 1 & 1 & \varepsilon & \varepsilon\end{bmatrix}.$$

We remark that by forcing a large mean first passage time in this way, we also cause some entries of the stationary vector to be extremely small. Since the entries of the stationary vector are sometimes interpreted in terms of the relative 'importance' of each state, perhaps it is not so notable on a grand scale if some mean first passage times to 'unimportant' states are large. It may be more interesting to fix a particular stationary vector w and to then determine bounds on the maximum mean first passage time for a matrix $T \in S_D$ with w as its stationary distribution vector. That is, we ask the question: assuming some long-term probability distribution of the chain, how bad must the mean first passage times of the chain (i.e. the short-term behaviour) be?

4.2 Maximum mean first passage time for a chain with a given stationary distribution

We begin by determining a lower bound on the maximum mean first passage time into state j in terms of the j^{th} entry of the stationary distribution vector.

Proposition 4.2.1. *Let $T = [t_{i,j}]$ be an $n \times n$ stochastic irreducible transition matrix, with stationary vector w and mean first passage matrix M. Then for every $1 \leq j \leq n$,*

$$\max_{\substack{1\leq i\leq n\\ i\neq j}} m_{i,j} \geq \frac{1}{w_j} - 1.$$

Equality is attained in this lower bound if and only if

1. *$t_{j,j} = 0$; and*

2. $t_{j,k}$ is nonzero only if $m_{k,j} = \frac{1}{w_j} - 1$.

Proof. Without loss of generality, suppose $j = n$. Partition off the last row and column of T, giving

$$T = \left[\begin{array}{c|c} T_{(n)} & (I - T_{(n)})\mathbb{1} \\ \hline r^\top & 1 - r^\top \mathbb{1} \end{array}\right].$$

From the eigenequation for $w^\top$, it follows readily that

$$w_n = \frac{1}{1 + r^\top (I - T_{(n)})^{-1}\mathbb{1}}. \tag{4.2}$$

We know from Proposition 2.4.2 that

$$(I - T_{(n)})^{-1}\mathbb{1} = \begin{bmatrix} m_{1,n} \\ m_{2,n} \\ \vdots \\ m_{n-1,n} \end{bmatrix}.$$

Hence we have

$$\begin{aligned} r^\top (I - T_{(n)})^{-1}\mathbb{1} &= \sum_{i=1}^{n-1} r_i m_{i,n} \\ &\leq \sum_{i=1}^{n-1} r_i \left(\max_{1 \leq i \leq n-1} m_{i,n} \right) \\ &= r^\top \mathbb{1} \left(\max_{1 \leq i \leq n-1} m_{i,n} \right) \\ &\leq \max_{1 \leq i \leq n-1} m_{i,n}, \end{aligned} \tag{4.3}$$

since $r^\top \mathbb{1} \leq 1$. We conclude from (4.2) that

$$\max_{1 \leq i \leq n-1} m_{i,n} \geq \frac{1}{w_n} - 1. \tag{4.4}$$

To investigate when equality holds in (4.4), simply examine the string of inequalities

in (4.3), and observe that equality holds in the first one if and only if $r_i > 0 \Rightarrow m_{i,n}$ is maximum. Equality holds in the second inequality in (4.3) if and only if $r^\top \mathbb{1} = 1$; i.e. $t_{n,n} = 0$. □

Proposition 4.2.1 furnishes a lower bound on the overall maximum mean first passage time.

Corollary 4.2.2. *Let T be an $n \times n$ stochastic irreducible matrix, with stationary vector w and mean first passage matrix $M = [m_{i,j}]$. Then*

$$\max_{i \neq j} m_{i,j} \geq \frac{1}{\min_k w_k} - 1. \tag{4.5}$$

Observe that we can think of this result in terms of an optimisation problem – if the stationary distribution has been specified, then that places a lower bound on the maximum off-diagonal entry in the mean first passage matrix. Thus, if T yields equality in (4.5) then T has optimal performance (in terms of mean first passage times) subject to having a specified long-term behaviour (i.e. stationary distribution).

Such a result is of great value in many applications of Markov chains, particularly in those where mean first passage times may be used to determine some key feature of the modelled system. For example, in the context of the vehicle traffic model in [20], the mean first passage times are used to represent average travel times between locations, a key aspect in the efficiency of the network. By producing a lower bound on the maximum expected travel time between two locations, we provide an indication of how well-connected the network might be.

Example 4.2.3. Let w be any probability vector, ordered so that w_1 is the smallest entry. Then the transition matrix

$$T = \frac{1}{1 - w_1}(\mathbb{1}w^\top - w_1 I)$$

is readily seen to yield equality in (4.5).

Example 4.2.4. Consider a stochastic companion matrix

$$T = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ t_1 & t_2 & t_3 & \cdots & t_n \end{bmatrix}$$

where the t_j's are nonnegative and sum to 1. It is straightforward to show that the stationary vector $w^\top$ of T is given by

$$w_j \;=\; \frac{\sum_{k=1}^{j} t_k}{\sum_{k=1}^{n}(n+1-k)t_k}, \qquad j = 1, \ldots, n.$$

Observe that the w_j's are nondecreasing, that $t_1 = \frac{w_1}{w_n}$, and that $t_j = \frac{w_j - w_{j-1}}{w_n}$, for $j = 2, \ldots, n$. Further, it can be shown that the mean first passage matrix M is given by

$$M = \begin{bmatrix} \frac{1}{w_1} & 1 & 2 & \cdots & n-2 & n-1 \\ \frac{1}{w_1} - 1 & \frac{1}{w_2} & 1 & 2 & \cdots & n-2 \\ \frac{1}{w_1} - 2 & \frac{1}{w_2} - 1 & \frac{1}{w_3} & 1 & \cdots & n-3 \\ \vdots & \vdots & \vdots & \ddots & & \vdots \\ \frac{1}{w_1} - (n-1) & \frac{1}{w_2} - (n-2) & \frac{1}{w_3} - (n-3) & \cdots & \frac{1}{w_{n-1}} - 1 & \frac{1}{w_n} \end{bmatrix}.$$

In particular, w_1 is the minimum entry in $w^\top$, and since $w_1 \leq \frac{1}{n}$, we also have $\frac{1}{w_1} - 1 \geq n - 1$; hence the maximum off-diagonal entry in M is $\frac{1}{w_1} - 1$, so that equality holds in (4.5).

The next example we consider is a very particular family of stochastic matrices, first discussed in [60] in the context of the characterisation of stochastic matrices T for which equality is attained in the following lower bound on Kemeny's constant:

$$\mathcal{K}(T) \geq \sum_{j=1}^{n}(j-1)w_j, \tag{4.6}$$

where the stationary vector $w^\top = \begin{bmatrix} w_1 & \cdots & w_n \end{bmatrix}$ is ordered so that the entries are in nondecreasing order. As we have already discussed, Kemeny's constant provides a measure of efficiency in a Markov chain, and so if this family of matrices can also be shown to attain equality in the lower bound on the mean first passage times given in (4.5), then these transition matrices represent Markov chains that can be considered to have optimal performance in two ways, subject to their having a specified stationary distribution.

Example 4.2.5. Let T be an irreducible stochastic matrix of order n with stationary distribution vector w, and suppose that the entries of w are in nondecreasing order. It is shown in [60] that equality holds in (4.6) for T if and only if T is permutation

equivalent to a matrix in the following family, for a fixed index k, $1 \leq k \leq n-1$:

$$\left[\begin{array}{cccc|cccc|c}
0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\
\frac{w_1}{w_2} & 0 & \cdots & 0 & \frac{w_2-w_1}{w_2} & 0 & \cdots & 0 & 0 & 0 \\
 & \ddots & & \vdots & \vdots & \vdots & & \vdots & \vdots & \\
0 & \cdots & \frac{w_{k-1}}{w_k} & 0 & \frac{w_k-w_{k-1}}{w_k} & 0 & \cdots & 0 & 0 & 0 \\
\hline
0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & 0 & 0 \\
0 & 0 & \cdots & 0 & 0 & 0 & 1 & & 0 & \\
\vdots & \vdots & & \vdots & \vdots & \vdots & & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\
\hline
0 & \cdots & 0 & \frac{w_k}{w_n} & \frac{w_{k+1}-w_k}{w_n} & \frac{w_{k+2}-w_{k+1}}{w_n} & \cdots & \frac{w_{n-2}-w_{n-3}}{w_n} & \frac{w_{n-1}-w_{n-2}}{w_n} & \frac{w_n-w_{n-1}}{w_n}
\end{array}\right].$$

To clarify the above, observe that the state space is partitioned as

$$\{1, \ldots, k\} \dot{\cup} \{k+1, \ldots, n-1\} \dot{\cup} \{n\}.$$

Note that there are two degenerate cases, when $k = 1$ and $k = n-1$; each produces a stochastic matrix with a companion matrix pattern.

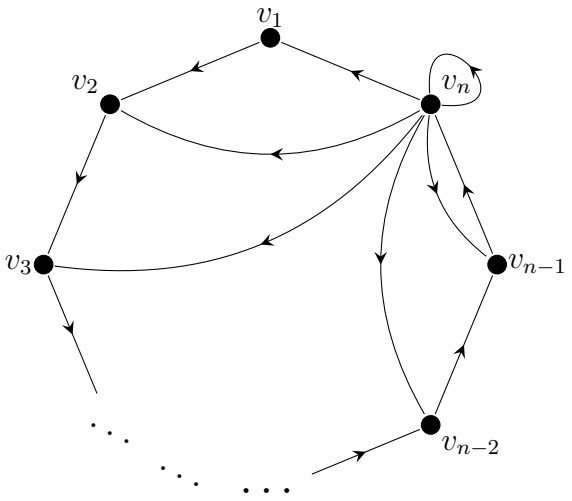
To prove that these matrices also yield equality in (4.5), we present the entries of the mean first passage matrix here, and leave it to the reader to confirm that this matrix is the unique solution to the equation (2.7).

Fix an index k. Then $m_{i,j}$ is given by:

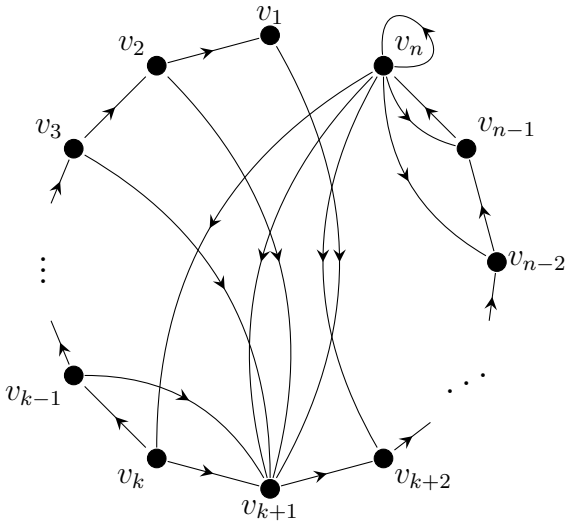
$$m_{i,j} = \begin{cases} \frac{1}{w_j}(1 - \sum_{r=1}^{j-1} w_r) + \frac{1}{w_i}(\sum_{r=1}^{i-1} w_r) & 1 \leq i < j \leq k; \\ \frac{1}{w_j} - \frac{1}{w_i}(\sum_{r=1}^{i-1} w_r) & 1 \leq j < i \leq k; \\ \frac{1}{w_j}(1 - \sum_{r=1}^{j-1} w_r) - (i-k) & k+1 \leq i \leq n,\ 1 \leq j \leq k; \\ (j-k) + \frac{1}{w_i}(\sum_{r=1}^{i-1} w_r) & 1 \leq i \leq k,\ k+1 \leq j \leq n; \\ j - i & k+1 \leq i < j \leq n; \\ \frac{1}{w_j} + (j-i) & k+1 \leq j < i \leq n; \\ \frac{1}{w_i} & i = j. \end{cases}$$

It may be determined that the largest off-diagonal entry of M occurs in the $(k+1, 1)$ position, and is equal to $\frac{1}{w_1} - 1$. We remark that results from Section 4.3 will render this a consequence of the fact that these matrices fall inside a larger family of stochastic matrices for which equality holds in (4.5).

These last examples clearly have very distinctive structure – see Fig. 4.2a and 4.2b for the directed graphs of these matrices. The structure of these examples indicates that the combinatorial influence of the directed graph of the transition matrix on the range of possible mean first passage times may be significant, and is worth investigating. That is the main objective of the rest of this chapter. We pose the following question: can we characterise the directed graphs D for which equality holds in the lower bound (4.5) for *every* irreducible $T \in \mathcal{S}_D$? An answer to this question will determine the types of networks for which any Markov chain is optimal in the sense of minimising the maximum mean first passage time between distinct states.



(a) The directed graph of the stochastic companion matrix of Example 4.2.4



(b) The directed graph of the transition matrix of Example 4.2.5

Figure 4.2: The structure of some transition matrices for which we know equality holds in the lower bound (4.5).

4.3 Directed graphs for which the maximum mean first passage time is minimised

Our first main result, Proposition 4.3.3, is a necessary condition on the cycle structure of directed graphs D for which equality holds in the lower bound (4.5) for all $T \in \mathcal{S}_D$. To prove it, we require the following definitions and a technical lemma, whose proof further reinforces the idea that there is a strong relationship between the directed graph and mean first passage times of associated Markov chains.

Definition 4.3.1. A directed graph D is said to be *minimally strong* if D is strongly connected and the removal of any arc in D results in a directed graph which is not strongly connected.

A matrix A is said to be *nearly reducible* if its directed graph $\mathcal{D}(A)$ is minimally strong, or equivalently, if A is an irreducible matrix such that setting any nonzero entry of A to 0 results in a reducible matrix.

Lemma 4.3.2. *Let D be a strongly connected directed graph on $n \geq 2$ vertices, labelled $v_1, v_2, \ldots, v_n$, and suppose that for some index j there exists an index $k \neq j$ such that for all irreducible $T \in \mathcal{S}_D$ with mean first passage matrix M,*

$$m_{k,j} = \max_{\substack{1 \leq l \leq n \\ l \neq j}} m_{l,j}. \tag{4.7}$$

Then:

(a) For every cycle in D which contains v_k but not v_j, if there is a vertex v_i on the cycle with outdegree greater than 1, then there is an arc from v_i to v_k in D.

(b) If there is a cycle in D containing both v_k and v_j, then there must be an arc from v_j to v_k in D.

Proof. Let D be a strongly connected digraph of order n such that the hypothesis (4.7) holds for all irreducible $T \in \mathcal{S}_D$. Without loss of generality, suppose $j = n$, and let $D \setminus \{v_n\}$ denote the digraph obtained from D by the removal of v_n and all incident arcs. We will assume that there is a cycle in $D \setminus \{v_n\}$ containing v_k which permits a vertex v_i with outdegree greater than one, such that (v_i, v_k) is not an arc in D. Then we will construct an irreducible matrix $\tilde{T} \in \mathcal{S}_D$ such that

$$e_k^\top (I - \tilde{T}_{(n)})^{-1} \mathbb{1} \; < \; \max_{1 \le l \le n-1} e_l^\top (I - \tilde{T}_{(n)})^{-1} \mathbb{1},$$

contradicting (4.7).

To this end, first consider a directed cycle of length l with the following weighted adjacency matrix C. Here, the weight of one arc in the cycle (and corresponding matrix entry) is equal to $a < 1$, while the remaining arcs on the cycle have weight 1:

$$C = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ a & 0 & 0 & \cdots & 0 \end{bmatrix}. \tag{4.8}$$

We have

$$
\begin{aligned}
(I-C)^{-1}\mathbb{1} &= \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 \\ 0 & 1 & -1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & -1 \\ -a & 0 & \cdots & 0 & 1 \end{bmatrix}^{-1} \mathbb{1} \\
&= \frac{1}{1-a} \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & a & 1 & \cdots & 1 \\ 1 & a & a & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & a & a & \cdots & a \end{bmatrix} \mathbb{1} \\
&= \frac{1}{1-a} \begin{bmatrix} l \\ a+(l-1) \\ 2a+(l-2) \\ \vdots \\ (l-1)a+1 \end{bmatrix}.
\end{aligned}
$$

Since $a < 1$, this results in a uniquely maximum entry in the first position.

Now construct a matrix S of order $n-1$ in the pattern of $D \setminus \{v_n\}$ so that for some permutation matrix P,

$$
PSP^\top = \left[\begin{array}{c|c} C & O \\ \hline X & N \end{array}\right] \tag{4.9}
$$

where C is as in (4.8), with some row of C other than the first corresponding to v_k, and X and N chosen appropriately so that the rows sum to 1 and N is nilpotent. To see that such a choice of X and N is possible, let $\hat{V}$ denote the subset of vertices in D

which are not contained in the cycle represented by C. We construct a digraph D_1 of D by choosing a maximal subdigraph for which the directed graph induced by $\hat{V}$ does not contain a cycle. Then any matrix in $\mathcal{S}_{D_1}$ has the appropriate form (4.9) when we remove the row and column corresponding to v_n; that is, the matrix N is nilpotent. This is to ensure that $(I-S)^{-1}$ exists.

We have

$$\begin{aligned} \max_{1\leq i\leq n-1} e_i^\top (I-S)^{-1}\mathbb{1} &\geq \max_{1\leq m\leq l} e_m^\top (I-C)^{-1}\mathbb{1} \\ &> e_k^\top (I-C)^{-1}\mathbb{1} \\ &= e_k^\top (I-S)^{-1}\mathbb{1}. \end{aligned} \tag{4.10}$$

We will now show the existence of an irreducible stochastic matrix $\tilde{T} \in \mathcal{S}_D$ such that $(I-\tilde{T}_{(n)})^{-1}$ is 'as close as we like' to $(I-S)^{-1}$ – that is, for a chosen matrix norm $\|\cdot\|$ and given $\varepsilon > 0$, we can find a matrix $\tilde{T}$ for which $\|(I-\tilde{T}_{(n)})^{-1} - (I-S)^{-1}\| < \varepsilon$.

Without loss of generality (and for ease of notation) suppose that the permutation matrix P above is the identity matrix. Then it is v_l which has outdegree greater than 1.

Let T be an $n \times n$ matrix such that $\mathcal{D}(T) \subseteq D$, and $T_{(n)} = S$. In particular, let

$$T = \left[\begin{array}{c|c|c} C & O & 0 \\ \hline X & N & y \\ \hline * & * & * \end{array}\right]$$

where $y = \mathbb{1} - X\mathbb{1} - N\mathbb{1}$ (for appropriately-sized vectors $\mathbb{1}$) and the last row may be chosen arbitrarily, so long as the row sums to 1, and $t_{n,i} \neq 0$ only if (v_n, v_i) is an arc in D. Constructed in this way, T is reducible, respects the directed graph D, and is

strictly substochastic – the l^{th} row sums to $a < 1$. Furthermore,

$$e_k^\top (I - T_{(n)})^{-1}\mathbb{1} < \max_{1\leq i\leq l} e_i^\top (I - T_{(n)})^{-1}\mathbb{1}, \quad \text{from (4.10)}.$$

We now construct a new stochastic matrix $\hat{T}$ from T which retains the property that $e_k^\top (I - \hat{T}_{(n)})^{-1}\mathbb{1}$ is not maximum. To do this, we need only focus on the l^{th} row of T, corresponding to the vertex v_l with outdegree greater than 1.

- *Case 1:* (v_l, v_n) is an arc in D.

  Then $\hat{T}$ may be constructed by setting $\hat{T} = T + (1-a)e_l e_n^\top$. In this case, $\hat{T}_{(n)} = T_{(n)}$.

- *Case 2:* (v_l, v_n) is not an arc in D.

  It may be assumed that there is an arc from v_l to v_{l+p}, for some $1 \leq p < n - l$ (as otherwise, since D is strongly connected, there is some other vertex v_m on the cycle from which such an arc exists). Then $\hat{T}$ is constructed by setting

  $$\hat{T} = T + (1-a)e_l e_{l+p}^\top.$$

  Then $\hat{T}_{(n)} = T_{(n)} + (1-a)e_l e_{l+p}^\top$ (where the vectors are resized), and by the Sherman-Morrison-Woodbury formula (see [41, Section 0.7.4]):

  $$(I - \hat{T}_{(n)})^{-1} = (I - T_{(n)})^{-1} + \frac{(1-a)(I - T_{(n)})^{-1} e_l e_{l+p}^\top (I - T_{(n)})^{-1}}{1 - (1-a)e_{l+p}^\top (I - T_{(n)})^{-1} e_l}.$$

  The row sums of $(I - \hat{T}_{(n)})^{-1}$ are obtained by multiplying on the right by $\mathbb{1}$:

  $$(I - \hat{T}_{(n)})^{-1}\mathbb{1} = (I - T_{(n)})^{-1}\mathbb{1} + \frac{(1-a)(I - T_{(n)})^{-1} e_l e_{l+p}^\top (I - T_{(n)})^{-1}\mathbb{1}}{1 - (1-a)e_{l+p}^\top (I - T_{(n)})^{-1} e_l}.$$

Considering only the first l row sums, we have on the right-hand side:

$$\frac{1}{1-a}\begin{bmatrix} l \\ a+(l-1) \\ 2a+(l-2) \\ \vdots \\ (l-1)a+1 \end{bmatrix} + \gamma_a \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ t \end{bmatrix},$$

where

$$\gamma_a = \frac{(1-a)e_{l+p}^\top (I - T_{(n)})^{-1}\mathbb{1}}{1-(1-a)e_{l+p}^\top (I-T_{(n)})^{-1}e_l},$$

i.e. a scalar. Hence the maximum entry in the first l positions of $(I-\hat{T}_{(n)})^{-1}\mathbb{1}$ still occurs in the first position, not the one corresponding to vertex v_k.

In either case $\hat{T}$ is a matrix in $\mathcal{S}_D$ for which

$$e_k^\top (I-\hat{T}_{(n)})^{-1}\mathbb{1} < \max_{1\le i\le n-1} e_i^\top (I-\hat{T}_{(n)})^{-1}\mathbb{1}. \tag{4.11}$$

Next consider that $\hat{T}$ may be a reducible member of $\mathcal{S}_D$. However, irreducible matrices in $\mathcal{S}_D$ are dense in $\mathcal{S}_D$, and so given $\delta > 0$, there exists $\tilde{T} \in \mathcal{S}_D$ irreducible such that $\|\hat{T}_{(n)} - \tilde{T}_{(n)}\| < \delta$.

Finally, recall that $f\colon B \mapsto B^{-1}$ is a continuous function on the set of real invertible matrices, and so for all $\varepsilon > 0$ there exists $\delta > 0$ such that $\|B_1 - B_2\| < \delta$ implies $\|B_1^{-1} - B_2^{-1}\| < \varepsilon$. Given $\varepsilon > 0$, we can find an irreducible $\tilde{T} \in \mathcal{S}_D$ so that $\|\hat{T}_{(n)} - \tilde{T}_{(n)}\| < \delta$. Then $\|(I-\hat{T}_{(n)}) - (I-\tilde{T}_{(n)})\| < \delta$, which implies

$$\|(I-\hat{T}_{(n)})^{-1} - (I-\tilde{T}_{(n)})^{-1}\| < \varepsilon.$$

Hence we conclude using (4.11) that there exists an irreducible matrix $\tilde{T} \in \mathcal{S}_D$ with

mean first passage times $M = [m_{i,j}]$ for which

$$m_{k,n} = e_k^\top (I - \tilde{T}_{(n)})^{-1}\mathbb{1} \; < \; \max_{1 \le i \le n-1} e_i^\top (I - \tilde{T}_{(n)})^{-1}\mathbb{1} = \max_{1 \le i \le n-1} m_{i,n},$$

contradicting our hypothesis (4.7). We conclude that if (4.7) holds for all $T \in \mathcal{S}_D$ for some digraph D, then D has the property that for any cycle containing v_k in $D \setminus \{v_j\}$, if a vertex v_i on the cycle has outdegree greater than 1 then (v_i, v_k) must be an arc in D.

To prove (b), suppose that (4.7) holds for all irreducible $T \in \mathcal{S}_D$, and that there is a cycle in D containing v_k and v_j, but that (v_j, v_k) is not an arc in D. Let v_m be the vertex on the cycle to which there is an arc from v_j. Then we can immediately construct a reducible $\hat{T} \in \mathcal{S}_D$ such that for some permutation matrix P,

$$P\hat{T}P^\top = \left[\begin{array}{c|ccccc} & & & X & & \\ N & & & & & \\ \hline & 0 & 1 & 0 & \cdots & 0 \\ & 0 & 0 & 1 & \cdots & 0 \\ O & \vdots & \vdots & \vdots & \ddots & \vdots \\ & 0 & 0 & 0 & \cdots & 1 \\ & 1 & 0 & 0 & \cdots & 0 \end{array}\right]$$

where v_j corresponds to the last row, v_m to the first row in the second diagonal block, and v_k to some other index in the second block of the partition. Without loss of generality, assume $P = I$, so that $j = n$. Clearly, if l is the length of the cycle in question (and hence the size of the second block in the partition) then $e_m^\top (I - \hat{T}_{(n)})^{-1}\mathbb{1} =$

$l-1$, while $e_k^\top(I-\hat{T}_{(n)})^{-1}\mathbb{1} < l-1$. Using a continuity argument as before, we may conclude the existence of an irreducible $\tilde{T} \in \mathcal{S}_D$ for which $m_{k,n} < \max_i m_{i,n}$, contradicting the hypothesis. Hence (v_j, v_k) must be an arc in D.

□

Proposition 4.3.3. *Let D be a minimally strong directed graph on n vertices, with the property that for any irreducible $T \in \mathcal{S}_D$ with stationary vector w and mean first passage matrix M,*

$$\max_{\substack{1\le i,j\le n\\ i\neq j}} m_{i,j} = \frac{1}{\min_k w_k} - 1.$$

Then D is a directed cycle.

Proof. Let D be minimally strong, and let $T \in \mathcal{S}_D$. Then T is nearly reducible, and by [9, Theorem 3.3.4] (and without loss of generality on the ordering of the rows and columns) T has the following form:

$$\left[\begin{array}{ccccc|c} 0 & 1 & 0 & \cdots & 0 & \\ 0 & 0 & 1 & \cdots & 0 & \\ \vdots & \vdots & \vdots & \ddots & \vdots & e_p e_k^\top \\ 0 & 0 & 0 & \cdots & 1 & \\ 0 & 0 & 0 & \cdots & 0 & \\ \hline & & ae_j e_1^\top & & & S \end{array}\right] \tag{4.12}$$

where the first diagonal block has order p ($1 \le p \le n-1$), and S is a substochastic, nearly reducible matrix of order $n-p$. In particular, if $\hat{D} = \mathcal{D}(S)$, then $S = \hat{S} - ae_j e_l^\top$, for some fixed $\hat{S} \in \mathcal{S}_{\hat{D}}$, $a \in (0,1)$, and index l such that $\hat{s}_{j,l} > a$. Moreover, $1 \le j,k \le n-p$, and $(p+j, p+k)$ is not an arc in D (as this would contradict the assumption

that D is minimally strong). Furthermore, note that if $p = n - 1$ then we are done, so henceforth take p to be at most $n - 2$. For ease of notation, let $v_1, v_2, \ldots, v_p$ denote the vertices corresponding to the first p rows and columns of T, and $\hat{v}_1, \hat{v}_2, \ldots, \hat{v}_{n-p}$ the vertices of $\hat{D}$.

The stationary vector w of this matrix T can be computed as

$$w^\top = \frac{1}{p + e_k^\top (I - S)^{-1} \mathbb{1}} \left[\begin{array}{c|c} \mathbb{1}_p^\top & e_k^\top (I - S)^{-1} \end{array} \right],$$

or using stochastic complementation (see Section 2.3) as

$$w^\top = \frac{1}{pa\tilde{w}_j + 1} \left[\begin{array}{c|c} a\tilde{w}_j \mathbb{1}_p^\top & \tilde{w}^\top \end{array} \right]$$

where $\tilde{w}$ is the stationary vector of the stochastic complement $\tilde{S} = S + ae_j e_k^\top = \hat{S} + ae_j(e_k - e_l)^\top$. Note that for sufficiently small values of a, the minimum entry in w occurs in the first p positions and the lower bound for the maximum mean first passage times is $\frac{1}{w_p} - 1$.

We claim that equality holds in the lower bound (4.5) for all matrices $T \in \mathcal{S}_D$ only if for all $\hat{S} \in \mathcal{S}_{\hat{D}}$,

$$\hat{m}_{k,j} = \max_{1 \le i \le n-p} \hat{m}_{i,j} \tag{4.13}$$

where $\hat{M}$ is the mean first passage matrix for $\hat{S}$.

Proof of claim: Fix $\hat{S} \in \mathcal{S}_{\hat{D}}$ and let $a \in (0, 1)$ be chosen sufficiently small so that when T is formed as in (4.12), the minimum entry of the stationary vector w of T occurs in the first p positions. Let M be the mean first passage matrix for T, and suppose that equality holds in (4.5). Now consider the mean first passage times into

state p, recalling that $m_{i,p} = e_i^\top (I - T_{(p)})^{-1} \mathbb{1}$:

$$
\begin{aligned}
(I - T_{(p)})^{-1} &= \left[\begin{array}{ccccc|c}
1 & -1 & 0 & \cdots & 0 & \\
0 & 1 & -1 & \cdots & 0 & \\
\vdots & \vdots & \ddots & \ddots & \vdots & O \\
0 & 0 & \cdots & 1 & -1 & \\
0 & 0 & \cdots & 0 & 1 & \\
\hline
\multicolumn{5}{c|}{} & \\
\multicolumn{5}{c|}{-a e_j e_1^\top} & I - S \\
\multicolumn{5}{c|}{} &
\end{array}\right]^{-1} \\
&= \left[\begin{array}{cccc|c}
1 & 1 & \cdots & 1 & \\
0 & 1 & \cdots & 1 & O \\
\vdots & \vdots & \ddots & \vdots & \\
0 & 0 & \cdots & 1 & \\
\hline
\multicolumn{4}{c|}{} & \\
\multicolumn{4}{c|}{J} & (I - S)^{-1} \\
\multicolumn{4}{c|}{} &
\end{array}\right]
\end{aligned}
$$

where J denotes the all-ones matrix of order $(n - p) \times (p - 1)$. Then

$$
(I - T_{(p)})^{-1} \mathbb{1} = \left[\begin{array}{c}
p - 1 \\
p - 2 \\
\vdots \\
1 \\
\hline
(p-1)\mathbb{1} + (I - S)^{-1} \mathbb{1}
\end{array}\right].
$$

So

$$\max_{\substack{1\le i\le n\\ i\neq p}} m_{i,p} = (p-1) + \max_{1\le i\le n-p} e_i^\top (I-S)^{-1}\mathbb{1},$$

while the lower bound on $\max_i m_{i,p}$ is

$$\frac{1}{w_p} - 1 = p + e_k^\top (I-S)^{-1}\mathbb{1} - 1.$$

Hence for equality to hold in the lower bound (4.5) on the mean first passage times of T as assumed, it is required that

$$e_k^\top (I-S)^{-1}\mathbb{1} = \max_{1\le i\le n-p} e_i^\top (I-S)^{-1}\mathbb{1}. \tag{4.14}$$

Observe, however, that $e_i^\top (I-S)^{-1}\mathbb{1} = m_{p+i,1}$, for $i = 1,\ldots,n-p$. Furthermore, since every path from a vertex in $\hat{D}$ to v_1 must pass through $\hat{v}_j$, it follows from the equality case of (4.1) that

$$m_{p+i,1} = m_{p+i,p+j} + m_{p+j,1} \quad \text{for all } i = 1,\ldots,n-p.$$

Hence (4.14) is equivalent to the condition that $m_{p+k,p+j} = \max_i m_{p+i,p+j}$. However, note that these mean first passage times are calculated as the sums of the lower rows of $(I - T_{(p+j)})^{-1}$ and that the principal submatrix $T_{(p+j)}$ has a lower left block of zeros, and its lower diagonal block is $S_{(j)}$. Recall that $S = \hat{S} - ae_j e_l^\top$, and hence $S_{(j)} = \hat{S}_{(j)}$. Hence

$$\begin{aligned} m_{p+i,p+j} &= e_i^\top (I - \hat{S}_{(j)})^{-1}\mathbb{1} \\ &= \hat{m}_{i,j}, \end{aligned}$$

where $\hat{M}$ is the mean first passage matrix of $\hat{S}$. Hence (4.14) is equivalent to the

condition that

$$\hat{m}_{k,j} = \max_{1 \leq i \leq n-p} \hat{m}_{i,j},$$

as claimed.

Suppose that $n - p \geq 2$. Using Lemma 4.3.2 applied to $\hat{D}$, it may be asserted that if (4.13) must hold for all $\hat{S} \in \mathcal{S}_{\hat{D}}$, then if $\mathcal{C} \subseteq \hat{D}$ is a cycle through $\hat{v}_k$ which does not contain $\hat{v}_j$, then there is exactly one vertex (say $\hat{v}_m$) with out-degree greater than one, and $(\hat{v}_m, \hat{v}_k)$ is also an arc in $\hat{D}$. Since $\hat{v}_j$ is not in $\mathcal{C}$, there is a path in $\hat{D}$ from $\hat{v}_m$ to $\hat{v}_j$ which does not use the arc $(\hat{v}_m, \hat{v}_k)$. The existence of such a path determines the construction of a path from $\hat{v}_m$ to $\hat{v}_k$ in D, via $\hat{v}_j$ and $v_1, v_2, \ldots, v_p$, which does not use the arc $(\hat{v}_m, \hat{v}_k)$. Hence if this arc is deleted from D, the directed graph remains strongly connected, contradicting the assumption that D is minimally strong.

In the case that there is no such cycle $\mathcal{C}$ – that is, every cycle through $\hat{v}_k$ in $\hat{D}$ also contains $\hat{v}_j$ – then from Lemma 4.3.2, there must be an arc from $\hat{v}_j$ to $\hat{v}_k$. This contradicts the hypothesis that D is minimally strong.

Hence we must have $n - p = 1$, and the lower diagonal block in (4.12) is trivial. Therefore the only minimally strong directed graph D for which equality can hold for all $T \in \mathcal{S}_D$ is the directed cycle on n vertices.

□

Since the question posed at the beginning of this section insists that *every* $T \in \mathcal{S}_D$ must satisfy equality in the lower bound on mean first passage times, this result places a huge restriction on the directed graph D. Since D is strongly connected, it must contain the directed n-cycle as a subdigraph, and no other minimally strong digraphs may appear as a subdigraph of D. Thus each such D satisfying our requirements is built on this underlying cycle. Recall that such a cycle passing through every vertex

of the directed graph exactly once is referred to as a *Hamilton cycle*.

Proposition 4.3.4. *Let D be a strongly connected directed graph on n vertices such that for every irreducible $T \in \mathcal{S}_D$ with stationary distribution vector w and mean first passage matrix M, equality holds in the lower bound* (4.5)*. Then D has a unique Hamilton cycle.*

Proof. The existence of a Hamilton cycle as a subdigraph of D is a corollary to Proposition 4.3.3. To show uniqueness of the Hamilton cycle, suppose that D has two distinct Hamilton cycles as subdigraphs. The adjacency matrices of these subdigraphs are both members of $\mathcal{S}_D$, which we denote T and T'. We assume without loss of generality that the vertices of D are ordered in such a way that

$$T = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

and that T' has its last row different from the last row of T.

The stationary vector of T and of T' is clearly equal to $w^\top = \frac{1}{n}\mathbb{1}^\top$, and it is easily seen that w is also the stationary vector of any convex combination of T and T'—that is, any matrix in $\mathcal{S}_D$ of the form

$$T_c := (1-c)T + cT', \quad \text{for } 0 \leq c \leq 1.$$

We now consider the mean first passage times for T_c: in particular the mean first passage times into state n, which are given by $(I - T_{c_{(n)}})^{-1}\mathbb{1}$. First, however, note that

$$(I - T_{(n)})^{-1} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}, \tag{4.15}$$

and that $m_{j,n} = n - j$.

Now

$$\begin{aligned} (I - T_{c_{(n)}})^{-1} &= (I - (1-c)T_{(n)} - cT'_{(n)})^{-1} \\ &= (I - T_{(n)} - c(T'_{(n)} - T_{(n)}))^{-1} \\ &= \left[(I - T_{(n)})(I - c(I - T_{(n)})^{-1}(T'_{(n)} - T_{(n)}))\right]^{-1} \\ &= [I - c(I - T_{(n)})^{-1}(T'_{(n)} - T_{(n)})]^{-1}(I - T_{(n)})^{-1} \\ &= [I + c(I - T_{(n)})^{-1}(T'_{(n)} - T_{(n)})](I - T_{(n)})^{-1} + \mathcal{O}(c^2) \end{aligned}$$

for small values of c. The maximum mean first passage time in column n then is given by the maximum entry of

$$\begin{aligned} (I - T_{c_{(n)}})^{-1}\mathbb{1} &= (I - T_{(n)})^{-1}\mathbb{1} + c(I - T_{(n)})^{-1}(T'_{(n)} - T_{(n)})(I - T_{(n)})^{-1}\mathbb{1} + \mathcal{O}(c^2) \\ &= \begin{bmatrix} n-1 \\ n-2 \\ \vdots \\ 1 \end{bmatrix} + c \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} (T'_{(n)} - T_{(n)}) \begin{bmatrix} n-1 \\ n-2 \\ \vdots \\ 1 \end{bmatrix} + \mathcal{O}(c^2). \end{aligned}$$

Recalling (4.15), it may be determined that the maximum entry occurs in the first row;

that is,

$$m_{1,n} = (n-1) + c\mathbb{1}^\top T'_{(n)} \begin{bmatrix} n-1 \\ n-2 \\ \vdots \\ 1 \end{bmatrix} - c \begin{bmatrix} 0 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} n-1 \\ n-2 \\ \vdots \\ 1 \end{bmatrix} + \mathcal{O}(c^2).$$

Since the column sums of T' are all equal to one, $\mathbb{1}^\top T'_{(n)} = \mathbb{1}^\top - e_j^\top$, where j is the index of the nonzero entry in the n^{th} row of T' (equivalently, the index of the vertex to which an arc issues from vertex n in the Hamilton cycle represented by T'). Hence

$$\begin{aligned} m_{1,n} &= n-1+c(\mathbb{1}^\top - e_j^\top) \begin{bmatrix} n-1 \\ n-2 \\ \vdots \\ 1 \end{bmatrix} - c\,\frac{n(n-1)}{2} + \mathcal{O}(c^2) \\ &= n-1+c\left(\frac{n(n-1)}{2} - (n-j) - \frac{(n-1)(n-2)}{2}\right) + \mathcal{O}(c^2) \\ &= n-1+c(j-1) + \mathcal{O}(c^2), \end{aligned}$$

and since by assumption j cannot equal 1, we have that for sufficiently small values of c, $m_{1,n} > n-1$.

Thus the existence of two Hamilton cycles in D produces a matrix $T_c \in \mathcal{S}_D$ for which the maximum mean first passage time is strictly greater than the lower bound, and we have a contradiction. □

4.3.1 Hessenberg cycles

In this section we discuss a particular class of directed graphs, first recalling the definition of a *lower Hessenberg matrix* to be an $n \times n$ matrix A such that $a_{i,j} \neq 0$ only if

$i + 1 \geq j$. An analogous definition holds for *upper Hessenberg matrices*, where matrix entries are nonzero only on the first subdiagonal and above.

Definition 4.3.5. Let D be a strongly connected directed graph on n vertices, with adjacency matrix A_D. D is said to be a *Hessenberg digraph* if there exists a permutation matrix P such that $PA_DP^\top$ is a (lower) Hessenberg matrix. D is called a *Hessenberg cycle* if D is Hessenberg and $e_n^\top(PA_DP^\top) = e_1$; that is, after some reordering of the rows, there is exactly one arc issuing from vertex v_n to vertex v_1.

Without loss of generality, we will assume when dealing with a Hessenberg digraph D that the vertices have been ordered in such a way that the adjacency matrix A_D is Hessenberg, so as to remove the need for the permutation matrix P. In addition, if D is a Hessenberg cycle, we assume without loss of generality that $e_n^\top A_D = e_1^\top$, for the same reason. If necessary, we may refer to D as a Hessenberg cycle *with respect to the index* j if it is the j^{th} vertex which corresponds to the last row when the permutation matrix is applied. We note also that the rows and columns of an upper Hessenberg matrix may be simultaneously permuted to produce a lower Hessenberg matrix; for this reason we have limited the definition above and the discussions hereafter to lower Hessenberg matrices.

An example of a Hessenberg cycle on six vertices may be seen in Figure 4.3, and since this example displays all possible arcs, any Hessenberg cycle on six vertices is a subdigraph of this one. Note in particular that a Hessenberg cycle on n vertices ordered in this way contains a unique Hamilton cycle of the form

$$1 \to 2 \to \cdots \to (n-1) \to n \to 1.$$

Remark 4.3.6. Notice that the directed graph of the matrix in Example 4.2.5 is a Hessenberg cycle with respect to the first vertex. The unique Hamilton cycle in this

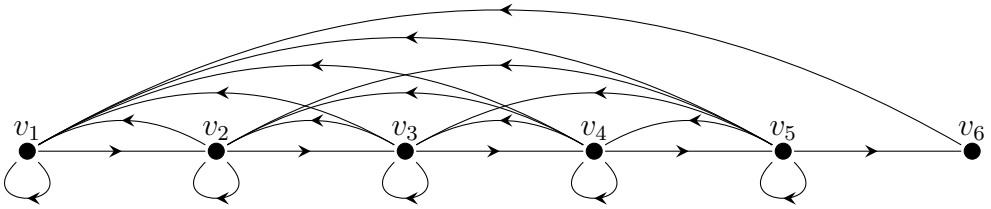


Figure 4.3: A Hessenberg cycle on six vertices, displaying all admissible arcs.

digraph (shown in Fig. 4.2b) is

$$(k+1) \to (k+2) \to \cdots \to (n-1) \to n \to k \to (k-1) \to \cdots \to 2 \to 1 \to (k+1).$$

This may be used to re-order the rows and columns of the transition matrix of Example 4.2.5 to obtain lower Hessenberg form, with last row equal to $e_1^\top$.

Proposition 4.3.7. *Let D be a Hessenberg cycle of order n. Then for all irreducible $T \in \mathcal{S}_D$ with stationary vector w,*

$$w_n \leq w_k, \qquad \text{for all } k = 1, \ldots, n.$$

Proof. The proof uses induction on n. Suppose D is a Hessenberg cycle on 2 vertices. Then every irreducible $T \in \mathcal{S}_D$ has the form

$$\begin{bmatrix} a & 1-a \\ 1 & 0 \end{bmatrix},$$

for some $a \in [0, 1)$. This has stationary vector

$$w = \begin{bmatrix} \frac{1}{2-a} & \frac{1-a}{2-a} \end{bmatrix}.$$

In this case $w_2 \leq w_1$ for any choice of a—i.e. for all $T \in \mathcal{S}_D$.

Now assume that for $m < n$, every stochastic $m \times m$ Hessenberg matrix T with $e_m^\top T = e_1$ with stationary vector w satisfies $w_m \leq w_k$ for all $k = 1, \ldots m$. Consider a Hessenberg cycle D on n vertices. For any $T \in \mathcal{S}_D$ with stationary vector w, we have the eigen-equation

$$\begin{bmatrix} w_1 & w_2 & \cdots & w_n \end{bmatrix} \begin{bmatrix} t_{1,1} & t_{1,2} & 0 & \cdots & 0 \\ t_{2,1} & t_{2,2} & t_{2,3} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_{n-1,1} & t_{n-1,2} & t_{n-1,3} & \cdots & t_{n-1,n} \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix} = \begin{bmatrix} w_1 & w_2 & \cdots & w_n \end{bmatrix}$$

giving

$$t_{1,1}w_1 + t_{2,1}w_2 + \ldots + w_n = w_1.$$

Hence $w_n \leq w_1$.

Now perform stochastic complementation (see Section 2.3) on the first row and column of T, in which case $S_1 = [1]$ and S_2 is a stochastic Hessenberg matrix of order $n-1$, with its $(n-1)^{th}$ row equal to $e_1^\top$. Recall that the stationary vector for T can be written in terms of the stationary vectors of the stochastic complements; in particular, $w^\top = [w_1 \mid \gamma\tilde{w}]$, where $\tilde{w}$ is the stationary vector for S_2. By the induction hypothesis, we know that

$$\tilde{w}_{n-1} \leq \tilde{w}_k \quad \text{for all } k = 1, \ldots, n-1.$$

But this implies that

$$\gamma\tilde{w}_{n-1} \leq \gamma\tilde{w}_k \quad \text{for all } k = 1, \ldots, n-1,$$

and hence

$$w_n \leq w_j, \quad \text{for all } j = 2, \ldots, n$$

and therefore by induction, the hypothesis holds for all Hessenberg cycles D. $\square$

Proposition 4.3.8. *Let D be a Hessenberg cycle of order n. Then for every irreducible $T \in \mathcal{S}_D$ with stationary vector w and mean first passage matrix $M = [m_{i,j}]$,*

$$\max_{\substack{1 \leq i,j \leq n \\ i \neq j}} m_{i,j} = m_{1,n} = \frac{1}{w_n} - 1.$$

Proof. Let D be a Hessenberg cycle and let $T \in \mathcal{S}_D$ with mean first passage matrix M and stationary vector w. First, observe from the equality case of (4.1) that

$$m_{n,n} = m_{n,1} + m_{1,n},$$

as every path from v_n to v_n must go through v_1. Furthermore, since the only arc issuing from v_n is to v_1, it follows that $m_{n,1} = 1$. Given that the mean first return time $m_{n,n} = \frac{1}{w_n}$, we obtain

$$m_{1,n} = \frac{1}{w_n} - 1.$$

Next, note that for a Hessenberg cycle D (as shown for example in Figure 4.3) it is clear that for $i < j$, any path from v_i to v_j must pass through every vertex indexed by integers between i and j. Therefore by (4.1),

$$m_{i,j} = m_{i,k} + m_{k,j}, \quad \text{for any } k,\ i < k < j. \tag{4.16}$$

We now show that $m_{1,n} \geq m_{i,j}$, for all $i, j = 1, \ldots, n$, $i \neq j$. First, suppose that

$i < j$. Then it follows from (4.16) that

$$m_{i,n} = m_{i,j} + m_{j,n}$$

and hence $m_{i,n} > m_{i,j}$ for $i < j < n$. It also follows from (4.16) that

$$m_{1,n} = m_{1,i} + m_{i,n}$$

and hence $m_{1,n} > m_{i,n}$. Therefore if $i < j$, we have shown that

$$m_{1,n} > m_{i,j}.$$

Now suppose that $i > j$. By (4.1),

$$m_{i,j} \leq m_{i,n} + m_{n,j}.$$

Since we have observed that $m_{n,1} = 1$, and $m_{n,j} = m_{n,1} + m_{1,j}$ by (4.16), we have

$$m_{i,j} \leq m_{i,n} + m_{1,j} + 1.$$

Now, any mean first passage time is at least 1. So $m_{j,i} \geq 1$, and hence from the above

$$m_{i,j} \leq m_{1,j} + m_{j,i} + m_{i,n}.$$

But if $i > j$, then every path in D from v_1 to v_i passes through vertex v_j. Hence $m_{1,j} + m_{j,i} = m_{1,i}$. We also observe that every path from v_1 to v_n passes through v_i,

and so $m_{1,i} + m_{i,n} = m_{1,n}$. Therefore

$$m_{i,j} \leq m_{1,n}.$$

□

Proposition 4.3.9. *Let D be a strongly connected directed graph such that the following hold:*

(a) D has a unique Hamilton cycle;

(b) there exists an index l such that for all irreducible $T \in \mathcal{S}_D$ with stationary vector w, $w_l = \min_k w_k$.

Then D is a Hessenberg cycle (with respect to the index l).

Proof. Let D be such a directed graph, satisfying conditions (a) and (b). Without loss of generality, we can assume

1. The unique Hamilton cycle is $v_1 \to v_2 \to \cdots \to v_n \to v_1$;
2. The index l for which $w_l = \min_k w_k$ for all $T \in \mathcal{S}_D$ with stationary vector w is $l := n$.

Now suppose that D is not a Hessenberg cycle. Then there are two cases to consider: either there is an arc (v_j, v_k) in D with $j+1 < k$, or there is more than one arc issuing from vertex n.

Case 1: Suppose there is an arc (v_j, v_k) in D with $j + 1 < k$. Then there exists a family of matrices $T_a \in \mathcal{S}_D$ such that $\mathcal{D}(T_a)$ consists only of the directed cycle as

above, and the arc (v_j, v_k). For $a \in (0,1)$, T_a is of the form:

$$T_a = \begin{bmatrix} 0 & 1 & 0 & \cdots & & & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & & & \cdots & 0 & 0 \\ \vdots & \vdots & & \ddots & & & & & \\ & & & & 1-a & \cdots & & a & \\ \vdots & \vdots & & & & \ddots & & & \\ & & & & & & & & 1 \\ 1 & 0 & 0 & \cdots & & & \cdots & 0 & 0 \end{bmatrix}.$$

It is easily seen by examination that $w^\top T_a = w^\top$ gives

$$w_n = w_j, \quad \text{and} \quad (1-a)w_j = w_{j+1}.$$

That is, $w_n = \frac{1}{1-a} w_{j+1}$. Hence $w_n > w_{j+1}$ for any choice of a, $0 < a < 1$, contradicting (b).

Case 2: Suppose that D contains an arc (v_n, v_k), some $k \neq n$. Then there exists a family of matrices $T_a \in \mathcal{S}_D$ of the form

$$T_a = \begin{bmatrix} 0 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 1 & \cdots & \cdots & 0 \\ \vdots & \vdots & & \ddots & & \vdots \\ \vdots & \vdots & & & \ddots & \vdots \\ 0 & 0 & \cdots & & \cdots & 1 \\ 1-a & 0 & \cdots & a & \cdots & 0 \end{bmatrix}.$$

Then the eigenequation for the stationary vector w of T_a produces

$$w_1 = (1-a)w_n,$$

and hence $w_1 < w_n$, contradicting (b) as before. □

The following corollary summarises the results from this section and provides a characterisation of all directed graphs D for which equality is attained in the lower bound (4.5) on $\max_{i \neq j} m_{i,j}$ for all $T \in \mathcal{S}_D$, with the extra stipulation that the stationary vectors of matrices in $\mathcal{S}_D$ must always have the minimum entry occurring in the same position.

Corollary 4.3.10. *D is a strongly connected directed graph on n vertices such that for every irreducible $T \in \mathcal{S}_D$ with stationary vector w and mean first passage matrix M:*

(a) $w_n = \min_k w_k$*;*

(b) $\max\limits_{\substack{1 \leq i,j \leq n \\ i \neq j}} m_{i,j} = \dfrac{1}{w_n} - 1,$

if and only if D is a Hessenberg cycle.

Remark 4.3.11. Let D be the Hessenberg cycle on n vertices with all possible arcs, and suppose we are given some probability vector $w = \begin{bmatrix} w_1 & w_2 & \cdots & w_n \end{bmatrix}^\top$ with $w_1 \geq w_2 \geq \cdots \geq w_n$. Then it is not difficult to show that there exists a parametrised family of matrices in $\mathcal{S}_D$ with w as their stationary distribution vector. This is determined simply by examining the eigenequation $w^\top T = w^\top$ for an arbitrary matrix T with the Hessenberg cycle pattern. In particular, the entries on the superdiagonal may

be expressed as

$$\begin{aligned} t_{j,j+1} &= \frac{w_{j+1}}{w_j}\sum_{k=1}^{j} t_{j+1,k} + \frac{w_{j+2}}{w_j}\sum_{k=1}^{j} t_{j+2,k} + \cdots + \frac{w_n}{w_j} \\ &= \sum_{i=1}^{n-j}\sum_{k=1}^{j} \frac{w_{j+1}}{w_j} t_{j+1,k}. \end{aligned}$$

Considering the diagonal entries of T to be constrained so that

$$t_{j,j} = 1 - \sum_{k=1}^{j-1} t_{j,k} - t_{j,j+1},$$

we can consider every entry below the main diagonal to be free parameters, constrained only by the fact that the matrix must be nonnegative and stochastic. Certainly this family is nonempty, as we may set all of these parameters to zero and still obtain a matrix $T \in \mathcal{S}_D$ with $w^\top T = w^\top$.

$M/G/1$ queues

Stochastic upper Hessenberg matrices arise as transition matrices for a Markov chain model of a certain type of queueing system, where customers arrive to the system, spend a certain amount of time waiting for service, and leave after they have been served. The model is as follows: let $\mathcal{S} = \{s_0, s_1, s_2, \ldots\}$ be our state space, where s_i denotes the state that there are i customers in the system, including one who is being served. Transitions between states are governed by arrivals and departures to and from the system; i.e. new customers joining the queue or customers leaving the queue once they have been served. Suppose that the length of a time-step is chosen so that at most one customer is served in a single time-step. Then $s_i \to s_j$ is a permitted transition if and only if $j > i$ (new arrivals), $j = i$ (one arrival and one departure), or $j = i - 1$ (no arrivals, one departure). Hence the transition matrix T is upper Hessenberg.

This Markov chain model of a queue is a description of the *embedded Markov chain* for an $M/G/1$ queue (see [3, Chapter 5]). This is a stochastic process of arrivals and departures where arrivals are assumed to be Markovian (governed by a Poisson process), service times have a general distribution, and there is one server. These assumptions allow the above Markov chain construction to describe the behaviour of the queueing system. Such models can be applied to familiar, mundane queues such as patients at a doctor's office, or vehicles awaiting service at a mechanic. They can also be used to examine communication systems, where 'customers' represent voice or data traffic awaiting transmission. These applications have existed since the very first publication on queueing theory (see [27]) and are adapted in recent times to be of use with modern technology, such as video transmission (see [63]) and web server performance (see [12]).

The result we have proven in this section applies to $M/G/1/K$ queues – that is, an $M/G/1$ queue with finite capacity K, resulting in a finite state space and transition matrix. This means that if the system has reached capacity (i.e. K customers are currently in the queue), any arriving customers must leave without joining the queue. The Hessenberg cycle which we have examined in this section represents a queueing system with the particular feature that once the system is empty, with zero customers waiting in the queue, it then fills to full capacity, in a 'bulk arrival'. Our result says that for queues of this type, the expected time to reach the state that there are no customers in the queue from the state that the queue is full is optimal, relative to the given stationary vector.

4.3.2 Non-Hessenberg digraphs which achieve equality

Our initial objective was to characterise all directed graphs D for which equality holds in the lower bound (4.5) for all irreducible $T \in \mathcal{S}_D$. The results of the previous section

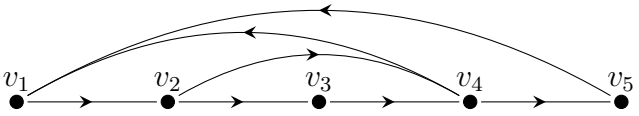


Figure 4.4: A non-Hessenberg digraph D on 5 vertices for which equality is attained in our lower bound for all $T \in \mathcal{S}_D$.

determine the family of so-called Hessenberg cycles as the characterisation of all such digraphs for which the additional condition holds: that the minimum entry of the stationary vector of a transition matrix in $\mathcal{S}_D$ always occurs in the same position.

Consider now the example D in Figure 4.4, which is not Hessenberg due to the arc $(2, 4)$ (and there is no permutation of the vertices resulting in a Hessenberg cycle). Any matrix T in $\mathcal{S}_D$ is of the form

$$T = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & a & 1-a & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1-b & 0 & 0 & 0 & b \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

for some $0 < a, b < 1$. The stationary vector of T is computed as

$$w^\top = \tfrac{1}{3+a+b} \begin{bmatrix} 1 & 1 & a & 1 & b \end{bmatrix}$$

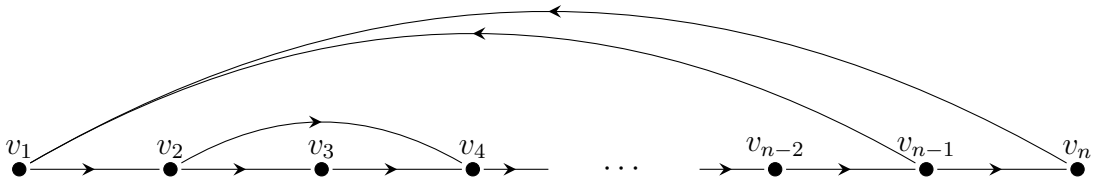


Figure 4.5: A non-Hessenberg digraph D on n vertices for which equality is attained in our lower bound for all $T \in \mathcal{S}_D$.

and the mean first passage matrix is

$$M = \begin{bmatrix} 3+a+b & 1 & \frac{3+b}{a}-1-b & 2+a & \frac{3+a}{b} \\ 2+a+b & 3+a+b & \frac{3+b}{a}-2-b & 1+a & \frac{3+a}{b}-1 \\ 2+b & 3+b & \frac{3+b}{a}+1 & 1 & \frac{3+a}{b}-1-a \\ 1+b & 2+b & \frac{3+b}{a} & 3+a+b & \frac{3+a}{b}-1-2a \\ 1 & 2 & \frac{3+b}{a}-b & 3+a & \frac{3+a}{b}+1 \end{bmatrix}.$$

The minimum entry of the stationary vector is either w_3 or w_5, depending on whether $a > b$ or $a < b$. Further, the maximum entry in the mean first passage matrix is either

$$m_{4,3} = \frac{3+b}{a} \quad \text{or} \quad m_{1,5} = \frac{3+a}{b},$$

which are $\frac{1}{w_3} - 1$ and $\frac{1}{w_5} - 1$ respectively. Moreover, when $a < b$, w_3 is minimum and $\max_{i \neq j} m_{i,j} = m_{4,3}$, and when $a > b$, w_5 is minimum and $\max_{i \neq j} m_{i,j} = m_{1,5}$. Note also that if $a = b$, $w_3 = w_5$ and these are both minimal, and equality holds in the lower bound (4.2.1) in both the third column and fifth column, and overall. Hence equality holds in the lower bound (4.5) for all $T \in \mathcal{S}_D$.

This example of order five can be generalised to a directed graph of order n with the same properties as D, shown in Figure 4.5. The stationary vector of a matrix in

this family is

$$w^\top = \tfrac{1}{(n-2)+a+b}\begin{bmatrix}1 & 1 & a & 1 & \cdots & 1 & b\end{bmatrix}$$

and the mean first passage matrix is

$$\begin{bmatrix}
(n-2)+a+b & 1 & \frac{(n-2)+b}{a}-(n-4)-b & 2+a & \cdots & (n-3)+a & \frac{(n-2)+a}{b} \\
(n-3)+a+b & (n-2)+a+b & \frac{(n-2)+b}{a}-(n-3)-b & 1+a & \cdots & (n-4)+a & \frac{(n-2)+a}{b}-1 \\
(n-3)+b & (n-3)+a+b & \frac{(n-2)+b}{a}+1 & 1 & \cdots & (n-4) & \frac{(n-2)+a}{b}-1-a \\
(n-4)+b & (n-3)+b & \frac{(n-2)+b}{a} & (n-2)+a+b & \cdots & (n-5) & \frac{(n-2)+a}{b}-2-a \\
\vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
2+b & 3+b & \frac{(n-2)+b}{a}-(n-6) & 4+a+b & \cdots & 1 & \frac{(n-2)+a}{b}-(n-4)-a \\
1+b & 2+b & \frac{(n-2)+b}{a}-(n-5) & 3+a+b & \cdots & (n-2)+a+b & \frac{(n-2)+a}{b}-(n-3)-a \\
1 & 2 & \frac{(n-2)+b}{a}-(n-5)-b & 3+a & \cdots & (n-2)+a & \frac{(n-2)+a}{b}+1
\end{bmatrix}.$$

Again, the minimum entry of the stationary vector depends on whether $a > b$ or $a < b$, and in either case (or the case of $a = b$), the maximum off-diagonal entry of the mean first passage matrix is $\frac{1}{\min_k w_k} - 1$.

Some observations

From the existence of the above class of examples, we can observe that the digraph characterisation problem becomes significantly more difficult when we relax the constraint that the minimum entry of the stationary vectors of these matrices occurs in a common position over the whole class. In particular, equality is attained in this class of examples due to the following features of the directed graphs in this class: Letting $\mathcal{J}$ denote the index set of indices j for which it is possible w_j is minimum for some $T \in \mathcal{S}_D$, we have

- for all $j \in \mathcal{J}$, the maximum entry in the j^{th} column of the mean first passage matrix (bar $m_{j,j}$) is $m_{j+1,j}$;

- for all $j \in \mathcal{J}$, $m_{j+1,j} = \frac{1}{w_j} - 1$;

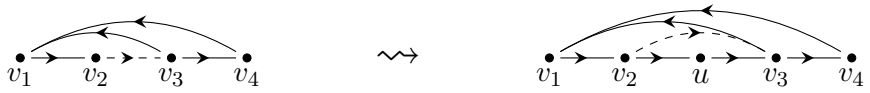


Figure 4.6: An illustration of a process for constructing the previous order 5 example from an order 4 Hessenberg cycle

- the set of candidates for maximum off-diagonal mean first passage time is $\{m_{j+1,j} \mid j \in \mathcal{J}\}$, and $m_{j+1,j}$ is the overall maximum precisely when $w_j = \min_k w_k$.

For these reasons, it would seem that to answer the more general question, results are sought on directed graphs for which equality holds in the column lower bound of Proposition 4.2.1 for all transition matrices respecting the digraph. Further, showing that these mean first passage times are maximum in the whole mean first passage matrix becomes difficult without the particular structure of a Hessenberg digraph and hence the tools used in Proposition 4.3.8, particularly the 'triangle inequality' for mean first passage times in (4.1).

A reasonable starting point would be to determine a method for constructing new families of directed graphs from the Hessenberg cycles, thereby using some of the tools we have already produced. Notice in Figure 4.6 that our order 5 example above is constructed from an order 4 Hessenberg cycle by introducing a new vertex u between vertices v_2 and v_3 on the Hamilton cycle, but retaining the original arc (v_2, v_3). This produces a non-Hessenberg directed graph which can then be examined for the property that mean first passage times are limited by the stationary vector, using the information we have about the mean first passage times of transition matrices respecting the original Hessenberg cycle. Note that a similar construction exists to create the order n non-Hessenberg digraph in Figure 4.5 from a Hessenberg cycle of order $n-1$. A developed construction method which is proven to produce families of new non-Hessenberg directed graphs with equality attainment in (4.5) would shed some light on the general characterisation question.

Chapter 5

Clustering behaviour in Markov chains

In the beginning of Chapter 4, we saw in Example 4.1.5 that we could attain large mean first passage times in a Markov chain by essentially restricting access to certain states in the chain by making transition probabilities between these sets of states extremely small. In that particular example, this also forced the corresponding entries of the stationary vector to be extremely small. However, this need not be the case. For example, consider the following stochastic irreducible matrix of order $2k$:

$$T = \frac{1}{k}\left[\begin{array}{c|c} (1-a)J & aJ \\ \hline aJ & (1-a)J \end{array}\right] \tag{5.1}$$

where each diagonal block is $k \times k$. The stationary vector of T is $w^\top = \frac{1}{2k}\mathbb{1}^\top$, while the mean first passage matrix for T is given by

$$M = \left[\begin{array}{c|c} (2k)J & (2k-2+\frac{1}{a})J \\ \hline (2k-2+\frac{1}{a})J & (2k)J \end{array}\right].$$

For small values of a, the behaviour of a Markov chain with such a transition matrix is clear. Beginning in an initial state s_i, for $1 \leq i \leq k$, the chain will remain in the subset of states $\{s_1, \ldots, s_k\}$ with high probability; i.e. the probability of the chain entering a state s_j with $k+1 \leq j \leq 2k$ is very small, and the expected time it will take the chain to reach a state in $\{s_{k+1}, \ldots, s_{2k}\}$ is large. Similarly, if the chain begins in $s_j \in \{s_{k+1}, \ldots, s_{2k}\}$, it remains in that set of states with high probability, and takes a long time on average to reach a state in $\{s_1, \ldots, s_k\}$. That is, there are mean first passage times for this chain that are very large, but this is not necessarily reflected in the entries of the stationary vector. In particular, our lower bound on $\max m_{i,j}$ from Chapter 4 is far from tight on many occasions.

The behaviour described for the Markov chain with transition matrix given in (5.1) is referred to as *clustering behaviour*. In this chapter, we determine a method for detecting such behaviour in a Markov chain using the eigenvalues and eigenvectors of the transition matrix. The main results are given in Theorems 5.2.1 and 5.3.1, and in Section 5.4 we give some remarks about the implementation of this method as an algorithm, and present some examples to illustrate the method. The content of this chapter has been submitted for publication and is under review. The results of Sections 5.2 and 5.3 can also be found in preliminary form in [28].

5.1 Introduction

Of great interest in many systems that can be modelled using Markov chains is the manifestation of clustering behaviour and how it may be predicted. Clustering behaviour is usually characterised by the existence of collections of states of the Markov chain for which the system, if starting in a state in a cluster, is unlikely to leave that collection of states in the short term (as in (5.1)). That is, the expected number of

time-steps until the chain is in a state outside of that cluster is relatively large. In the extreme, this results in a *nearly uncoupled* system; that is, the stochastic matrix in question can be considered as a perturbed block diagonal matrix, where the diagonal blocks represent the clusters or *almost invariant aggregates* of the chain. It is not difficult to show that for such a matrix, the second-largest (or *subdominant*) eigenvalue(s) must be close to 1 due to the continuity of eigenvalues. However, much of the work regarding the determination of this clustered behaviour or *near uncoupling* is concerned with the converse question: given that a stochastic irreducible matrix T has eigenvalues λ close to 1, what can be said about the clustering behaviour of the Markov chain represented by T? This is the question that we consider in this chapter.

In a stochastic model of molecular dynamics, clusters are referred to as *metastable states*, representing different conformations of the molecule. Identification of these metastable states is extremely important in drug design (see [24]) and biomolecular research (see [72]). An algorithm for this purpose, based on *Perron cluster analysis* (that is, analysing the cluster of eigenvalues around the Perron eigenvalue or spectral radius 1), is developed in [23], and improved upon in [25]. However, the Markov chains considered in these models are always reversible, and hence the eigenvalues of the stochastic matrices are always real. An attempt to generalise without relying on the reversibility assumption is given in [33], which uses the singular value decomposition instead of the eigendecomposition of the matrix. In [79], further assumptions were found to be necessary for this algorithm to work correctly.

We return again to the Markov chain model for an urban traffic network presented in [20]. Clustering in such a network corresponds to 'communities' in the network, and it is measured in this model using Kemeny's constant and the second largest (real) eigenvalue of the transition matrix, which is found to be the basis of an expression of an upper bound on the transition probabilities from one subset of states to another,

and also a bound on the mean first passage times between those subsets. Since we cannot depend on the assumption of real eigenvalues in this model of road traffic—or in any general Markov chain model—we wish to generalise the result in [20] to the case that the stochastic matrix representing the chain has complex eigenvalues.

We now give an expository discussion of the main theoretical result in [20, Theorem A.1], regarding evidence of clustering in a Markov chain derived from the existence of a real eigenvalue near 1. The method of proof of this result inspires the results in this chapter.

Theorem 5.1.1 ([20])**.** *Let T be an irreducible stochastic matrix and suppose that $\lambda \in \mathbb{R}$ is an eigenvalue of T. Let $v = [v_1^\top \mid v_2^\top | \mathbf{0}^\top]^\top$ be a corresponding λ eigenvector (with $v_1 > 0$ and $v_2 < 0$) and partition the matrix T conformally as*

$$\left[\begin{array}{c|c|c} T_{11} & T_{12} & T_{13} \\ \hline T_{21} & T_{22} & T_{23} \\ \hline T_{31} & T_{32} & T_{33} \end{array}\right]$$

and label the subsets of the partition as $\mathcal{J}_1, \mathcal{J}_2$, and $\mathcal{J}_3$ respectively. Then:

(a) $\rho(T_{11}), \rho(T_{22}) > \lambda$.

(b) There are subsets $\hat{\mathcal{J}}_1 \subseteq \mathcal{J}_1$, $\hat{\mathcal{J}}_2 \subseteq \mathcal{J}_2$, and positive vectors $\hat{z}_1^\top, \hat{z}_2^\top$ with supports on $\hat{\mathcal{J}}_1, \hat{\mathcal{J}}_2$ respectively such that $\hat{z}_1^\top \mathbb{1} = \hat{z}_2^\top \mathbb{1} = 1$ and

$$\sum_{i \in \hat{\mathcal{J}}_1} \hat{z}_1(i) \sum_{j \notin \hat{\mathcal{J}}_1} t_{i,j} = 1 - \rho(T_{11}) \leq 1 - \lambda, \tag{5.2}$$

and

$$\sum_{i \in \hat{\mathcal{J}}_2} \hat{z}_2(i) \sum_{j \notin \hat{\mathcal{J}}_2} t_{i,j} = 1 - \rho(T_{22}) \leq 1 - \lambda. \tag{5.3}$$

(c) For any $j \in \hat{\mathcal{J}}_2$,

$$\sum_{i \in \hat{\mathcal{J}}_1} \hat{z}_1(i) m_{i,j} \geq \frac{1}{1 - \rho(T_{11})} \geq \frac{1}{1 - \lambda} \tag{5.4}$$

and for any $j \in \hat{\mathcal{J}}_1$,

$$\sum_{i \in \hat{\mathcal{J}}_2} \hat{z}_2(i) m_{i,j} \geq \frac{1}{1 - \rho(T_{22})} \geq \frac{1}{1 - \lambda}, \tag{5.5}$$

where $m_{i,j}$ *are entries of the mean first passage matrix.*

We first remark that the bounds in this theorem hold for any real eigenvalue λ of T. However, the result is intended to provide evidence of clustering in a system when λ is close to 1. The justification for this primarily relies on parts (b) and (c) of the above; (b) essentially implies that transitions out of a certain subset of the index set of T_{11} are rare (that is, the corresponding transition probabilities are small) if λ is close to 1, while (c) indicates that the expected times for the system to move from one subset of states to the other are large.

Proof. (a) From the eigenequation $Tv = \lambda v$ we have

$$\begin{aligned} T_{11}v_1 + T_{12}v_2 &= \lambda v_1 \\ \Rightarrow \quad T_{11}v_1 &= \lambda v_1 - T_{12}v_2. \end{aligned}$$

Let z be a left Perron vector for T_{11}, so that

$$z^\top T_{11} = \rho(T_{11}) z^\top.$$

Then

$$\begin{aligned} \rho(T_{11})z^\top v_1 &= \lambda z^\top v_1 - z^\top T_{12} v_2 \\ \Rightarrow \quad (\rho(T_{11}) - \lambda) z^\top v_1 &= -z^\top T_{12} v_2. \end{aligned}$$

Now, z, v_1, T_{12} are nonnegative, and v_2 is negative. Hence $z^\top v_1$, $-z^\top T_{12} v_2$ are nonnegative vectors, so $\rho(T_{11}) - \lambda$ must also be nonnegative; that is, $\rho(T_{11}) \geq \lambda$.

An analogous argument applies to $\rho(T_{22})$.

(b) We say an index set $\mathcal{J}$ is the *support* of a vector x if $\mathcal{J}$ consists of the indices j for which $x(j) > 0$.

Let $z_1^\top$ be a left Perron vector for T_{11}, normalised so that $z_1^\top \mathbb{1} = 1$. Partition $\mathcal{J}_1$ as $\hat{\mathcal{J}}_1 \dot{\cup} \check{\mathcal{J}}_1$ where $\hat{\mathcal{J}}_1$ is the support of z_1. Denote the corresponding subvector as $\hat{z}_1$. Let $z_2^\top$ be a left Perron vector for T_{22}, normalised so that $z_2^\top \mathbb{1} = 1$ and similarly, partition $\mathcal{J}_2$ as $\hat{\mathcal{J}}_2 \dot{\cup} \check{\mathcal{J}}_2$ where $\hat{\mathcal{J}}_2$ is the support of z_2. Denote the corresponding subvector as $\hat{z}_2$.

Then T can be further partitioned (again without loss of generality on the ordering of the rows and columns) as

$$\left[\begin{array}{c|c|c|c|c} T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1} & T_{\hat{\mathcal{J}}_1\check{\mathcal{J}}_1} & T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_2} & T_{\hat{\mathcal{J}}_1\check{\mathcal{J}}_2} & T_{\hat{\mathcal{J}}_1\mathcal{J}_3} \\ \hline T_{\check{\mathcal{J}}_1\hat{\mathcal{J}}_1} & T_{\check{\mathcal{J}}_1\check{\mathcal{J}}_1} & T_{\check{\mathcal{J}}_1\hat{\mathcal{J}}_2} & T_{\check{\mathcal{J}}_1\check{\mathcal{J}}_2} & T_{\check{\mathcal{J}}_1\mathcal{J}_3} \\ \hline T_{\hat{\mathcal{J}}_2\hat{\mathcal{J}}_1} & T_{\hat{\mathcal{J}}_2\check{\mathcal{J}}_1} & T_{\hat{\mathcal{J}}_2\hat{\mathcal{J}}_2} & T_{\hat{\mathcal{J}}_2\check{\mathcal{J}}_2} & T_{\hat{\mathcal{J}}_2\mathcal{J}_3} \\ \hline T_{\check{\mathcal{J}}_2\hat{\mathcal{J}}_1} & T_{\check{\mathcal{J}}_2\check{\mathcal{J}}_1} & T_{\check{\mathcal{J}}_2\hat{\mathcal{J}}_2} & T_{\check{\mathcal{J}}_2\check{\mathcal{J}}_2} & T_{\check{\mathcal{J}}_2\mathcal{J}_3} \\ \hline T_{\mathcal{J}_3\hat{\mathcal{J}}_1} & T_{\mathcal{J}_3\check{\mathcal{J}}_1} & T_{\mathcal{J}_3\hat{\mathcal{J}}_2} & T_{\mathcal{J}_3\check{\mathcal{J}}_2} & T_{\mathcal{J}_3\mathcal{J}_3} \end{array}\right].$$

Consider the vector $z^\top = [\hat{z}_1^\top \mid \mathbf{0}^\top \mid \mathbf{0}^\top \mid \mathbf{0}^\top \mid \mathbf{0}^\top]$ and the expression $z^\top T \mathbb{1}$ in this partitioned form. Since T is stochastic, and $\hat{z}_1$ has been normalised so that

$\hat{z}_1^\top \mathbb{1} = 1$, we have

$$\begin{aligned} \hat{z_1}^\top T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1}\mathbb{1} + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\check{\mathcal{J}}_1}\mathbb{1} + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_2}\mathbb{1} + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\check{\mathcal{J}}_2}\mathbb{1} + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\mathcal{J}_3}\mathbb{1} &= 1 \\ \Rightarrow \quad \rho(T_{11}) + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\check{\mathcal{J}}_1}\mathbb{1} + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_2}\mathbb{1} + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\check{\mathcal{J}}_2}\mathbb{1} + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\mathcal{J}_3}\mathbb{1} &= 1. \end{aligned}$$

Now $1 - \lambda \geq 1 - \rho(T_{11}) = \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\check{\mathcal{J}}_1}\mathbb{1} + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_2}\mathbb{1} + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\check{\mathcal{J}}_2}\mathbb{1} + \hat{z}_1^\top T_{\hat{\mathcal{J}}_1\mathcal{J}_3}\mathbb{1}$, and the inequality follows.

An analogous argument holds for $\rho(T_{22})$, by considering the expression

$$[\mathbf{0}^\top \mid \hat{z}_2^\top \mid \mathbf{0}^\top \mid \mathbf{0}^\top \mid \mathbf{0}^\top]T\mathbb{1}$$

in its partitioned form.

(c) Choose an index j in $\hat{\mathcal{J}}_2$. Then for any $i \in \mathcal{J}_1$ the mean first passage time $m_{i,j}$ is given by $e_i^\top (I - T_{(j)})^{-1}\mathbb{1}$. But

$$e_i^\top (I - T_{(j)})^{-1}\mathbb{1} \geq e_i^\top (I - T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1})^{-1}\mathbb{1},$$

since $T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1}$ is a submatrix of $T_{(j)}$. Hence

$$\sum_{i\in\hat{\mathcal{J}}_1} \hat{z}_1(i)m_{i,j} \geq \hat{z}_1^\top (I - T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1})^{-1}\mathbb{1}.$$

Since $\rho(T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1}) < 1$, we have

$$\begin{aligned}
\hat{z}_1^\top (I - T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1})^{-1}\mathbb{1} &= \hat{z}_1^\top \left(\sum_{k=0}^{\infty} T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1}^k\right)\mathbb{1} \\
&= \left(\sum_{k=0}^{\infty} (\rho(T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1}))^k \hat{z}_1^\top\right)\mathbb{1} \\
&\geq \left(\sum_{k=0}^{\infty} \rho(T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1})^k\right) \\
&= \frac{1}{1-\rho(T_{\hat{\mathcal{J}}_1\hat{\mathcal{J}}_1})} \\
&\geq \frac{1}{1-\lambda}.
\end{aligned}$$

An analogous argument holds for any index j chosen from $\hat{\mathcal{J}}_2$.

□

The drawback of this result is that lower bounds for $\rho(T_{11})$ and $\rho(T_{22})$ are restricted to the case of a real eigenvalue and its corresponding eigenvector. Our question is this: can any clustering behaviour be determined from a complex eigenvalue and corresponding eigenvector? That is, given $\lambda \in \mathbb{C}$ an eigenvalue of T where $\lambda = \alpha + i\beta$, some α, β, can we:

(i) define a conformal partition of a corresponding eigenvector for λ and the matrix T;

(ii) determine lower bounds for the spectral radii of T_{11} and T_{22} (the principal submatrices determined by the index set of this partition); and

(iii) conclude equivalent statements about the clustering properties of T in Theorem 5.1.1, parts (b) and (c).

A brief examination of the proof of Theorem 5.1.1 will determine that indeed, (b) and (c) are proven independent of the fact that λ is real; moreover, given lower bounds for

$\rho(T_{11}), \rho(T_{22})$, these may be substituted for λ in (5.2), (5.3), (5.4) and (5.5).

The remainder of this chapter is structured as follows: in Section 5.2, we establish a method for determining a conformal partition using the real part of the complex eigenvector corresponding to the eigenvector $\lambda = \alpha + i\beta$ and the corresponding lower bounds. This is our main result, presented in a discursive format and formalised in the statement of Theorem 5.2.1 at the end of the section; in particular, we do not supply a formal proof. In Section 5.3, we describe a parallel method for determining a conformal partition using the imaginary part of the eigenvector corresponding to λ, which can produce entirely new evidence of clustering behaviour in the Markov chain corresponding to the transition matrix in question. Since the approach is analogous to that in Section 5.2, this is presented in less detail, and again formalised in Theorem 5.3.1, without a formal proof.

Finally, we remark that this work is inspired by the empirical observations in [29] which anticipated that clustering behaviour could be detected from complex eigenvectors. A rationale is given in Section 2.2 of [29] as to why this may be plausible, although we will emphasise later in Remark 5.3.2 that the mere existence of complex eigenvalues of large modulus or close to 1 is not sufficient to conclude the presence of clustering behaviour. Furthermore, in a simulated model of a bus network, the authors of [29] demonstrate that clusters in the Markov chain can be determined by visual inspection of the second eigenvector. We will analyse this example further in Section 5.4 using the theory developed in Sections 5.2 and 5.3.

5.2 Clustering information obtained from the sign pattern of the real part of an eigenvector

Suppose that T is an irreducible stochastic matrix of order n with an eigenvalue $\lambda = \alpha + i\beta$. It will be important later to consider α to be close to 1, and β close to 0, but for now we assume only that $\alpha, \beta > 0$. Let $x + iy$ be a corresponding eigenvector for T, where $x, y \in \mathbb{R}^n$. It follows from equating real and complex coefficients in the standard eigenequation that

$$Tx = \alpha x - \beta y \tag{5.6}$$

and

$$Ty = \beta x + \alpha y. \tag{5.7}$$

Now consider the following: we partition the system (i.e. the matrix T and the vectors x and y) according to where x is positive, negative, and zero. That is, we have (without loss of generality regarding a re-ordering of the rows and columns)

$$\left[\begin{array}{c|c|c} T_{11} & T_{12} & T_{13} \\ \hline T_{21} & T_{22} & T_{23} \\ \hline T_{31} & T_{32} & T_{33} \end{array}\right] \left[\begin{array}{c} x_1 \\ \hline x_2 \\ \hline 0 \end{array}\right] = \left[\begin{array}{c} \alpha x_1 - \beta y_1 \\ \hline \alpha x_2 - \beta y_2 \\ \hline -\beta y_3 \end{array}\right]$$

where $x_1 > 0$ and $x_2 < 0$, entrywise. Let $\mathcal{J}_1, \mathcal{J}_2, \mathcal{J}_3$ denote the index sets of the partition. Note that $\mathcal{J}_3$ may be empty.

This gives:

$$T_{11}x_1 + T_{12}x_2 = \alpha x_1 - \beta y_1,$$

and since $T_{12}x_2$ is entrywise nonpositive,

$$T_{11}x_1 \quad \geq \quad \alpha x_1 - \beta y_1.$$

Now consider the diagonal matrix $X_1 := \mathrm{diag}(x_1)$, and observe that $T_{11}x_1 = T_{11}X_1\mathbb{1}$. Furthermore, from the above,

$$X_1^{-1}T_{11}X_1\mathbb{1} \quad \geq \quad X_1^{-1}(\alpha x_1 - \beta y_1).$$

By a well-known result (see [76, Cor.1 to Thm.1]) we know that the spectral radius of a nonnegative matrix lies between its minimum and maximum row sums; hence

$$\rho(X_1^{-1}T_{11}X_1) \quad \geq \quad \min(X_1^{-1}T_{11}X_1\mathbb{1}) \quad \geq \quad \min_j \left(\frac{\alpha x_1(j) - \beta y_1(j)}{x_1(j)} \right)$$

(where $x_i(j)$ denotes the j^{th} entry of x_i, for example). Since T_{11} and $X_1^{-1}T_{11}X_1$ are diagonally similar matrices, their spectral radii are equal, and it follows that

$$\rho(T_{11}) \quad \geq \quad \alpha - \beta \max_j \left(\frac{y_1(j)}{x_1(j)} \right). \tag{5.8}$$

Similarly, we may show that

$$\rho(T_{22}) \quad \geq \quad \alpha - \beta \max_j \left(\frac{y_2(j)}{x_2(j)} \right). \tag{5.9}$$

We pause here to note two things. The first is that if α is close to 1, and β close to 0, then these lower bounds are each close to 1, indicating that the states indexed by $\mathcal{J}_1$ and $\mathcal{J}_2$ display some clustering behaviour in the Markov chain represented by T, in the manner described in Theorem 5.1.1, parts (b) and (c).

The second thing to note is that it is vital to our further discussion on these clusters

that we assume that

$$\alpha x_1 - \beta y_1 > 0 \quad \text{and} \quad \alpha x_2 - \beta y_2 < 0, \tag{5.10}$$

in order that the lower bounds in (5.8) and (5.9) are positive. We will consider (5.10) as an additional hypothesis that must be satisfied in order to state the result, because although (5.8) and (5.9) still hold in the case that (5.10) does not, they are worthless to us, since the spectral radius will always be nonnegative. Therefore this result (and subsequent results) are only relevant in the case that the hypotheses in (5.10) hold.

5.2.1 Expanding the index sets of the partition

It is possible to optimise the bounds in (5.8) and (5.9) by adding a little flexibility in how the partition is determined. We allow the option of expanding the first cluster indexed by $\mathcal{J}_1$ to include indices corresponding to positive entries of y_3. Similarly, we expand the second index set $\mathcal{J}_2$ by including entries corresponding to negative entries of y_3.

Formally, we define the new partition index sets as

$$\tilde{\mathcal{J}}_1 = \mathcal{J}_1 \cup \{j \mid y_3(j) > 0\}, \text{ and } \tilde{\mathcal{J}}_2 = \mathcal{J}_2 \cup \{j \mid y_3(j) < 0\}.$$

Equivalently, we may consider the vector $x + ty$ for some $t > 0$ and partition, as before, according to where $x + ty$ is positive, negative, and zero, producing the respective partition sets $\tilde{\mathcal{J}}_1, \tilde{\mathcal{J}}_2$, and $\tilde{\mathcal{J}}_3 = \{j \mid x(j) = y(j) = 0\}$. In particular, we must choose $t > 0$ sufficiently small to achieve the above; we require

$$t < \frac{-x(j)}{y(j)}, \quad \text{for all } j \text{ such that } x(j)y(j) < 0.$$

This ensures that $x(j) + ty(j) > 0$ for all $j \in \tilde{\mathcal{J}}_1$, and that $x(j) + ty(j) < 0$ for all $j \in \tilde{\mathcal{J}}_2$.

Considering $T(x + ty)$, and partitioning with respect to where $x + ty$ is positive, negative, and zero, using (5.6) and (5.7) we obtain:

$$\left[\begin{array}{c|c|c} \tilde{T}_{11} & \tilde{T}_{12} & \tilde{T}_{13} \\ \hline \tilde{T}_{21} & \tilde{T}_{22} & \tilde{T}_{23} \\ \hline \tilde{T}_{31} & \tilde{T}_{32} & \tilde{T}_{33} \end{array}\right] \left[\begin{array}{c} \tilde{x}_1 + t\tilde{y}_1 \\ \hline \tilde{x}_2 + t\tilde{y}_2 \\ \hline 0 \end{array}\right] = \left[\begin{array}{c} \alpha(\tilde{x}_1 + t\tilde{y}_1) + \beta(t\tilde{x}_1 - \tilde{y}_1) \\ \hline \alpha(\tilde{x}_2 + t\tilde{y}_2) + \beta(t\tilde{x}_2 - \tilde{y}_2) \\ \hline (\alpha t - \beta)\tilde{y}_3 \end{array}\right], \tag{5.11}$$

where $\tilde{T}_{ij}$ denote the submatrices corresponding to the new partition with index sets $\tilde{\mathcal{J}}_1, \tilde{\mathcal{J}}_2, \tilde{\mathcal{J}}_3$.

Note that this 'repartition' is not substantially different; we simply allow the option of including some extra states in the cluster by including indices corresponding to positive entries of y_3 to $\mathcal{J}_1$, and indices corresponding to negative entries of y_3 to $\mathcal{J}_2$. Moreover, $\mathcal{J}_1 \subseteq \tilde{\mathcal{J}}_1$ and $\mathcal{J}_2 \subseteq \tilde{\mathcal{J}}_2$. Interpreting in terms of prospective clustering behaviour, we are simply allowing the possible addition of more states into our existing index set to determine more information about the clustering behaviour of our chain.

Proceeding as before, we have from (5.11):

$$\begin{aligned} \tilde{T}_{11}(\tilde{x}_1 + t\tilde{y}_1) &\geq \alpha(\tilde{x}_1 + t\tilde{y}_1) + \beta(t\tilde{x}_1 - \tilde{y}_1) \\ \Rightarrow \quad \rho(\tilde{T}_{11}) &\geq \alpha + \beta \min_j \left(\frac{t\tilde{x}_1(j) - \tilde{y}_1(j)}{\tilde{x}_1(j) + t\tilde{y}_1(j)}\right), \end{aligned} \tag{5.12}$$

and similarly

$$\rho(\tilde{T}_{22}) \geq \alpha + \beta \min_j \left(\frac{t\tilde{x}_2(j) - \tilde{y}_2(j)}{\tilde{x}_2(j) + t\tilde{y}_2(j)}\right). \tag{5.13}$$

These lower bounds are increasing functions of t, and so they are optimised by taking

the limit as t approaches

$$\min\left\{\frac{-x(j)}{y(j)}\,\middle|\, x(j)y(j)<0\right\}. \tag{5.14}$$

If the set above is empty, then t is unbounded. This occurs if and only if wherever x is positive, y is positive, and where x is negative, y is negative. It follows that our lower bounds would then be

$$\rho(\tilde{T}_{11}) \quad \geq \quad \alpha+\beta\min_j\left(\frac{\tilde{x}_1(j)}{\tilde{y}_1(j)}\right),$$

and

$$\rho(\tilde{T}_{22}) \quad \geq \quad \alpha+\beta\min_j\left(\frac{\tilde{x}_2(j)}{\tilde{y}_2(j)}\right),$$

by taking the limit as $t\to\infty$.

As in the first case, we need to ensure that the right-hand side of (5.12) is positive in order for our conclusions to be worthwhile. It is not difficult to show that if $\mathcal{J}_1=\tilde{\mathcal{J}}_1$, the first hypothesis in (5.10) is sufficient to ensure positivity, but if $\mathcal{J}_1$ is a proper subset of $\tilde{\mathcal{J}}_1$, the additional case that $\tilde{x}_1(j)=0$ and $\tilde{y}_1(j)>0$ is considered. In this case we obtain the additional restriction that

$$t>\frac{\beta}{\alpha}.$$

Since t is also bounded above by (5.14), it is necessary that $\frac{\beta}{\alpha}$ is also strictly less than these. In other words, it is necessary that

$$\alpha x_1+\beta y_1>0 \qquad \text{and} \qquad \alpha x_2+\beta y_2<0. \tag{5.15}$$

It remains to consider the possibility that, in our lower bounds (5.12) and (5.13),

we divide by zero when choosing t equal to the minimum entry of the set in (5.14). Of course, by choosing t in this way, we do set at least one entry of either the vector $\tilde{x}_1 + t\tilde{y}_1$ or the vector $\tilde{x}_2 + t\tilde{y}_2$ equal to zero, but since we choose the minimum entry of

$$\frac{t\tilde{x}_i - \tilde{y}_i}{\tilde{x}_i + t\tilde{y}_i}$$

for $i = 1, 2$, this only presents issues if *every* entry of either $\tilde{x}_1 + t\tilde{y}_1$ or $\tilde{x}_2 + t\tilde{y}_2$ is equal to zero. This means that linear dependence occurs between the vectors $\tilde{x}_i$ and $\tilde{y}_i$ for $i = 1$ or $i = 2$. This presents yet another condition: that the vectors x_i and y_i must be linearly independent.

Finally, we note that there is a possibility that no extra states are included in one or both of the clusters; that is, $\tilde{\mathcal{J}}_1 = \mathcal{J}_1$, or $\tilde{\mathcal{J}}_2 = \mathcal{J}_2$. In this case, it is easily shown that the new lower bounds (5.12) and (5.13) are an improvement on the lower bounds (5.8) and (5.9), respectively.

5.2.2 An alternate expansion of the index sets of the partition

We now consider an alternate partition derived from the index sets $\mathcal{J}_1$ and $\mathcal{J}_2$, where we allow the inclusion of indices corresponding to negative entries of y_3 to $\mathcal{J}_1$, and positive entries of y_3 to $\mathcal{J}_2$. That is, we define new index sets

$$\overline{\mathcal{J}}_1 = \mathcal{J}_1 \cup \{j \mid y_3(j) < 0\} \text{ and } \overline{\mathcal{J}}_2 = \mathcal{J}_2 \cup \{j \mid y_3(j) > 0\}.$$

This is equivalent to considering the vector $x + ty$, where t is negative and sufficiently small, and partitioning according to where $x+ty$ is positive, negative and zero, denoting these new index sets $\overline{\mathcal{J}}_1, \overline{\mathcal{J}}_2, \overline{\mathcal{J}}_3$. This may provide a different partition than before, but the computation of the lower bounds is exactly the same. Since we observed that

the expressions for the lower bounds in (5.12) and (5.13) were increasing in t, and t is negative, we choose $t \to 0$ to optimise these lower bounds for the spectral radii.

We now summarize the results of this section in the following theorem:

Theorem 5.2.1. *Let T be an $n \times n$ irreducible and stochastic matrix, let $\lambda = \alpha + i\beta$ be an eigenvalue of T, with $\alpha, \beta > 0$, and let $x+iy$ be a right eigenvector of T corresponding to λ. For $k = 1, 2, 3$, let $\mathcal{J}_k$ denote the index sets obtained by partitioning according to where x is positive, negative and zero (respectively), and let x_k and y_k denote the subvectors of x and y corresponding to the index set $\mathcal{J}_k$. Also, let*

$$\tilde{\mathcal{J}}_1 = \mathcal{J}_1 \cup \{j \mid y_3(j) > 0\}, \quad \tilde{\mathcal{J}}_2 = \mathcal{J}_2 \cup \{j \mid y_3(j) < 0\}$$

and

$$\overline{\mathcal{J}}_1 = \mathcal{J}_1 \cup \{j \mid y_3(j) < 0\}, \quad \overline{\mathcal{J}}_2 = \mathcal{J}_2 \cup \{j \mid y_3(j) > 0\}.$$

and let $\tilde{x}_k, \tilde{y}_k$, and $\bar{x}_k, \bar{y}_k$ be the subvectors of x and y corresponding to the index sets $\tilde{\mathcal{J}}_k$ and $\overline{\mathcal{J}}_k$, respectively. Finally, let $T_{kk}, \tilde{T}_{kk}$ and $\overline{T}_{kk}$ be the principal submatrices of T corresponding to the index sets $\mathcal{J}_k, \tilde{\mathcal{J}}_k$, and $\overline{\mathcal{J}}_k$. Then:

1. *If $\alpha x_1 - \beta y_1 > 0$,*

   (i) $\rho(T_{11}) \geq \alpha - \beta \cdot \max_j \left\{ \dfrac{y_1(j)}{x_1(j)} \right\}$.

   (ii) If $y_1 > 0$ and $y_2 < 0$, then

$$\rho(\tilde{T}_{11}) \geq \alpha + \beta \cdot \min_j \left\{ \frac{\tilde{x}_1(j)}{\tilde{y}_1(j)} \right\}.$$

Otherwise, if x_1 and y_1 are linearly independent, $\alpha x_1 + \beta y_1 > 0$, and

$\alpha x_2 + \beta y_2 < 0$, *then*

$$\rho(\tilde{T}_{11}) \geq \alpha + \beta \cdot \min_j \left\{ \frac{t\tilde{x}_1(j) - \tilde{y}_1(j)}{\tilde{x}_1(j) + t\tilde{y}_1(j)} \right\},$$

where $t > 0$ *and is bounded above by*

$$\min \left\{ \frac{-x(j)}{y(j)} \,\middle|\, x(j)y(j) < 0 \right\}.$$

(iii) $\rho(\overline{T}_{11}) \geq \alpha - \beta \cdot \max_j \left\{ \dfrac{\bar{y}_1(j)}{\bar{x}_1(j)} \right\}.$

2. *If* $\alpha x_2 - \beta y_2 < 0$,

   (i) $\rho(T_{22}) \geq \alpha - \beta \cdot \max_j \left\{ \dfrac{y_2(j)}{x_2(j)} \right\}.$

   (ii) If $y_1 > 0$ *and* $y_2 < 0$, *then*

   $$\rho(\tilde{T}_{22}) \geq \alpha + \beta \cdot \min_j \left\{ \frac{\tilde{x}_2(j)}{\tilde{y}_2(j)} \right\}.$$

   Otherwise, if x_2 *and* y_2 *are linearly independent,* $\alpha x_1 + \beta y_1 > 0$, *and* $\alpha x_2 + \beta y_2 < 0$, *then*

   $$\rho(\tilde{T}_{22}) \geq \alpha + \beta \cdot \min_j \left\{ \frac{t\tilde{x}_2(j) - \tilde{y}_2(j)}{\tilde{x}_2(j) + t\tilde{y}_2(j)} \right\},$$

   where $t > 0$ *and is bounded above by*

   $$\min \left\{ \frac{-x(j)}{y(j)} \,\middle|\, x(j)y(j) < 0 \right\}.$$

   (iii) $\rho(\overline{T}_{22}) \geq \alpha - \beta \cdot \max_j \left\{ \dfrac{\bar{y}_2(j)}{\bar{x}_2(j)} \right\}.$

5.3 Clustering information obtained from the sign pattern of the imaginary part of an eigenvector

We could also begin by partitioning the system with respect to where y is positive, negative, and zero. This potentially gives an entirely different partition, and we use the same approach to find lower bounds for the spectral radii of the submatrices of T corresponding to the index sets of this partition. For the purpose of avoiding congested notation, we will re-use y_1, y_2, x_1, x_2, and x_3 in this section to denote the components of the vectors y and x once the system has been partitioned, where this time it is understood that $y_1 > 0$ and $y_2 < 0$. Similarly, the submatrices T_{ij} now represent something different than in Sections 5.1 and 5.2.

In particular, we consider:

$$\left[\begin{array}{c|c|c} T_{11} & T_{12} & T_{13} \\ \hline T_{21} & T_{22} & T_{23} \\ \hline T_{31} & T_{32} & T_{33} \end{array}\right] \left[\begin{array}{c} y_1 \\ \hline y_2 \\ \hline 0 \end{array}\right] = \left[\begin{array}{c} \beta x_1 + \alpha y_1 \\ \hline \beta x_2 + \alpha y_2 \\ \hline \beta x_3 \end{array}\right]$$

where $y_1 > 0$ and $y_2 < 0$, entrywise. Let $\mathcal{J}_1, \mathcal{J}_2, \mathcal{J}_3$ denote the index sets of the partition. This equation produces, in the same way as before, the following inequalities:

$$\begin{aligned} \rho(T_{11}) &\geq \alpha + \beta \min_j \left(\frac{x_1(j)}{y_1(j)} \right) \\ \rho(T_{22}) &\geq \alpha + \beta \min_j \left(\frac{x_2(j)}{y_2(j)} \right). \end{aligned}$$

We are once again in a situation where, if $\alpha \approx 1$ and $\beta \approx 0$, these lower bounds are close to 1, indicating clustering behaviour in the Markov chain represented by the transition matrix T.

Note that we require new hypotheses in order to ensure these lower bounds are

positive. In particular, we need

$$\alpha y_1 + \beta x_1 > 0 \quad \text{and} \quad \alpha y_2 + \beta x_2 < 0. \tag{5.16}$$

Pursuing the same analysis with repartitioning results in the following theorem:

Theorem 5.3.1. *Let T be an $n \times n$ irreducible and stochastic matrix, let $\lambda = \alpha + i\beta$ be an eigenvalue of T, with $\alpha, \beta > 0$, and let $x+iy$ be a right eigenvector of T corresponding to λ. For $k = 1, 2, 3$, let $\mathcal{J}_k$ denote the index sets obtained by partitioning according to where y is positive, negative and zero (respectively), and let x_k and y_k denote the subvectors of x and y corresponding to the index set $\mathcal{J}_k$. Also, let*

$$\tilde{\mathcal{J}}_1 = \mathcal{J}_1 \cup \{j \mid x_3(j) > 0\}, \quad \tilde{\mathcal{J}}_2 = \mathcal{J}_2 \cup \{j \mid x_3(j) < 0\}$$

and

$$\overline{\mathcal{J}}_1 = \mathcal{J}_1 \cup \{j \mid x_3(j) < 0\}, \quad \overline{\mathcal{J}}_2 = \mathcal{J}_2 \cup \{j \mid x_3(j) > 0\}.$$

and let $\tilde{x}_k, \tilde{y}_k$, and $\bar{x}_k, \bar{y}_k$ be the subvectors of x and y corresponding to the index sets $\tilde{\mathcal{J}}_k$ and $\overline{\mathcal{J}}_k$, respectively. Finally, let $T_{kk}, \tilde{T}_{kk}$ and $\overline{T}_{kk}$ be the principal submatrices of T corresponding to the index sets $\mathcal{J}_k, \tilde{\mathcal{J}}_k$, and $\overline{\mathcal{J}}_k$. Then:

1. *If $\alpha y_1 + \beta x_1 > 0$,*

   (i) $\rho(T_{11}) \geq \alpha + \beta \cdot \min_j \left\{ \dfrac{x_1(j)}{y_1(j)} \right\}$.

   (ii) $\rho(\tilde{T}_{11}) \geq \alpha + \beta \cdot \min_j \left\{ \dfrac{\tilde{x}_1(j)}{\tilde{y}_1(j)} \right\}$.

   (iii) If $x_1 < 0$ and $x_2 > 0$, then

   $$\rho(\overline{T}_{11}) \geq \alpha - \beta \cdot \max_j \left\{ \frac{\bar{y}_1(j)}{\bar{x}_1(j)} \right\}.$$

Otherwise, if x_1 and y_1 are linearly independent, $\alpha y_1 - \beta x_1 > 0$, and $\alpha y_2 - \beta x_2 < 0$, then

$$\rho(\overline{T}_{11}) \geq \alpha + \beta \cdot \min_j \left\{ \frac{\bar{x}_1(j) - s\bar{y}_1(j)}{s\bar{x}_1(j) + \bar{y}_1(j)} \right\},$$

where $s < 0$ and is bounded below by

$$\min \left\{ \frac{-y(j)}{x(j)} \,\middle|\, x(j)y(j) > 0 \right\}.$$

2. *If $\alpha y_2 + \beta x_2 < 0$,*

   (i) $\rho(T_{22}) \geq \alpha + \beta \cdot \min_j \left\{ \dfrac{x_2(j)}{y_2(j)} \right\}.$

   (ii) $\rho(\tilde{T}_{22}) \geq \alpha + \beta \cdot \min_j \left\{ \dfrac{\tilde{x}_2(j)}{\tilde{y}_2(j)} \right\}.$

   (iii) If $x_1 < 0$ and $x_2 > 0$, then

$$\rho(\overline{T}_{22}) \geq \alpha - \beta \cdot \max_j \left\{ \frac{\bar{y}_2(j)}{\bar{x}_2(j)} \right\}.$$

   Otherwise, if x_2 and y_2 are linearly independent, $\alpha y_1 - \beta x_1 > 0$, and $\alpha y_2 - \beta x_2 < 0$, then

$$\rho(\overline{T}_{22}) \geq \alpha + \beta \cdot \min_j \left\{ \frac{\bar{x}_2(j) - s\bar{y}_2(j)}{s\bar{x}_2(j) + \bar{y}_2(j)} \right\},$$

   where $s < 0$ and is bounded below by

$$\min \left\{ \frac{-y(j)}{x(j)} \,\middle|\, x(j)y(j) > 0 \right\}.$$

Remark 5.3.2. We note here the importance of the hypotheses in (5.10) and (5.16), and stress that it is not sufficient to simply determine an eigenvalue of the transition

matrix which is sufficiently close to 1 and conclude that the associated Markov chain must exhibit clustering behaviour.

It is easily determined that the $n \times n$ transition matrix

$$T = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

has eigenvalues $\{e^{\frac{2\pi ji}{n}} \mid j = 0, 1, \ldots, n-1\}$, and hence for n large enough, T will have an eigenvalue $\lambda = e^{\frac{2\pi i}{n}}$ close to 1, with large real part and small imaginary part. However, the Markov chain represented by T has no clustering behaviour, since the chain transitions cyclically through the states in a deterministic fashion.

The eigenvector $x + iy$ corresponding to $\lambda = e^{\frac{2\pi i}{n}} = \cos(\frac{2\pi}{n}) + i\sin(\frac{2\pi}{n})$ is

$$\begin{bmatrix} \cos(0) \\ \cos(\frac{2\pi}{n}) \\ \cos(\frac{4\pi}{n}) \\ \vdots \\ \cos(\frac{2(n-1)\pi}{n}) \end{bmatrix} + i \begin{bmatrix} \sin(0) \\ \sin(\frac{2\pi}{n}) \\ \sin(\frac{4\pi}{n}) \\ \vdots \\ \sin(\frac{2(n-1)\pi}{n}) \end{bmatrix}.$$

Partitioning the system with respect to the sign pattern of x as in Section 5.2, we have

$$x_1 = \begin{bmatrix} \cos(0) \\ \cos(\frac{2\pi}{n}) \\ \vdots \\ \cos(\frac{2k\pi}{n}) \\ \cos(-\frac{2k\pi}{n}) \\ \vdots \\ \cos(-\frac{2\pi}{n}) \end{bmatrix}, \qquad y_1 = \begin{bmatrix} \sin(0) \\ \sin(\frac{2\pi}{n}) \\ \vdots \\ \sin(\frac{2k\pi}{n}) \\ \sin(-\frac{2k\pi}{n}) \\ \vdots \\ \sin(-\frac{2\pi}{n}) \end{bmatrix},$$

where $k = \lfloor \frac{n-1}{4} \rfloor$.

Let $\alpha + i\beta = \lambda = \cos(\frac{2\pi}{n}) + i\sin(\frac{2\pi}{n})$. Considering the first of the hypotheses in (5.10), we have that each entry of $\alpha x_1 + \beta y_1$ is of the form

$$\cos(\tfrac{2\pi}{n})\cos(\tfrac{2\pi j}{n}) - \sin(\tfrac{2\pi}{n})\sin(\tfrac{2\pi j}{n}) = \cos(\tfrac{2\pi(j+1)}{n})$$

for $j \in \{-k, \ldots, -1, 0, 1, \ldots, k\}$. Hence there is an entry of the vector $\alpha x_1 - \beta y_1$ which is negative (in particular, the $k+1$ entry), and so the hypothesis does not hold. Similarly, $\alpha x_2 - \beta y_2$ can be found to have a positive entry; furthermore due to the structure of the matrix and its eigenvectors, it is similarly determined that the hypotheses do not hold for the other case of partitioning with respect to y. Hence we conclude nothing about clustering behaviour of the Markov chain with transition matrix T, as expected.

5.4 Simulations and examples

In this section we produce some numerical examples, determined with a degree of randomness, in order to test this method of detecting clusters. To produce such examples for which we can test this process, we require irreducible stochastic matrices which have complex eigenvalues appropriately close to 1, and which have a certain degree of clustered structure built in. To design an appropriate matrix with a prescribed eigenvalue, we make use of the following technique, which is described below in a general matrix theory setting but is more well-known in spectral graph theory in the context of an *equitable partition* of the adjacency matrix of a graph (see [7, Section 2.3]).

Consider a square block-partitioned matrix

$$A = \left[\begin{array}{c|c|c|c} A_{11} & A_{12} & \cdots & A_{1m} \\ \hline A_{21} & A_{22} & \cdots & A_{2m} \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline A_{m1} & A_{m2} & \cdots & A_{mm} \end{array}\right]$$

and suppose that A has been partitioned into these blocks in such a way that each block A_{ij} has constant row sums $b_{i,j}$. That is, $A_{ij}\mathbb{1}_{k_j} = b_{i,j}\mathbb{1}_{k_i}$ (where k_i is the number of rows in A_{ij}).

Now consider that λ is an eigenvalue of A with right eigenvector $[v_1\mathbb{1}_{k_1}^\top \mid v_2\mathbb{1}_{k_2}^\top \mid \cdots \mid v_m\mathbb{1}_{k_m}^\top]^\top$ if and only if

$$\begin{bmatrix} b_{1,1} & b_{1,2} & \cdots & b_{1,m} \\ b_{2,1} & b_{2,2} & \cdots & b_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ b_{m,1} & b_{m,2} & \cdots & b_{m,m} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_m \end{bmatrix} = \lambda \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_m \end{bmatrix}.$$

That is, the eigenvalues of this quotient matrix $B = [b_{i,j}]$ are contained in the spectrum of A. We make use of this technique here by determining a 3×3 matrix with appropriate eigenvalues to act as the quotient matrix, and then constructing a larger matrix where the first two diagonal blocks represent clusters of the chain.

Consider the 3×3 matrix

$$B = \begin{bmatrix} \frac{5}{6} & 0 & \frac{1}{6} \\ \frac{3}{4} & \frac{1}{6} & \frac{1}{12} \\ \frac{2}{3} - 12t^2 & \frac{1}{3} + 12t^2 & 0 \end{bmatrix}$$

which, for any $t \in [0, \frac{\sqrt{2}}{6}]$, is nonnegative, stochastic, and irreducible, with eigenvalues $1, \pm it$. Taking a convex combination of this matrix and the identity will produce a 3×3 matrix

$$C := (1 - s)I + sB, \qquad 0 \leq s \leq 1$$

which has eigenvalues $1, (1 - s) \pm i(st)$.

Now let T_{11}, T_{22} and T_{33} be irreducible stochastic matrices of orders n_1, n_2, and n_3 respectively. Further, let T_{ij} be an $n_i \times n_j$ rectangular row-stochastic matrix, for $i, j \in \{1, 2, 3\}, i \neq j$. Then

$$T = \left[\begin{array}{c|c|c} c_{11}T_{11} & c_{12}T_{12} & c_{13}T_{13} \\ \hline c_{21}T_{21} & c_{22}T_{22} & c_{23}T_{23} \\ \hline c_{31}T_{31} & c_{32}T_{32} & c_{33}T_{33} \end{array}\right]$$

is an irreducible stochastic matrix of order $n_1 + n_2 + n_3$ which has in its spectrum the complex eigenvalues $(1 - s) \pm i(st)$.

For s chosen appropriately, these eigenvalues are close to 1. Furthermore, the diagonal blocks of T represent potential clusters, in that the probability of transitioning

to another state indexed in the same block is high ($\geq 1-s$) relative to the probability of transitioning to a state indexed in another block. Note that although these transition matrices are constructed to have certain properties, we emphasise that this construction may involve many elements of randomness in order to effectively test the method presented in this chapter. The random elements are as follows.

- t is chosen uniformly at random from the interval $[0, \frac{\sqrt{2}}{6}]$.
- s is chosen uniformly at random from the interval $[0, 0.2]$, so that the complex eigenvalue λ under consideration has real part $\alpha \in [0.8, 1]$ and imaginary part $\beta \in [0, \frac{\sqrt{2}}{30}]$.
- The order n of T is fixed. The integer n_1 is chosen at random from $\{3, 4, \ldots, \lfloor \frac{n}{2} \rfloor\}$. The integer n_2 is chosen at random from $\{3, 4, \ldots n-n_1-3\}$, and $n_3 := n-n_1-n_2$. These integers are chosen in this way to avoid trivial or degenerate cases.
- The matrices T_{ij} are chosen as uniform stochastic random matrices respecting a zero pattern determined randomly with density $p := 0.7$.

We present a single example in detail that has been constructed in this way in order to illustrate both the construction and the analysis of the eigenvectors which produces the partitions and associated potential clusters.

Example 5.4.1. T is a 100×100 matrix, with $n_1 = 32$, $n_2 = 53$, and $n_3 = 15$. T has an eigenvalue $\lambda = 0.9067 + 0.0106i$; i.e. the values of s and t chosen are 0.0933 and 0.1138, respectively.

A heat map for T is given in Fig. 5.1, which illustrates the clustering behaviour of the Markov chain with transition matrix T. The index sets of the constructed clusters are $\{1, 2, \ldots, 32\}$, $\{33, 34, \ldots, 85\}$ and $\{86, 87, \ldots, 100\}$.

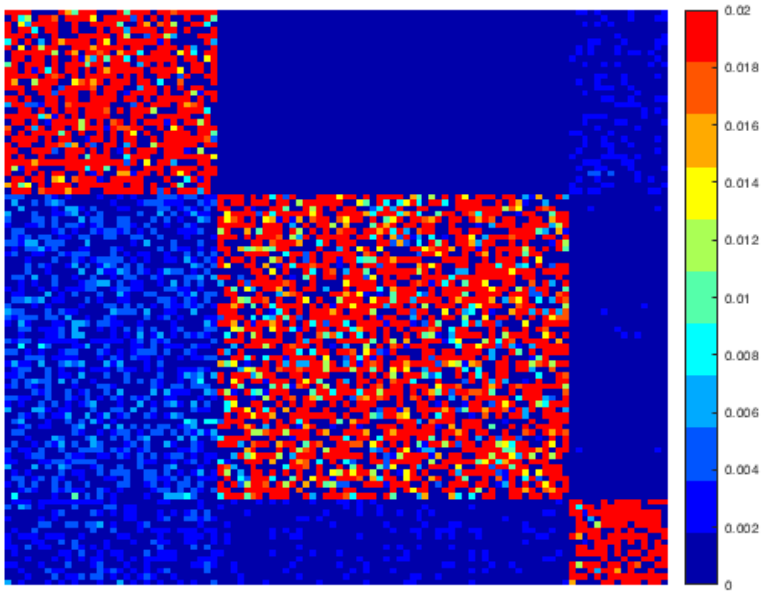


Figure 5.1: A heat map of the transition matrix T in Example 5.4.1. Evidence of clustering behaviour is indicated by the largely red blocks on the diagonal, indicating high probability of staying within one group of states, and low probability (blue) of leaving.

The results of the analysis according to Theorem 5.2.1 are summarized in the following table:

Thm 5.2.1	index set	spectral radius	lower bound
1(i)	$\{1, 2, \ldots, 32\}$	0.9844	0.9052
1(ii)	$\{1, 2, \ldots, 32\}$	0.9844[1]	0.9844[1]
1(iii)	$\{1, 2, \ldots, 32\}$	0.9844	0.9052
2(i)	$\{33, 34, \ldots, 100\}$	0.9348	0.8932
2(ii)	$\{33, 34, \ldots, 100\}$	0.9348	0.9150
2(iii)	$\{33, 34, \ldots, 100\}$	0.9348	0.8932

We see that the partitions determined according to Theorem 5.2.1 recover the first

[1]The spectral radius and the lower bound in this case differ in the 10^{-15} position.

cluster exactly, and present the second two clusters together with evidence of clustering behaviour on the union of those two sets of states. Note that although the 'repartitioning' process of Theorem 5.2.1 does not actually change the partitions, the calculation of the lower bounds in both cases is an improvement on the initial lower bound.

The results of the analysis according to Theorem 5.3.1 are summarized in the following table:

Thm 5.3.1	index set	spect. rad.	lower bound
1(i)	hypothesis not satisfied: $\alpha y_1 + \beta x_1 \not> 0$	-	-
1(ii)	hypothesis not satisfied: $\alpha y_1 + \beta x_1 \not> 0$	-	-
1(iii)	hypothesis not satisfied: $\alpha y_1 + \beta x_1 \not> 0$	-	-
2(i)	$\{33, \ldots, 85, 88, 89, 90, 99\}$	0.9224	0.9150
2(ii)	$\{33, \ldots, 85, 88, 89, 90, 92, 99\}$	0.9224	0.9150
2(iii)	hypothesis not satisfied: $\alpha y_2 - \beta x_2 \not< 0$	-	-

In this case, certain hypotheses do not hold, and hence we obtain less information about the clustering behaviour of this matrix from the partitions obtained with respect to the sign pattern of the imaginary part of the eigenvector. However, we note that while in the previous analysis, the second and third constructed clusters were presented as a single cluster, we see some differentiation here in that the partition obtained from Theorem 5.3.1 2(i) produces the index set $\{33, \ldots, 85, 88, 89, 90, 99\}$ with equally strong evidence of clustering on this subset of the state space, which is essentially composed of the second constructed cluster, plus four states from the third constructed cluster.

We produce 10,000 such matrices with in-built clustered structure, then run this same analysis of the eigenvectors corresponding to eigenvalues close to 1 using Theorems 5.2.1 and 5.3.1. The MATLAB code is given in Appendix A. The goal is to determine how frequently we can recover the clusters that we constructed, and to determine

lower bounds on the spectral radii of the corresponding submatrices. The magnitude of these lower bounds is an indicator of the 'tightness' of the detected cluster, in the manner described in Theorem 5.1.1, parts (b) and (c).

Our results are as follows:

- The first cluster is recovered exactly in 99.61% of cases.
- The second cluster is recovered exactly in 8.55% of cases.
- The third cluster is recovered exactly in 0.31% of cases.
- The first and second clusters are both recovered exactly in 8.38% of cases. The first and third are recovered exactly in 0.2% of cases. The second and third are never both recovered exactly in the same simulation; neither are all three ever recovered exactly using this analysis.
- In *every* case that the first cluster is recovered, the second and third clusters are both partially recovered in that they are each produced in some larger subset of states on which the Markov chain displays clustering behaviour. In 96.47% of these cases where the second cluster is not recovered, the second cluster is produced by this algorithm, along with some states from the third cluster, as an index set of states on which the Markov chain displays clustering behaviour, in a similar manner as discussed in Example 5.4.1. This occurs with the third cluster in only 3 cases out of a total of 9103.

We note that in the extreme majority of these examples, the first constructed cluster is recovered exactly, and the second and third are often grouped together as a single cluster. We expect that this is an artefact of the particular 3×3 matrix used to produce these examples. In particular, the spectral radii of the submatrices corresponding to the first, second and third clusters are $1 - \frac{s}{6}$, $1 - \frac{5s}{6}$, and $1 - s$, respectively. Hence it is

not unexpected that the first cluster is recovered more frequently, as by this measure alone it represents a 'stronger' or 'tighter' cluster than the others.

As a final remark, we observe that once this tightest cluster is determined, we could use a 'divide-and-conquer' approach and consider a principal submatrix with the rows and columns corresponding to this cluster removed. Renormalising the rows of this matrix (in some appropriate manner) will produce a stochastic transition matrix which represents a parallel Markov chain acting only on the states of the second and third cluster. It is possible that we could then perform a similar analysis on this new matrix, if it had eigenvalues appropriately close to one, and there is a chance that we could recover the second and third clusters separately. There are several ways in which renormalisation could be performed, but the simplest is to scale each row so that it sums to 1.

To illustrate, we refer to Example 5.4.1, whose first cluster on the states $\{1, 2, \ldots, 32\}$ was recovered exactly. We consider the matrix $\hat{T}$ constructed as above by renormalising the principal submatrix obtained from T by deleting the first 32 rows and columns. This matrix has an eigenvalue equal to 0.9437. By considering the sign pattern of the associated eigenvector and applying Theorem 5.1.1, we conclude evidence of clustering behaviour on the states indexed by $\{33, 34, \ldots, 85\}$ and $\{86, 87, \ldots, 100\}$; that is, we recover both constructed clusters exactly.

Example 5.4.2. In this example, we apply Theorems 5.2.1 and 5.3.1 to the transition matrix for a simulated bus network discussed in [29] in which states represent bus stops in a network and transition probabilities are simulated probabilities of passengers moving from one stop to another through the bus network. In [29], the authors observed evidence of clustering behaviour based on the mean first passage matrix (shown in Fig. 5.2a) and observed that the eigenvector corresponding to the eigenvalue of second largest modulus (which was, in this case, complex) could be used to determine these

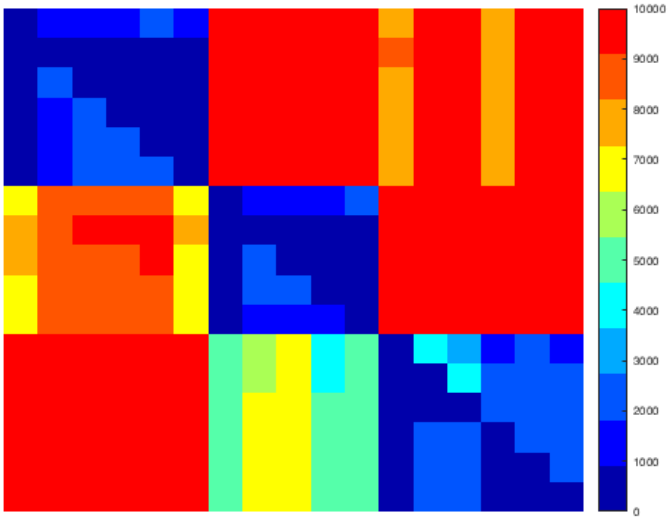
clusters. A plot of the entries of this vector is given in Fig. 5.2b in which it can clearly be seen that the entries are clustered, with clusters indexed by $\{1, 2, \ldots, 6\}$, $\{7, 8, \ldots, 11\}$, and $\{12, 13, \ldots, 17\}$, which are the subsets of states for which the mean first passage times seem to predict clustering.

The following tables summarize the findings of Theorems 5.2.1 and 5.3.1 with regard to this eigenvalue $\lambda = 0.9998 + 0.0001i$ and its corresponding eigenvector. With some examination of this information, one can recover all three clusters.

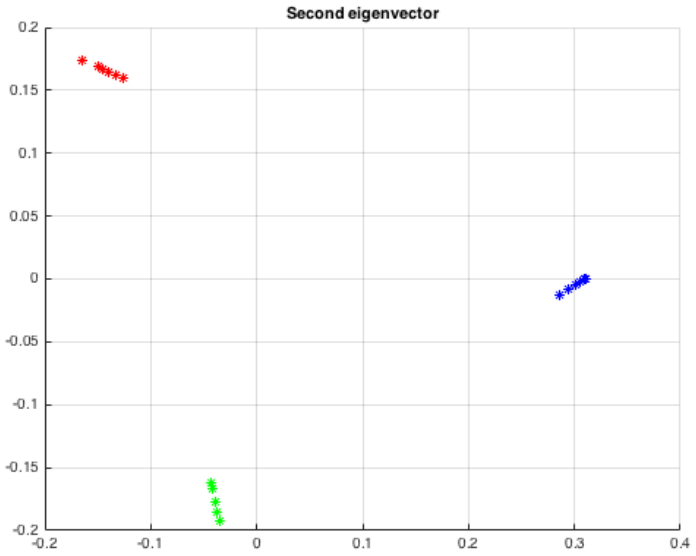
Thm 5.2.1	index set	spectral radius	lower bound
1(i)	$\{12, 13, \ldots, 17\}$	0.9998	0.9997
1(ii)	$\{12, 13, \ldots, 17\}$	0.9998[1]	0.9998[1]
1(iii)	$\{12, 13, \ldots, 17\}$	0.9998	0.9997
2(i)	$\{1, 2, \ldots, 11\}$	0.9999	0.9996
2(ii)	$\{1, 2, \ldots, 11\}$	0.9999	0.9996
2(iii)	$\{1, 2, \ldots, 11\}$	0.9999	0.9996

Thm 5.3.1	index set	spect. rad.	lower bound
1(i)	$\{7, 8, \ldots, 16\}$	0.9999	0.9997
1(ii)	$\{7, 8, \ldots, 17\}$	0.9999	0.9997
1(iii)	$\{7, 8, \ldots, 16\}$	0.9999	0.9996
2(i)	$\{1, 2, \ldots, 6\}$	0.9999[2]	0.9999[2]
2(ii)	$\{1, 2, \ldots, 6\}$	0.9999[3]	0.9999[3]
2(iii)	$\{1, 2, \ldots, 6, 17\}$	0.9999	0.9996

[1]The spectral radius and the lower bound in this case differ in the 10^{-6} position.
[2]The spectral radius and the lower bound in this case differ in the 10^{-5} position.
[3]The spectral radius and the lower bound in this case differ in the 10^{-5} position.



(a) Heat map of the mean first passage matrix for the transition matrix of the simulated bus network. Evidence of clustering behaviour is given by the relatively low (blue) values for mfp times between states in the same cluster, and high values for mfp times between clusters.



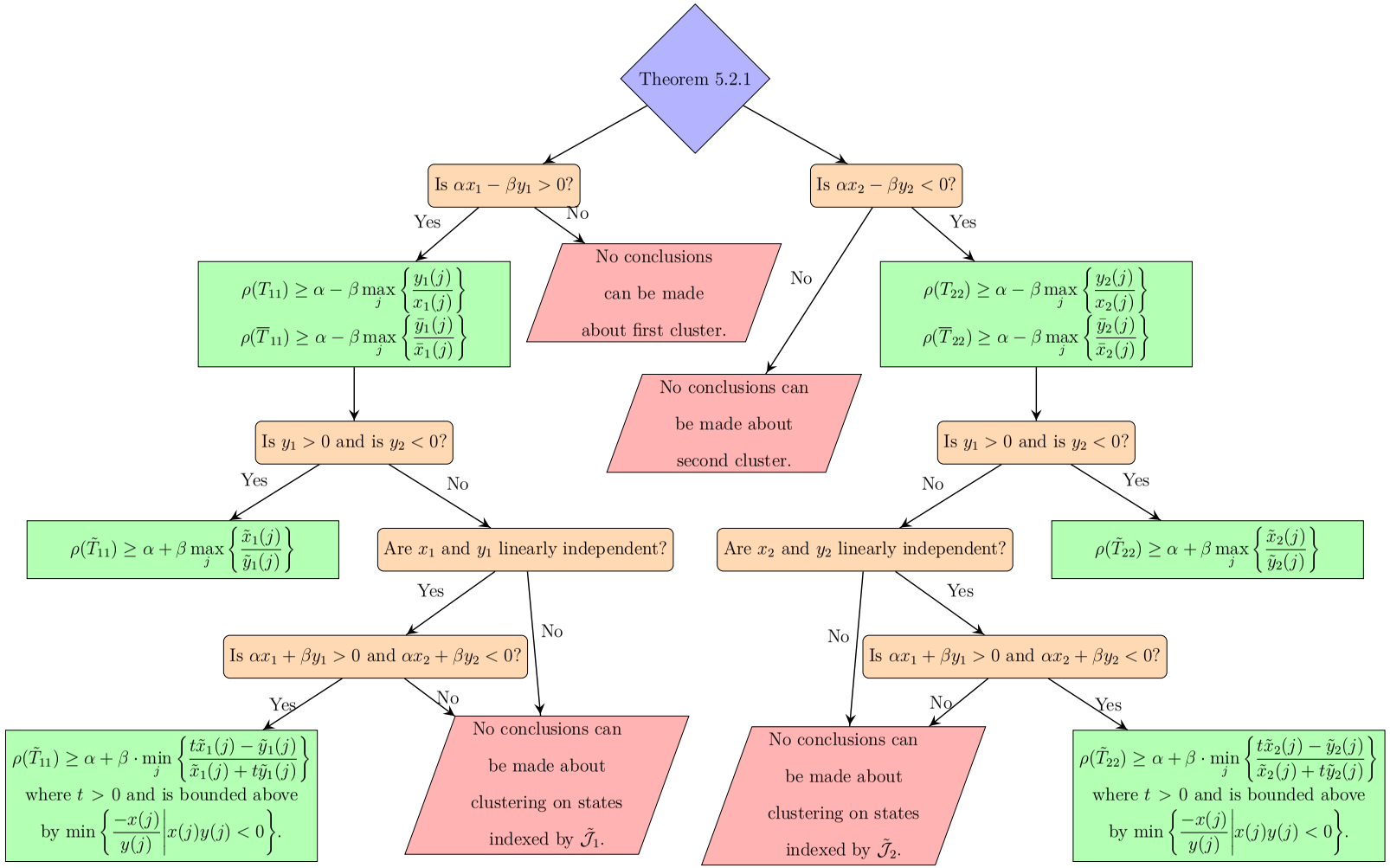
(b) Entries of the eigenvector corresponding to the eigenvalue of second-largest modulus

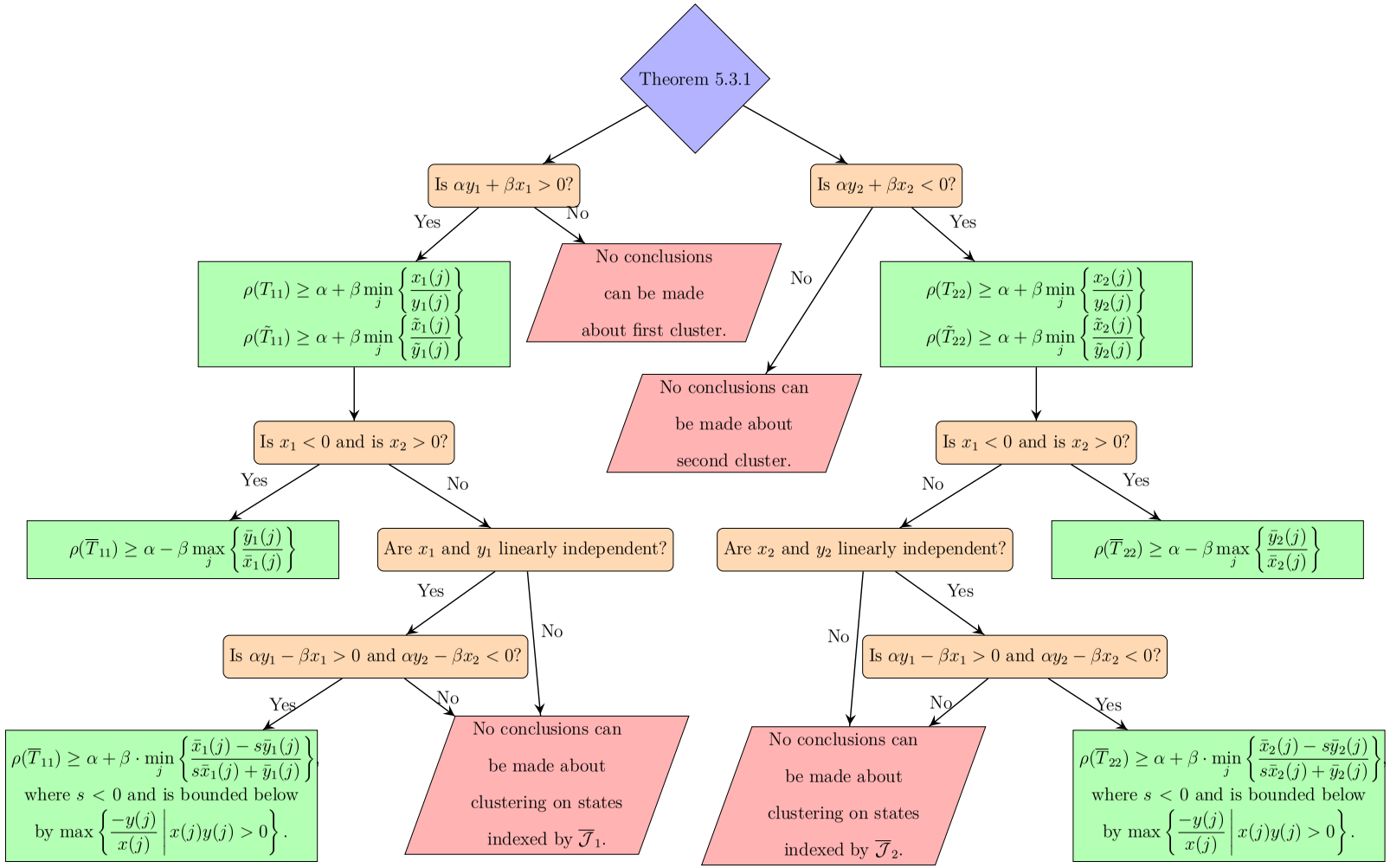
Figure 5.2: Evidence of clustering in the transition matrix for the bus network in [29], discussed in Example 5.4.2.

Remark 5.4.3. It is perhaps worth noting that the manifestation of clustering behaviour in a Markov chain does not depend at all on the combinatorial structure of the transition matrix, in that a dense matrix could display the same level of clustering behaviour as a sparse one. For this reason, the results of this chapter do not seem to fit with the general theme of the other chapters. However, this thesis seeks to determine the influence of a given directed graph, and we have determined a lack of influence in this case, regarding clustering properties of a Markov chain. In addition, we remark that these results are partially inspired by a classical result in combinatorial matrix theory by Fiedler. The eigenvalues of the *Laplacian matrix* of an undirected graph may be used to determine clustering behaviour – in particular, the second smallest eigenvalue is referred to as the *algebraic connectivity* of the graph, and the corresponding eigenvector contains some structural information about the graph (see [30, 31]). Furthermore, there are similar results for the *normalised Laplacian* $\mathcal{L}$ of a graph $\mathcal{G}$ (see [10] for a recent survey). The normalised Laplacian is more closely connected with finite Markov chains, in that the eigenvalues of the normalised Laplacian are related to the eigenvalues of the probability transition matrix $T_{\mathcal{G}}$ of the *random walk* on the graph $\mathcal{G}$. In particular, μ is an eigenvalue of $\mathcal{L}$ if and only if $1 - \mu$ is an eigenvalue of $T_{\mathcal{G}}$.

Flowcharts for Theorem 5.2.1 and Theorem 5.3.1

On the next two pages, we provide flowcharts for each of Theorem 5.2.1 and Theorem 5.3.1 that clearly display the dependencies of the lower bounds on the technical hypotheses.


Theorem 5.2.1
Is $\alpha x_1 - \beta y_1 > 0$?
Is $\alpha x_2 - \beta y_2 < 0$?
Yes
No
No
Yes
No conclusions can be made about first cluster.
$\rho(T_{11}) \geq \alpha - \beta \max_j \left\{ \frac{y_1(j)}{x_1(j)} \right\}$
$\rho(\overline{T}_{11}) \geq \alpha - \beta \max_j \left\{ \frac{\bar{y}_1(j)}{\bar{x}_1(j)} \right\}$
No conclusions can be made about second cluster.
$\rho(T_{22}) \geq \alpha - \beta \max_j \left\{ \frac{y_2(j)}{x_2(j)} \right\}$
$\rho(\overline{T}_{22}) \geq \alpha - \beta \max_j \left\{ \frac{\bar{y}_2(j)}{\bar{x}_2(j)} \right\}$
Is $y_1 > 0$ and is $y_2 < 0$?
Is $y_1 > 0$ and is $y_2 < 0$?
Yes
No
No
Yes
$\rho(\tilde{T}_{11}) \geq \alpha + \beta \max_j \left\{ \frac{\tilde{x}_1(j)}{\tilde{y}_1(j)} \right\}$
Are x_1 and y_1 linearly independent?
Are x_2 and y_2 linearly independent?
$\rho(\tilde{T}_{22}) \geq \alpha + \beta \max_j \left\{ \frac{\tilde{x}_2(j)}{\tilde{y}_2(j)} \right\}$
Yes
No
No
Yes
Is $\alpha x_1 + \beta y_1 > 0$ and $\alpha x_2 + \beta y_2 < 0$?
Is $\alpha x_1 + \beta y_1 > 0$ and $\alpha x_2 + \beta y_2 < 0$?
Yes
No
No
Yes
$\rho(\tilde{T}_{11}) \geq \alpha + \beta \cdot \min_j \left\{ \frac{t\tilde{x}_1(j) - \tilde{y}_1(j)}{\tilde{x}_1(j) + t\tilde{y}_1(j)} \right\}$
where $t > 0$ and is bounded above by $\min \left\{ \frac{-x(j)}{y(j)} \middle| x(j)y(j) < 0 \right\}$.
No conclusions can be made about clustering on states indexed by $\tilde{\mathcal{J}}_1$.
No conclusions can be made about clustering on states indexed by $\tilde{\mathcal{J}}_2$.
$\rho(\tilde{T}_{22}) \geq \alpha + \beta \cdot \min_j \left\{ \frac{t\tilde{x}_2(j) - \tilde{y}_2(j)}{\tilde{x}_2(j) + t\tilde{y}_2(j)} \right\}$
where $t > 0$ and is bounded above by $\min \left\{ \frac{-x(j)}{y(j)} \middle| x(j)y(j) < 0 \right\}$.


Theorem 5.3.1
Is $\alpha y_1 + \beta x_1 > 0$?
Is $\alpha y_2 + \beta x_2 < 0$?
Yes
No
No
Yes
No conclusions can be made about first cluster.
$\rho(T_{11}) \geq \alpha + \beta \min_j \left\{ \frac{x_1(j)}{y_1(j)} \right\}$
$\rho(\tilde{T}_{11}) \geq \alpha + \beta \min_j \left\{ \frac{\tilde{x}_1(j)}{\tilde{y}_1(j)} \right\}$
No conclusions can be made about second cluster.
$\rho(T_{22}) \geq \alpha + \beta \min_j \left\{ \frac{x_2(j)}{y_2(j)} \right\}$
$\rho(\tilde{T}_{22}) \geq \alpha + \beta \min_j \left\{ \frac{\tilde{x}_2(j)}{\tilde{y}_2(j)} \right\}$
Is $x_1 < 0$ and is $x_2 > 0$?
Is $x_1 < 0$ and is $x_2 > 0$?
Yes
No
No
Yes
$\rho(\overline{T}_{11}) \geq \alpha - \beta \max_j \left\{ \frac{\bar{y}_1(j)}{\bar{x}_1(j)} \right\}$
Are x_1 and y_1 linearly independent?
Are x_2 and y_2 linearly independent?
$\rho(\overline{T}_{22}) \geq \alpha - \beta \max_j \left\{ \frac{\bar{y}_2(j)}{\bar{x}_2(j)} \right\}$
Yes
No
Yes
No
Is $\alpha y_1 - \beta x_1 > 0$ and $\alpha y_2 - \beta x_2 < 0$?
Is $\alpha y_1 - \beta x_1 > 0$ and $\alpha y_2 - \beta x_2 < 0$?
Yes
No
No
Yes
$\rho(\overline{T}_{11}) \geq \alpha + \beta \cdot \min_j \left\{ \frac{\bar{x}_1(j) - s\bar{y}_1(j)}{s\bar{x}_1(j) + \bar{y}_1(j)} \right\}$, where $s < 0$ and is bounded below by $\max \left\{ \frac{-y(j)}{x(j)} \,\middle|\, x(j)y(j) > 0 \right\}$.
No conclusions can be made about clustering on states indexed by $\overline{\mathcal{J}}_1$.
No conclusions can be made about clustering on states indexed by $\overline{\mathcal{J}}_2$.
$\rho(\overline{T}_{22}) \geq \alpha + \beta \cdot \min_j \left\{ \frac{\bar{x}_2(j) - s\bar{y}_2(j)}{s\bar{x}_2(j) + \bar{y}_2(j)} \right\}$, where $s < 0$ and is bounded below by $\max \left\{ \frac{-y(j)}{x(j)} \,\middle|\, x(j)y(j) > 0 \right\}$.

Chapter 6

Perturbation analysis of Kemeny's constant

Kemeny's constant is an extremely useful measure of how well-connected the states of a Markov chain are. While we have seen in the previous two chapters that the mean first passage times can be used to determine how well-connected two distinct states are, Kemeny's constant gives a better measure of the average performance of the whole Markov chain in terms of the length of a trip between a randomly-chosen initial state and a randomly-chosen destination state. Note that the probability distribution with which the states are chosen is given by the stationary distribution vector, and so 'important' states in the chain are weighted more highly. This means that Kemeny's constant can, for instance, distinguish between the two types of examples with large mean first passage times that we have briefly discussed in the introductions of the last two chapters. In Example 4.1.5, Kemeny's constant will be relatively small, and the chain is still considered to be well-connected, but in the example in (5.1) at the beginning of the previous chapter, Kemeny's constant will certainly be large, indicating the presence of clustering.

As discussed in Section 2.8, there are many applications of Markov chains to real dynamical systems, including urban road network dynamics (see [20]), molecular conformation dynamics (see [24]), and the spread of infectious disease (see [1]). In each of these, Kemeny's constant is a valuable measure: in urban road networks, the value of $\mathcal{K}(T)$ provides insight into how well-connected the urban area is; in molecular conformational dynamics, the value of $\mathcal{K}(T)$ could indicated the presence or absence of metastable sets (which is extremely useful in computational drug design); in an infectious disease setting, $\mathcal{K}(T)$ provides a measure of how quickly epidemic levels are approached.

Given the utility of Kemeny's constant in practical applications, it is worthwhile to consider how sensitive it is to perturbations in the transition probabilities. For those modeling with Markov chains using real data, the transition probabilities derived from these data are usually only sample estimates, and not true values. The transition matrix of this model can then be viewed as a perturbation of the 'true' transition matrix, and answering the question of how sensitive the calculation of $\mathcal{K}(T)$ is to errors in the data gives a measure of confidence in the computed value for Kemeny's constant.

Furthermore, there have been surprising insights into the behaviour of Kemeny's constant when a transition in the chain is removed entirely. In [61], the authors considered the random walk on an undirected graph, and the value of Kemeny's constant for this Markov chain. A family of undirected graphs was found for which almost every member of the family had a *Braess edge*; that is, an edge which could be added into the graph that would *increase* Kemeny's constant—that is, reduce the connectedness of the Markov chain, as measured by Kemeny's constant. The name comes from *Braess' paradox*, which is a well-known phenomenon in urban traffic modelling, and refers to the idea that in practice, closing a major road in a network can sometimes decrease

average travel times. For this reason, and in keeping with the theme of this thesis, we are particularly interested in the structure of the matrices for which Kemeny's constant behaves erratically under perturbation.

In this chapter, we develop a structured condition number for Kemeny's constant, and determine some bounds which provide some insight into the transition matrices for which Kemeny's constant is poorly-conditioned. We also explore the value of this structured condition number for some infinite families of matrices. The results of this chapter are original to this thesis.

6.1 Introduction to conditioning problems in Markov chain theory

Suppose T is an irreducible stochastic matrix representing a Markov chain, with stationary vector w. Then suppose that T is perturbed to form some new irreducible stochastic matrix $\tilde{T}$, with stationary vector $\tilde{w}$. How different can w and $\tilde{w}$ be, relative to the magnitude of the perturbation? An answer to this question determines how sensitive the long-term behaviour of a system modelled by a Markov chain can be to small changes in the transition probabilities.

The above problem is referred to as *conditioning* of the stationary vector, and is formalised as follows: Given T, an irreducible stochastic matrix with stationary vector w, we wish to determine some function $f(T)$, such that if $\tilde{T} = T + E$ is also irreducible, nonnegative and stochastic with stationary vector $\tilde{w}$, then for some appropriate p, q,

$$\|w - \tilde{w}\|_p \leq \|E\|_q \cdot f(T). \tag{6.1}$$

This function $f(T)$ is referred to as a *condition number*. The norms we will most

frequently discuss are the ∞-norm and the 1-norm. We recall that for any real $n \times n$ matrix A,

$$\|A\|_\infty = \max_{i=1,\ldots,n} \sum_{j=1}^{n} |a_{i,j}|,$$

and

$$\|A\|_1 = \max_{j=1,\ldots,n} \sum_{i=1}^{n} |a_{i,j}|,$$

so that $\|A^\top\|_1 = \|A\|_\infty$. The matrix norm $\|\cdot\|_\infty$ is sometimes referred to as the *absolute row sum norm*. For more on vector and matrix norms, see [41, Chapter 5].

The group inverse of $I - T$ is valuable in answering questions regarding the conditioning of the stationary vector due to the following argument.

Given T, w, $\tilde{T}$ and $\tilde{w}$ as above (so that $\tilde{T} = T + E$), from the eigenequation $\tilde{w}^\top \tilde{T} = \tilde{w}^\top$, it follows that $\tilde{w}^\top(T+E) = \tilde{w}^\top$, and so $\tilde{w}^\top E = \tilde{w}^\top(I-T)$. Multiplying on the right by $Q^\# = (I-T)^\#$, we have $\tilde{w}^\top E Q^\# = \tilde{w}^\top Q Q^\#$. Since $I - QQ^\#$ is the eigenprojection of Q onto the eigenspace corresponding to the eigenvalue 0, $QQ^\# = I - \mathbb{1}w^\top$ (from Theorem 2.5.2 (e).) Hence

$$\tilde{w}^\top E Q^\# = \tilde{w}^\top(I - \mathbb{1}w^\top) = \tilde{w}^\top - w^\top.$$

It is from this relationship that many condition numbers of the type in (6.1) are derived; hence this $f(T)$ is frequently some function of the entries of the group inverse $(I-T)^\#$.

Originally, Schweitzer approached this problem using the fundamental matrix of the chain, $Z = (I - T + \mathbb{1}w^\top)^{-1}$, and showed in [73] that

$$\|\tilde{w} - w\|_1 \leq \|Z\|_\infty \|E\|_\infty.$$

This was followed by Meyer in [69], who instead used the group inverse $Q^\#$ and showed

that

$$\|\tilde{w} - w\|_1 \leq \|Q^{\#}\|_\infty \|E\|_\infty.$$

Succeeding these are a long list of improvements to and variations of these condition numbers, along with new approaches to analysing the sensitivity of the stationary vector by determining bounds on the condition numbers in terms of the eigenvalues of the matrix (see [67]) and the mean first passage times (see [17]), as well as determining the sensitivity of a single entry of the stationary distribution vector (see [49]). A survey is given in [18], and we also refer the reader to further work since then in [56, 49].

We now give two examples of condition numbers on the stationary vector.

Let T be an irreducible stochastic matrix, and let $Q = I - T$. Define

$$\mathfrak{c}_1(T) := \frac{1}{2} \max_{1 \leq i,j \leq n} \sum_{k=1}^{n} |q^{\#}_{i,k} - q^{\#}_{j,k}|, \tag{6.2}$$

and

$$\mathfrak{c}_2(T) := \frac{1}{2} \max_{1 \leq i,j \leq n} (q^{\#}_{j,j} - q^{\#}_{i,j}). \tag{6.3}$$

Both $\mathfrak{c}_1(T)$ and $\mathfrak{c}_2(T)$ act as condition numbers, proven by Seneta (see [75]) and by Haviv and Van der Heyden (see [39]), respectively. In particular:

Theorem 6.1.1 ([39, 75])**.** *Let T be an irreducible stochastic matrix with stationary vector w, and let $\tilde{T} = T + E$ also be an irreducible stochastic matrix for some matrix E, with stationary vector $\tilde{w}$. Then:*

(a)

$$\|\tilde{w} - w\|_1 \leq \|E\|_\infty \mathfrak{c}_1(T).$$

(b)

$$\|\tilde{w} - w\|_\infty \leq \|E\|_\infty \mathfrak{c}_2(T).$$

Note that $\mathfrak{c}_1(T)$ is also a special case of the *coefficient of ergodicity* of the group inverse $Q^{\#}$ (see [74, 75]), and is sometimes denoted as $\tau(Q^{\#})$.

The body of work on perturbation analysis and condition numbers for stationary distribution vectors has grown and developed since the 1960s. At this point there has been extensive research on the conditioning properties of the stationary vector, and the field is well-established. In this chapter, we begin the development of a body of work on perturbation analysis and condition numbers for Kemeny's constant. That is, we wish to tackle the question of how sensitive Kemeny's constant is to perturbations or errors in the transition probabilities of the Markov chain, for a given transition matrix T. More formally, given an irreducible stochastic matrix T and perturbing matrix E (such that $T+E$ is also stochastic and irreducible), can we determine an upper bound for $|\mathcal{K}(T+E)-\mathcal{K}(T)|$ in terms of $\|E\|$ (for some choice of norm $\|\cdot\|$) and some function of T? In the following sections we will prove some preliminary results to this end, and determine a *structured condition number* for $\mathcal{K}(T)$—that is, a condition number under the restriction that the size of the perturbation is small.

Remark 6.1.2. Note that in [75], it is shown that for an irreducible stochastic matrix T of order n, with eigenvalues $1, \lambda_2, \ldots, \lambda_n$,

$$\mathfrak{c}_1(T) \leq \sum_{j=2}^{n} \frac{1}{1-\lambda_j},$$

i.e. $\mathfrak{c}_1(T) \leq \mathcal{K}(T)$. Therefore

$$\|\tilde{w} - w\|_1 \leq \|E\|_\infty \mathcal{K}(T)$$

so that Kemeny's constant is itself a condition number for the stationary distribution of the chain.

6.2 A structured condition number for Kemeny's constant

Throughout this section, T is considered to be a nonnegative stochastic matrix of order n with 1 as an algebraically simple eigenvalue, and w denotes the stationary vector of T. Let E denote some perturbation matrix of T; that is, E is an $n \times n$ matrix whose rows sum to zero, such that $\tilde{T} = T + E$ is also nonnegative and stochastic, with 1 as an algebraically simple eigenvalue. Let $Q = I - T$, and $\tilde{Q} = I - \tilde{T}$.

In [69], the following is proven to give an expression for $\tilde{Q}^{\#}$ in terms of $Q^{\#}$ and E.

Theorem 6.2.1 ([69]). *Let T, E, $\tilde{T}$, w, Q, and $\tilde{Q}$ be defined as above. Then $I - EQ^{\#}$ is invertible, and*

$$\tilde{Q}^{\#} = Q^{\#}(I - EQ^{\#})^{-1} - \mathbb{1}w^{\top}(I - EQ^{\#})^{-1}Q^{\#}(I - EQ^{\#})^{-1}.$$

We now use this perturbation formula to derive an expression for $\mathcal{K}(T + E)$.

Lemma 6.2.2. *Let T, E, $\tilde{T}$, Q, $\tilde{Q}$ be defined as above. If $\rho(EQ^{\#}) < 1$, then*

$$\mathcal{K}(\tilde{T}) = \mathcal{K}(T) + \sum_{j=1}^{\infty} \text{trace}\left(Q^{\#}(EQ^{\#})^{j}\right).$$

Proof. Recall that $\mathcal{K}(T) = \text{trace}(I - T)^{\#}$. Hence from Theorem 6.2.1,

$$\begin{aligned} \mathcal{K}(T + E) &= \text{trace}(\tilde{Q}^{\#}) \\ &= \text{trace}(Q^{\#}(I - EQ^{\#})^{-1}) - \text{trace}(\mathbb{1}w^{\top}(I - EQ^{\#})^{-1}Q^{\#}(I - EQ^{\#})^{-1}). \end{aligned}$$

Then since the trace of any rank-one matrix $uv^{\top}$ is $v^{\top}u$,

$$\text{trace}(\mathbb{1}w^{\top}(I - EQ^{\#})^{-1}Q^{\#}(I - EQ^{\#})^{-1}) = w^{\top}(I - EQ^{\#})^{-1}Q^{\#}(I - EQ^{\#})^{-1}\mathbb{1}.$$

Now, $I - EQ^{\#}$ is invertible, and if $\rho(EQ^{\#}) < 1$, then

$$(I - EQ^{\#})^{-1} = I + EQ^{\#} + (EQ^{\#})^2 + (EQ^{\#})^3 + \cdots$$

and $(I - EQ^{\#})^{-1}\mathbb{1} = \mathbb{1}$. Further,

$$\text{trace}(\mathbb{1}w^{\top}(I - EQ^{\#})^{-1}Q^{\#}(I - EQ^{\#})^{-1}) = 0,$$

since $Q^{\#}\mathbb{1} = 0$. So

$$\begin{aligned}
\mathcal{K}(\tilde{T}) &= \text{trace}(\tilde{Q}^{\#}) \\
&= \text{trace}(Q^{\#}(I - EQ^{\#})^{-1}) \\
&= \text{trace}(Q^{\#} + Q^{\#}EQ^{\#} + Q^{\#}(EQ^{\#})^2 + \cdots) \\
&= \text{trace}(Q^{\#}) + \sum_{j=1}^{\infty} \text{trace}(Q^{\#}(EQ^{\#})^j) \\
&= \mathcal{K}(T) + \sum_{j=1}^{\infty} \text{trace}(Q^{\#}(EQ^{\#})^j).
\end{aligned}$$

□

Remark 6.2.3. It is well-known (see [41, Theorem 5.6.9]) that for any matrix norm $\|\cdot\|$ and $n \times n$ matrix A,

$$\rho(A) \leq \|A\|.$$

That is, given any matrix norm $\|\cdot\|$, it is a sufficient condition for Lemma 6.2.2 that $\|EQ^{\#}\| < 1$. Consequently, by the submultiplicativity of matrix norms, it is hence sufficient that $\|E\| < \frac{1}{\|Q^{\#}\|}$. Thus for any matrix norm, if $\|E\|$ is sufficiently small, the expression for $\mathcal{K}(\tilde{T})$ given in the result above will hold. We will typically use the absolute row sum norm $\|\cdot\|_{\infty}$.

Definition 6.2.4. Let T be an irreducible stochastic matrix. The *structured condition number for Kemeny's constant* is defined as

$$\mathcal{C}(T) := \limsup_{\varepsilon \to 0} \left\{ \frac{|\mathcal{K}(T+E) - \mathcal{K}(T)|}{\varepsilon} \,\middle|\, T+E \text{ irreducible and stochastic, } \|E\|_\infty \leq \varepsilon \right\}.$$

The structured condition number for $\mathcal{K}(T)$ may be interpreted as a measure of the maximum change in $\mathcal{K}(T)$ when T undergoes some perturbation, where it is assumed that the norm of the perturbing matrix is vanishingly small. This lends itself more to the application of considering numerical errors in a computational setting, with $\mathcal{C}(T)$ interpreted in terms of how robust the calculation of $\mathcal{K}(T)$ is. Analogous work has been done with conditioning of the stationary distribution (see [40]).

Theorem 6.2.5. *Let T be an irreducible stochastic $n \times n$ matrix; let $Q = I - T$; and let $q_{i,j}^{\#(2)}$ denote the (i,j) entry of $(Q^\#)^2$. Then*

$$\mathcal{C}(T) \;=\; \frac{1}{2} \sum_{j=1}^{n} \max \left\{ \max_i \{q_{i,j}^{\#(2)}\} - \alpha(j),\; \beta(j) - \min_i \{q_{i,j}^{\#(2)}\} \right\}, \tag{6.4}$$

where

$$\begin{aligned} \alpha(j) &:= \min_i \{q_{i,j}^{\#(2)} | t_{j,i} > 0\}; \\ \beta(j) &:= \max_i \{q_{i,j}^{\#(2)} | t_{j,i} > 0\}. \end{aligned}$$

Proof. Let T be an irreducible stochastic matrix of order n, and let E be a matrix of order n with zero row sums, such that $\tilde{T} = T + E$ is irreducible, nonnegative and stochastic, and $\|E\|_\infty \leq \varepsilon$. From Lemma 6.2.2, we have

$$\mathcal{K}(\tilde{T}) - \mathcal{K}(T) = \sum_{j=1}^{n} \operatorname{trace}(Q^\# (E Q^\#)^j).$$

We first concentrate our attention on $\mathrm{trace}(Q^{\#}EQ^{\#}) = \mathrm{trace}(E(Q^{\#})^2)$. Representing the rows of E by $u_i^\top$, $i = 1, \ldots, n$, and letting e_j denote the j^{th} standard basis vector, we can write

$$\mathrm{trace}(E(Q^{\#})) = \sum_{j=1}^{n} u_j^\top (Q^{\#})^2 e_j.$$

For every j, $u_j = e_j^\top E$ can be written as $x^\top - y^\top$, where x and y are nonnegative vectors, and $x^\top \mathbb{1} = y^\top \mathbb{1} \leq \frac{\varepsilon}{2}$. Note that if $y_i > 0$, then $t_{j,i} > 0$, since $T + E$ is nonnegative.

Fixing j, we have

$$\begin{aligned} u_j^\top (Q^{\#})^2 e_j &= x^\top (Q^{\#})^2 e_j - y^\top (Q^{\#})^2 e_j \\ &= \sum_{l=1}^{n} x_l q_{l,j}^{\#(2)} - \sum_{l=1}^{n} y_l q_{l,j}^{\#(2)} \\ &\leq \sum_{l=1}^{n} x_l \cdot \max_l \{q_{l,j}^{\#(2)}\} - \sum_{l=1}^{n} y_l \cdot \alpha(j) \end{aligned}$$

where $\alpha(j) = \min_l \{q_{l,j}^{\#(2)} \mid t_{j,l} > 0\}$. Therefore

$$u_j^\top (Q^{\#})^2 e_j \leq \frac{\varepsilon}{2} \left(\max_l \{q_{l,j}^{\#(2)}\} - \alpha(j) \right). \tag{6.5}$$

Also consider that

$$\begin{aligned} u_j^\top (Q^{\#})^2 e_j &= \sum_{l=1}^{n} x_l q_{l,j}^{\#(2)} - \sum_{l=1}^{n} y_l q_{l,j}^{\#(2)} \\ &\geq \sum_{l=1}^{n} x_l \cdot \min_l \{q_{l,j}^{\#(2)}\} - \sum_{l=1}^{n} y_l \cdot \beta(j) \end{aligned}$$

where $\beta(j) = \max_l \{q_{l,j}^{\#(2)} \mid t_{j,l} > 0\}$. Therefore

$$u_j^\top (Q^{\#})^2 e_j \geq \frac{\varepsilon}{2} \left(\min_l \{q_{l,j}^{\#(2)}\} - \beta(j) \right). \tag{6.6}$$

Hence from (6.5) and (6.6),

$$|u_j^\top (Q^\#)^2 e_j| \leq \frac{\varepsilon}{2} \cdot \max\left\{\max_l\{q_{l,j}^{\#(2)}\} - \alpha(j), \beta(j) - \min_l\{q_{l,j}^{\#(2)}\}\right\},$$

and so

$$\begin{aligned} |\operatorname{trace}(Q^\# E Q^\#)| &\leq \sum_{j=1}^n |u_j^\top (Q^\#)^2 e_j| \\ &\leq \frac{\varepsilon}{2}\sum_{j=1}^n \max\left\{\max_i\{q_{i,j}^{\#(2)}\} - \alpha(j),\ \beta(j) - \min_i\{q_{i,j}^{\#(2)}\}\right\}. \quad (6.7) \end{aligned}$$

Finally, we conclude

$$\begin{aligned} \frac{|\mathcal{K}(\tilde{T}) - \mathcal{K}(T)|}{\varepsilon} &= \frac{1}{\varepsilon}\left|\operatorname{trace}(Q^\# E Q^\#) + \sum_{j=2}^n \operatorname{trace}(Q^\#(EQ^\#)^j)\right| \\ &\leq \frac{1}{2}\sum_{j=1}^n \max\left\{\max_i\{q_{i,j}^{\#(2)}\} - \alpha(j),\ \beta(j) - \min_i\{q_{i,j}^{\#(2)}\}\right\} + \mathcal{O}(\varepsilon), \end{aligned}$$

and hence as $\varepsilon \to 0$, the supremum is bounded above by

$$\frac{1}{2}\sum_{j=1}^n \max\left\{\max_i\{q_{i,j}^{\#(2)}\} - \alpha(j),\ \beta(j) - \min_i\{q_{i,j}^{\#(2)}\}\right\}. \quad (6.8)$$

To show that the supremum is in fact equal to (6.8), it suffices to show that for any matrix T, there is some matrix E for which this bound is achieved by $|\operatorname{trace}(Q^\# E Q^\#)|$. We will demonstrate how to choose the matrix E—in particular, the u_j—so that equality holds in the upper bound (6.7) on $|\operatorname{trace}(Q^\# E Q^\#)|$.

Fix j, and for conciseness, let $\mathfrak{a}_j = \max_i\{q_{i,j}^{\#(2)}\} - \alpha(j)$, and $\mathfrak{b}_j = \beta(j) - \min_i\{q_{i,j}^{\#(2)}\}$.

Let r_1 be the index such that

$$q^{\#(2)}_{r_1,j} = \alpha(j) = \min_l\{q^{\#(2)}_{l,j} \mid t_{j,l} > 0\},$$

and r_2 be the index such that

$$q^{\#(2)}_{r_2,j} = \beta(j) = \max_l\{q^{\#(2)}_{l,j} \mid t_{j,l} > 0\}.$$

Let s_1 be the index such that

$$q^{\#(2)}_{s_1,j} = \max_l\{q^{\#(2)}_{l,j}\},$$

and s_2 be the index such that

$$q^{\#(2)}_{s_2,j} = \min_l\{q^{\#(2)}_{l,j}\}.$$

Then the row vector $u_j^\top = e_j^\top E$ is chosen as follows:

$$u_j^\top = \begin{cases} \frac{\varepsilon}{2}(e_{s_1}^\top - e_{r_1}^\top) & \text{if } \max\{\mathfrak{a}_j, \mathfrak{b}_j\} = \mathfrak{a}_j; \\ \\ \frac{\varepsilon}{2}(e_{s_2}^\top - e_{r_2}^\top) & \text{if } \max\{\mathfrak{a}_j, \mathfrak{b}_j\} = \mathfrak{b}_j. \end{cases}$$

Then

$$u_j^\top (Q^\#)^2 e_j = |u_j^\top (Q^\#)^2 e_j| = \max\{\mathfrak{a}_j, \mathfrak{b}_j\}.$$

Choosing in this way for each j, we have $E = \sum_{j=1}^n u_j e_j^\top$, with $\|E\|_\infty = \varepsilon$, and with

$$|\operatorname{trace}(Q^\# E Q^\#)| = \frac{\varepsilon}{2}\sum_{j=1}^n \max\left\{\max_i\{q^{\#(2)}_{i,j}\} - \alpha(j),\ \beta(j) - \min_i\{q^{\#(2)}_{i,j}\}\right\}.$$

Furthermore the (i,j) entry of E is negative only if $t_{i,j} > 0$; hence $T + E$ is nonnegative (for appropriate ε). $\square$

We present the following example to illustrate the distinction between a condition number and a structured condition number and why it is important to keep in mind that the structured condition number only provides information of value when it is assumed that the norm of the perturbing matrix is small.

Example 6.2.6. Consider the 2×2 stochastic matrix

$$T = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

which has $\mathcal{K}(T) = \frac{1}{2}$. Furthermore,

$$Q^{\#} = \begin{bmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{1}{4} \end{bmatrix} \quad \text{and} \quad (Q^{\#})^2 = \begin{bmatrix} \frac{1}{8} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{1}{8} \end{bmatrix}.$$

Hence $\mathcal{C}(T)$ can be calculated to be $\frac{1}{4}$.

Now consider the perturbing matrix

$$E = \begin{bmatrix} a & -a \\ -a & a \end{bmatrix},$$

for $0 < a < 1$ so that $\|E\|_\infty = 2a$ and

$$\tilde{T} = T + E = \begin{bmatrix} a & 1-a \\ 1-a & a \end{bmatrix}$$

which is a stochastic matrix with eigenvalues $1, 2a-1$. Hence $\mathcal{K}(\tilde{T}) = \frac{1}{2-2a}$, and

$$\begin{aligned} |\mathcal{K}(\tilde{T}) - \mathcal{K}(T)| &= \frac{a}{2-2a} \\ &= \frac{\|E\|_\infty}{4-4a} \\ &> \frac{1}{4}\|E\|_\infty = \mathcal{C}(T)\|E\|_\infty. \end{aligned}$$

In fact, as $a \to 1$, the associated Markov chain with transition matrix $\tilde{T}$ approaches a chain which is completely decoupled, and so $\mathcal{K}(\tilde{T}) \to \infty$.

While the expression of $\mathcal{C}(T)$ in Theorem 6.2.5 is accurate, it is a complex expression and provides little insight into the nature of Kemeny's constant and how it acts under perturbation of the transition probabilities. We provide below an upper bound which does supply some insight, after the following technical lemma, of which a proof may be found in [52, Lemma 5.3.4].

Lemma 6.2.7. *Let v be a vector in $\mathbb{R}^n$ such that $v^\top \mathbb{1} = 0$.*

(a) Suppose that A is an $n \times n$ matrix with complex entries. Then

$$\|A^\top v\|_1 \leq \|v\|_1 \cdot \tfrac{1}{2} \max_{i,j} \sum_{k=1}^{n} |a_{i,k} - a_{j,k}|.$$

(b) Suppose that $z \in \mathbb{C}^n$. Then

$$|v^\top z| \leq \|v\|_1 \cdot \max_{i,j} \frac{|z_i - z_j|}{2}.$$

Theorem 6.2.8.

$$\mathcal{C}(T) \leq n \cdot \mathfrak{c}_1(T) \cdot \mathfrak{c}_2(T). \tag{6.9}$$

Proof. Let T be an irreducible stochastic matrix of order n, and let E be a matrix with

zero row sums such that $\tilde{T} = T + E$ is also irreducible and stochastic. We consider

$$\text{trace}(Q^{\#}EQ^{\#}) = \text{trace}(E(Q^{\#})^2) = \sum_{i=1}^{n} e_i^{\top} E(Q^{\#})^2 e_i.$$

For any i, we have from Lemma 6.2.7(b):

$$\begin{aligned} |e_i^{\top} E(Q^{\#})^2 e_i| &\leq \|e_i^{\top} EQ^{\#}\|_1 \cdot \max_{j,k} \left(\frac{q_{j,i}^{\#} - q_{k,i}^{\#}}{2} \right) \\ &= \tfrac{1}{2} \|e_i^{\top} EQ^{\#}\|_1 \cdot \max_{k} (q_{i,i}^{\#} - q_{k,i}^{\#}), \end{aligned}$$

since $q_{i,i}^{\#} > q_{j,i}^{\#}$, for all i, and $j \neq i$.

Next, consider that

$$\begin{aligned} \|e_i^{\top} EQ^{\#}\|_1 &= \|(Q^{\#})^{\top} E^{\top} e_i\|_1 \\ &\leq \|E^{\top} e_i\|_1 \cdot \tfrac{1}{2} \max_{i,j} \sum_{k=1}^{n} |q_{i,k}^{\#} - q_{j,k}^{\#}| \quad \text{(by Lemma 6.2.7(a))} \\ &= \|e_i^{\top} E\|_1 \mathfrak{c}_1(T). \end{aligned}$$

Hence

$$|e_i^{\top} E(Q^{\#})^2 e_i| \leq \tfrac{1}{2} \|e_i^{\top} E\|_1 \mathfrak{c}_1(T) \max_{k} (q_{i,i}^{\#} - q_{k,i}^{\#}).$$

Finally, we have

$$\begin{aligned}
|\operatorname{trace}(E(Q^{\#})^2)| &= \left|\sum_{i=1}^{n} e_i^\top E(Q^{\#})^2 e_i\right| \\
&\leq \sum_{i=1}^{n} |e_i^\top E(Q^{\#})^2 e_i| \\
&\leq \tfrac{1}{2}\sum_{i=1}^{n} \|e_i^\top E\|_1 \mathfrak{c}_1(T) \max_k (q_{i,i}^{\#} - q_{k,i}^{\#}) \\
&\leq \tfrac{1}{2}\|E\|_\infty \mathfrak{c}_1(T) \sum_{i=1}^{n} \max_k (q_{i,i}^{\#} - q_{k,i}^{\#}) \\
&\leq \tfrac{1}{2}\|E\|_\infty \mathfrak{c}_1(T) \cdot n \max_{i,k} (q_{i,i}^{\#} - q_{k,i}^{\#}) \\
&= n\|E\|_\infty \mathfrak{c}_1(T)\mathfrak{c}_2(T) \qquad \text{(from (6.3))}.
\end{aligned}$$

It follows that $\mathcal{C}(T) \leq n \cdot \mathfrak{c}_1(T)\mathfrak{c}_2(T)$. □

Remark 6.2.9. Since we have observed in Remark 6.1.2 that $\mathfrak{c}_1(T) \leq \mathcal{K}(T)$ this means that

$$\mathcal{C}(T) \leq n \cdot \mathcal{K}(T)\mathfrak{c}_2(T).$$

This furnishes another relative bound, where both the original size of Kemeny's constant and the size of the perturbation are taken into account. That is,

$$\limsup_{\varepsilon \to 0} \left\{ \frac{|\mathcal{K}(T+E) - \mathcal{K}(T)|}{\varepsilon \cdot \mathcal{K}(T)} \,\middle|\, T + E \text{ irreducible and stochastic, } \|E\|_\infty \leq \varepsilon \right\} \leq n \cdot \mathfrak{c}_2(T).$$

6.3 Examples

In this section, we investigate the structured condition number $\mathcal{C}(T)$ for some infinite families of matrices. We also examine the upper bound of Theorem 6.2.8 and determine some families for which $\mathcal{C}(T)$ is on the same order of magnitude as this upper bound.

Example 6.3.1. Let $w = \begin{bmatrix} w_1 & w_2 & \cdots & w_n \end{bmatrix}^\top$ be any positive vector such that $\sum_i w_i =$

1, and form T as a convex combination of the identity matrix and the rank-one stochastic matrix $\mathbb{1}w^\top$; that is, for some $c \in [0,1]$,

$$T = cI + (1-c)\mathbb{1}w^\top.$$

Then letting $Q = I - T$, we have $Q = (1-c)(I - \mathbb{1}w^\top)$ and so

$$Q^\# = \frac{1}{1-c}(I - \mathbb{1}w^\top)$$

and

$$(Q^\#)^2 = \frac{1}{(1-c)^2}(I - \mathbb{1}w^\top).$$

Then it is easily calculated that

$$\begin{aligned} \mathcal{C}(T) &= \frac{1}{2}\sum_{j=1}^{n} \frac{1}{(1-c)^2} \\ &= \frac{n}{2(1-c)^2}. \end{aligned}$$

Meanwhile,

$$\mathfrak{c}_1(T) = \frac{1}{1-c}, \quad \text{and} \quad \mathfrak{c}_2(T) = \frac{1}{2(1-c)}.$$

Hence the upper bound (6.9) is $\frac{n}{2(1-c)^2}$, coinciding with the value of $\mathcal{C}(T)$.

Example 6.3.2. Consider the Markov chain whose transition matrix is the adjacency

matrix of the directed cycle

$$T = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

That is, we consider the random walk on the directed cycle on n vertices. To determine $\mathcal{C}(T)$, we require $(Q^{\#})^2$. In fact, we require the maximum and minimum entries of each column of $(Q^{\#})^2$, along with $\alpha(j)$ and $\beta(j)$, which in this example are both equal to $q^{\#(2)}_{j+1,j}$, for each $j = 1, \ldots, n-1$, and $\alpha(n) = \beta(n) = q^{\#(2)}_{1,n}$.

Since T is an example of a periodic Markov chain, there is an expression for the group inverse of $I - T$ (see [55]) which we can use, producing

$$Q^{\#} = \frac{1}{2n} \begin{bmatrix} n-1 & n-3 & n-5 & \cdots & -(n-3) & -(n-1) \\ -(n-1) & n-1 & n-3 & n-5 & \cdots & -(n-3) \\ -(n-3) & -(n-1) & n-1 & n-3 & \cdots & -(n-5) \\ & & & & & \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ & & & & & \\ n-3 & n-5 & \cdots & -(n-3) & -(n-1) & n-1 \end{bmatrix}.$$

Alternatively,

$$q^{\#}_{i,j} = \begin{cases} \frac{n-1}{2n} - \frac{j-i}{n}, & \text{if } i \leq j; \\ \frac{n-1}{2n} - \frac{n-j+i}{n}, & \text{if } i > j. \end{cases}$$

Since $Q^{\#}$ is a circulant matrix (that is, each row is a shift to the right of the one

preceding it), $(Q^{\#})^2$ will also be a circulant matrix. Hence every term in the sum indexed by j in (6.4) is equal, and it suffices to determine only the first term, and then multiply by $\frac{1}{2}n$; that is,

$$\mathcal{C}(T) = \frac{n}{2} \max\left\{ \max_i\{q_{i,1}^{\#(2)}\} - \alpha(1), \beta(1) - \min_i\{q_{i,1}^{\#(2)}\} \right\}.$$

Some tedious computation produces

$$q_{k,1}^{\#(2)} = \frac{1}{4n^2}\left(-\frac{1}{3}n^3 + (2k-4)n^2 - \frac{23}{3}n + (8k-2k^2)n \right),$$

and it is not difficult to show that

$$\min_k q_{k,1}^{\#(2)} = q_{n,1}^{\#(2)} = -\frac{n^2-1}{12n},$$

while

$$\max_k q_{k,1}^{\#(2)} = \begin{cases} q_{\frac{n+4}{2},1}^{\#(2)} = \dfrac{n^2+2}{24n} & \text{if } n \text{ is even;} \\ \\ q_{\frac{n+5}{2},1}^{\#(2)} = \dfrac{n^2-1}{24n} & \text{if } n \text{ is odd.} \end{cases}$$

Hence

$$\mathcal{C}(T) = \begin{cases} \dfrac{n^2}{16} & \text{if } n \text{ is even;} \\ \dfrac{n^2-1}{16} & \text{if } n \text{ is odd.} \end{cases}$$

However, with some computation we find

$$\mathfrak{c}_1(T) = \begin{cases} \dfrac{n}{4} & \text{if } n \text{ is even;} \\ \dfrac{n^2-1}{4n} & \text{if } n \text{ is odd;} \end{cases}$$

and $\mathfrak{c}_2(T) = \frac{n-1}{2n}$. The upper bound for $\mathcal{C}(T)$ given in Theorem 6.2.8 is then equal to

$$\begin{cases} \dfrac{n^2-n}{8} & \text{if } n \text{ is even;} \\ \dfrac{n^3-n^2-n+1}{8n} & \text{if } n \text{ is odd;} \end{cases}$$

Hence for n large enough,

$$\mathcal{C}(T) \sim \frac{1}{2} n \mathfrak{c}_1(T) \mathfrak{c}_2(T).$$

Example 6.3.3. Consider the random walk on the path on n vertices. The transition matrix of this Markov chain is

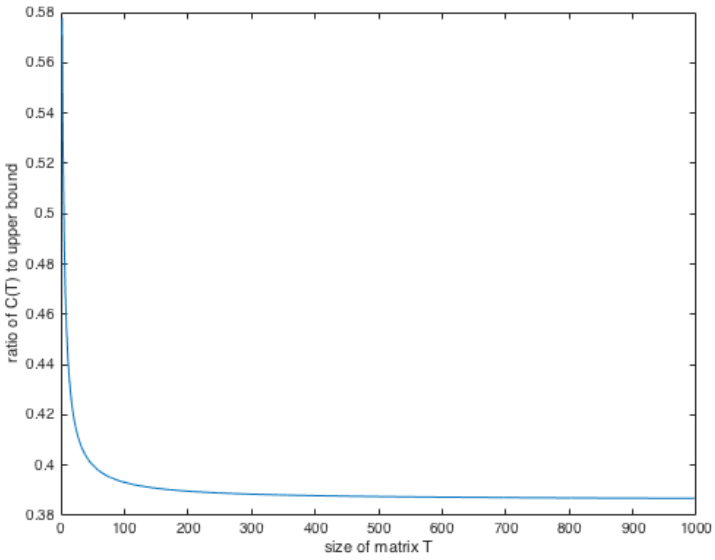
$$T = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \cdots & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & \cdots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & 0 & \cdots & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$

The group inverse of $I - T$ and its square do not follow as neat a pattern as the previous example, so we do not produce here a closed-form expression for $\mathcal{C}(T)$ or the upper bound. Instead, see in Fig. 6.1a of the values of the ratio of the upper bound to $\mathcal{C}(T)$ for values of n up to $n = 1000$. This appears to indicate that for n large enough,

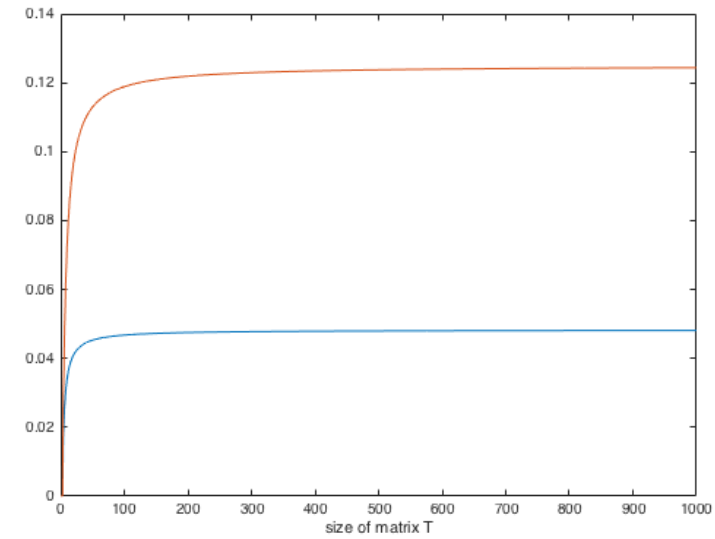
$$\mathcal{C}(T) \sim \gamma n \mathfrak{c}_1(T) \mathfrak{c}_2(T),$$

for some $\gamma \approx 0.38$.

Note that the order of magnitude of both $\mathcal{C}(T)$ and the upper bound appears to be n^4. We display evidence of this in Fig. 6.1b, a plot of $\mathcal{C}(T)/n^4$ and $n\mathfrak{c}_1(T)\mathfrak{c}_2(T)/n^4$, for



(a) The ratio of the structured condition number $\mathcal{C}(T)$ to the upper bound in (6.9).



(b) The ratio of both the upper bound (in red) and the structured condition number $\mathcal{C}(T)$ (in blue) to n^4.

Figure 6.1: Numerical examination of the structured condition number for T the transition matrix for the random walk on the path on n vertices.

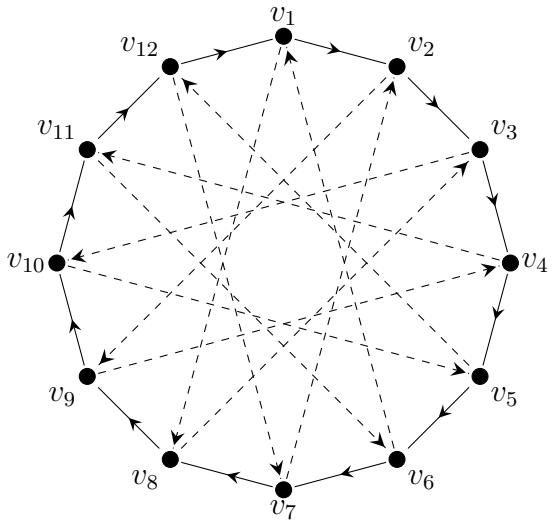


Figure 6.2: The directed cycle on 12 vertices, for which a 'bad' perturbation introduces new transitions displayed here as dashed arcs.

values of n up to $n = 1000$. Such a high order of magnitude indicates that Kemeny's constant is extremely poorly-conditioned for the random walk on a path on n vertices.

In each of these examples where the conditioning of Kemeny's constant is poor, the structure of the transition matrix is very specific. Furthermore, the perturbation which produces such a large difference in Kemeny's constant breaks the structure completely. In the directed cycle example, this perturbation introduces many new possible transitions into the chain, taking what is essentially a deterministic process and making it much more stochastic; see Fig. 6.2 for the new transitions introduced under this perturbation to the directed cycle on 12 vertices.

It is natural to ask about the conditioning of Kemeny's constant where perturbations must respect the given structure of the transition matrix; that is, given D the directed graph of T, consider only perturbations $T + E$ of T where $T + E \in \mathcal{S}_D$. However, we remark that there is an entire family of directed graphs given in [15] for which the value of $\mathcal{K}(T)$ depends only on the directed graph, and not on the values of the transition probabilities. Directed graphs with this property are characterised by the

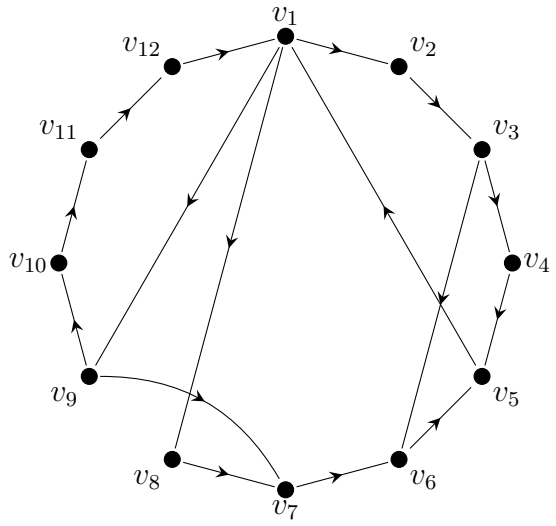


Figure 6.3: A directed graph D on 12 vertices for which every $T \in \mathcal{S}_D$ has $\mathcal{K}(T)$ equal to 10.

following conditions:

1. Every vertex of D has positive outdegree.

2. There exists an integer k such that all cycles of D have length k.

3. There is a vertex in D that lies on every cycle in D.

Then $\mathcal{K}(T) = \frac{2n-k+1}{2}$, for all irreducible $T \in \mathcal{S}_D$, where n is the number of vertices in D. An example of such a directed graph is displayed in Fig. 6.3.

Chapter 7

Concluding remarks and future directions

In this chapter we will briefly describe some extensions of the work completed in Chapters 3 through 6, with an emphasis on the extensions of the preliminary work on perturbation analysis of Kemeny's constant completed in Chapter 6.

In Chapter 3, we discussed the problem of characterising the set of all possible stationary vectors of irreducible stochastic matrices in $\mathcal{S}_D$. We were able to produce algorithmically from a directed graph D a list of conditions under which a given probability vector w would be the stationary vector for an irreducible stochastic matrix T respecting this directed graph D, and for a given admissible vector w, we can determine the matrices $T \in \mathcal{S}_D$ which have w as stationary distribution vector.

This problem was motivated by the idea that in many real-world applications, the underlying network of possible transitions between states is predetermined, and it is of interest to determine the range of possible long-term behaviours of the system given this constraint, and to be able to produce a matrix T respecting the given network, which has a certain desirable stationary distribution. A specific example was given

of an urban road network, where the values of transition probabilities can perhaps be manipulated through, say, the timing of traffic lights, while the network itself is given and must be respected. While there may be a degree of control over the transition probabilities in this way, it is probably more realistic to specify an interval $[p_1, p_2]$ for each transition probability $t_{i,j}$, and to determine the long-term behaviours of a system where the transition probabilities can range, but not too far. Note that in the coming age of driverless cars, there may be more control over the behaviour of traffic in the network, if such vehicles can be directed to travel in a way that benefits the overall efficiency of the network.

This specification of an interval also makes sense in the context of the other types of examples we considered, such as population growth in Section 3.5. It is unlikely that we can obtain complete control over the life cycle of an organism and determine how quickly it progresses to the next stage; rather, it is far more likely that these biologically-determined parameters can be influenced within a certain specified range. This problem could be approached using more complex techniques in convex polytopes; see [38] for a discussion on the sets of eigenvectors of *intervals* of matrices.

In Chapter 4, we determined a lower bound on the maximum mean first passage time between distinct states of a Markov chain in terms of the stationary distribution of the chain. We also characterised the directed graphs for which equality always holds in this lower bound for $T \in \mathcal{S}_D$, but only under the extra assumption that the minimum entry of the stationary distribution vector always occurs at the same index. The obvious next step is to attempt to characterise these directed graphs without this extra assumption, and we have made several observations to that end in Section 4.3.2.

It is natural to ask how the values of certain Markov chain parameters dictate the values of others, and this is what we have done in Chapter 4, where a given

stationary vector places a certain restriction on $\max_{i \neq j} m_{i,j}$. Given the stationary vector $w = \begin{bmatrix} w_1 & \cdots & w_n \end{bmatrix}^\top$ of a transition matrix T, where $w_1 \leq \cdots \leq w_n$, it is shown in [60] that this places the restriction on $\mathcal{K}(T)$ that

$$\mathcal{K}(T) \geq \sum_{j=1}^{n} (j-1) w_j.$$

Another problem that we could consider would be the following: Suppose T is an irreducible stochastic matrix, and let $\mathcal{K}(T)$ be given. Can we determine meaningful lower bounds on $\max_{i \neq j} m_{i,j}$ in terms of $\mathcal{K}(T)$? This problem is motivated by the fact that $\mathcal{K}(T)$ gives a measure of global connectivity, but that the wider-ranging mean first passage times give more information about connectivity between specific states. While an optimal low value for $\mathcal{K}(T)$ may be a primary goal in a setting such as the urban road network, it may be a secondary goal to ensure that the expected time to get from one location to another is as low as possible. It is likely that some techniques from the work in Chapter 4 could apply here, and that for this problem, the combinatorial structure of T will similarly play a role in establishing when $\mathcal{K}(T)$ and $\max_{i \neq j} m_{i,j}$ are more closely related.

In Chapter 5 we determined a way to find indications of clustering behaviour in a Markov chain whose transition matrix has complex eigenvalues that are close to 1. This involves partitioning the matrix based on the sign pattern of a vector associated with the eigenvectors of the transition matrix, and while Theorems 5.2.1 and 5.3.1 may be rather involved, they can effectively be used to determine clustering behaviour in a Markov chain. A natural extension of this process is to generalise it to a situation where we may have many clusters, not just two. We tested the process on a class of simulated examples where there were three constructed clusters, and found that

our method is excellent at detecting at least one, and often two of the three clusters. However, as remarked at the end of Chapter 7, a divide-and-conquer approach could be used in the case that we have many clusters. The next step would be to formalise this process and produce a robust divide-and-conquer algorithm for detecting multiple clusters in a Markov chain.

In Chapter 6, we began the development of a body of work on the perturbation analysis of Kemeny's constant, mirroring that of condition numbers for the stationary vector. We have scratched the surface with this structured condition number of Kemeny's constant, and it has given insight into what methods can be used to further this research area. It seems the bounds we have developed have some dependence on the square of the group inverse of $(I - T)$, which is known to be related to the variances of first passage times (see [11, Theorem 8.4.4]). This could be an interesting avenue to explore. Furthermore, given the multiple expressions and interpretations for $\mathcal{K}(T)$, there are many interesting ways to attack the following general problem.

Problem. *Let T be an irreducible stochastic matrix, and suppose $\tilde{T} = T + E$ is some perturbation of T—that is, E is a matrix with zero row sums such that $T + E$ is also nonnegative, stochastic, and irreducible. Determine some function f of T for which*

$$|\mathcal{K}(\tilde{T}) - \mathcal{K}(T)| \leq \|E\|_\infty \cdot f(T).$$

A related subproblem of the above is that of the influence of certain transitions in the Markov chain on the value of $\mathcal{K}(T)$. That is, suppose we perturb the transition matrix T precisely so that the transition probability from s_i to s_j is decreased, and the transition probability from s_i to s_k is increased. How large is the change in Kemeny's constant, relative to the size of this change?

Problem. *Let T be an irreducible stochastic matrix, and suppose $t_{i,j} > 0$, for some i, j. Fix a, $0 < a \leq t_{i,j}$, and set $E = a \cdot e_i(e_k - e_j)^\top$. Determine some function g of T for which*

$$|\mathcal{K}(T + E) - \mathcal{K}(T)| \leq a \cdot g(T).$$

If a is fixed in the above problem to be equal to $t_{i,j}$ the 'perturbation' amounts to removing the possibility of a transition from s_i to s_j. Thus an answer to the above problem would determine the relative importance of that transition is to the overall connectivity of the system, when compared to the transition from s_i to s_k. Note that another variant of this would be to re-distribute the probability of moving from s_i to s_j across all states immediately accessible from s_i in some appropriate way.

Problem. *Let T be an irreducible stochastic matrix, and suppose $t_{i,j} > 0$, for some i, j. Set $a = t_{i,j}$, and let u be some appropriate nonnegative vector, normalized by $u^\top \mathbb{1} = 1$. Set $E = a \cdot e_i(u - e_j)^\top$, where e_r denotes the r^{th} standard basis vector. Determine some function h of T for which*

$$|\mathcal{K}(T + E) - \mathcal{K}(T)| \leq a \cdot h(T).$$

The above problem is motivated by the urban road network application of a Markov chain, where removing this transition amounts to closing a road in the network, and this redistribution vector u describes how the existing traffic is diverted. A measure of the change in Kemeny's constant given this perturbation will describe how the global connectivity of the network is affected by this closure. Note that there may be several appropriate choices of u—for example; the weight of this transition could be distributed uniformly across all other $t_{i,k}$, $k \neq j$, for which $t_{ik} > 0$. Alternatively, u could be chosen so that the part of the weight $t_{i,j}$ transferred to the (i, k) entry $t_{i,k}$ is proportional to the 'importance' of state s_k—i.e. proportional to w_k, the k^{th} entry of the stationary

distribution vector.

Note that it is not necessarily the case that Kemeny's constant will increase given this 'road closure'. In fact, there are many instances of a road closure leading to increased connectivity in an urban setting. This phenomenon is known as *Braess' paradox*. Instances of Braess' paradox for random walks on simple undirected graphs have been studied previously, both in terms of Kemeny's constant (see [61]) and other measures of connectivity in an undirected graph (see, for example, [26]).

Given the above remark, we list one last problem in this area:

Problem. *Let T be an irreducible stochastic matrix, and suppose $t_{i,j} > 0$, for some i, j. Set $a = t_{i,j}$, and let u be some nonnegative vector with $u^\top \mathbb{1} = a$. Set $E = a \cdot e_i(u - e_j)^\top$, where e_r denotes the r^{th} standard basis vector. For what choices of i, j, and vector u is $\mathcal{K}(T + E) < \mathcal{K}(T)$?*

This problem can perhaps be more well-defined by considering only transition matrices respecting a given directed graph, and determining those directed graphs D for which there is always some instance of Braess' paradox given the removal of a particular arc.

Appendix A

MATLAB code

In this appendix we include annotated MATLAB code for the numerical experiments that were used to illustrate the results in this thesis.

A.1 Code pertaining to Chapter 3

```
1 function [C, inverses, T0s] = xconditions(D)
2 %This will be the function that takes the adjacency matrix of the
     directed graph, D, and produces C, the matrix of component
     conditions to be satisfied, and inverses, a cell array where each
     entry inverses{i} is a cell array corresponding to component i,
     containing the inverse incidence matrices of all spanning trees of
     component i in the bipartite graph.
3
4 n = size(D, 1);
5
6 %adjacency matrix of B(D)
```

```
B = [[zeros(n), D]; [D.' , zeros(n)]];
%find the connected components of B(D)
[~, C1] = graphconncomp(sparse(B)); %vector with i'th entry the
    component to which vertex i belongs
k = max(C1);

%construct vertex sets of components
V = cell(1, k);
for i = 1:k
    V{i} = find(C1 == i);
end

%construct C, matrix of component equations
C = zeros(k, 2*n);
if k > 1
    for i = 1:k
        C(i, V{i}(V{i} <= n)) = 1;
        C(i, V{i}(V{i} > n)) = -1;
    end
end

%construct matrices representing induced subgraphs that are the
    components
A = cell(1, k);
for i = 1:k
    A{i} = B(V{i}, V{i});
```

```
end

%compute the set inverses{i} for each component i
T0s = cell(1, k);
inverses = cell(1, k);
for i = 1:k
    [T0, E, T] = all_spanning_trees(A{i});
    T0s{i} = V{i}(T0);
    inverses{i} = incidenceinverses(T0, E, T);
end

end
```

```
function [T0, E, T] = all_spanning_trees(A)

[T0, E, cand, leave] = DFSmethod(A, 1);

T = NaN(0, 2);
find_child()

function find_child()

if isempty(leave)
    return;
else

```

```
Q = dlnode.empty;
e = leave(length(leave)).Data; %last entry of leave
delete(leave(length(leave))) %delete e from leave
leave(length(leave)) = [];

while ~isempty(cand{e})
    g = cand{e}(length(cand{e})).Data; %last entry of cand{e}
    delete(cand{e}(length(cand{e}))) %delete g from cand{e}
    cand{e}(length(cand{e})) = [];

    %add g to the beginning of Q
    if ~isempty(Q)
        Q(length(Q) + 1) = Q(length(Q));
        for i = 2:(length(Q)-1)
            Q(length(Q) + 1 - i) = Q(length(Q) - i);
        end
        Q(1) = dlnode(g);
        Q(1).insertBefore(Q(2))
    else
        Q(1) = dlnode(g);
    end

    T(size(T, 1) + 1, :) = [-e, +g];

    sub_child(e, g)

```

```
40      T(size(T, 1) + 1, :) = [+e, -g];
41
42  end
43
44  %move all entries of Q to cand{e} - i.e. reconstruct cand{e} to what it
        was before
45  if isempty(cand{e})
46      cand{e} = Q;
47  else
48      cand{e}(length(cand{e})).insertBefore(Q(1))
49      cand{e} = [cand{e} Q];
50  end
51
52  sub_child(e, e)
53
54  %add e to the end of leave
55  if isempty(leave)
56      leave(1) = dlnode(e);
57  else
58      leave(length(leave) + 1) = dlnode(e);
59      insertAfter(leave(length(leave)), leave(length(leave)-1))
60  end
61
62  end
63  end
64
```

```
65 function sub_child(e, g)
66
67 if isempty(cand{e})
68     find_child()
69 else
70     if  E(g, 1) <= E(datadl(cand{e}(1)), 1)
71         find_child()
72     else
73         f = find(E(:, 2) == E(g, 1), 1);
74
75         if ~isempty(cand{f})
76             %Create set S = {e' in cand{e} | E(e', 1) < E(g, 1)}
77             Y = datadl(cand{e});
78             S = find(E(Y, 1) < E(g, 1));%Note this is just an index set
                   of Y
79
80             %Merge S into cand{f}
81             for i= 1:length(S)
82                 cand{f} = insertdl(dlnode(Y(S(i))), cand{f});
83             end
84
85             find_child()
86
87             %delete all entries of S from cand{f}
88             F = datadl(cand{f});
89             I = NaN(1, 0);
```

```
90              for i = 1:length(S)
91                  if nnz(F == Y(S(i))) > 0
92                      I(length(I) + 1) = find(F == Y(S(i))); %finds the
                            indices of all entries of S that are in F
93                  end
94              end
95              I = sort(I);
96              for j = 1:length(I)
97                  delete(cand{f}(I(length(I)+1-j)))
98                  cand{f}(I(length(I) + 1 - j)) = [];
99              end
100
101             clear S;
102         else %cand{f} is empty
103             %Set cand{f} = {e' in cand{e} | E(e', 1) < E(g, 1)}
104             Y = datadl(cand{e});
105             M = find(E(Y, 1) < E(g, 1));
106             cand{f}(1) = dlnode(Y(M(1)));
107             for i = 2:length(M)
108                 cand{f}(i) = dlnode(Y(M(i)));
109                 insertAfter(cand{f}(i), cand{f}(i-1))
110             end
111
112             leave = insertdl(dlnode(f), leave); % insert f to leave
113
114             find_child()
```

```
115
116             %delete f from leave
117             m = find(datadl(leave) == f);
118             delete(leave(m))
119             leave(m) = [];
120
121             cand{f} = dlnode.empty;
122         end
123     end
124 end
125 end
126 end
```

```
1  function [number, edgenumber, cand, leave] =  DFSmethod(A, v)
2  % an attempt at writing the DFS script I need to find a min spanning
       tree of A and order the vertices and edges appropriately, as well as
        constructing the initial candidate sets for each edge, and the set
       of edges which we may delete from T0 (leave).
3
4  %Initialise values
5  c = 1; %index number for the number set below
6  number = NaN(1, length(A)); %vertex numbers - the order will determine
       T0
7  edgenumber = [0, 0]; %edge numbers
8  Q = zeros(0, 2); %a set to deposit edges NOT in T0, before ordering them
        and adding them to edgenumber
```

```
9
10 DFS(v, 0)
11
12 %defining a depth first search alg. to find T0 and order vertices and
       edges in G(A)
13 function DFS(v, u)
14 number(c) = v;
15 for w = 1:length(A)
16     if ismember(w, adj(A, v))
17         if ismember(w, number) == 0
18             edgenumber(c, :) = [v, w];
19             c = c + 1;
20             DFS(w, v);
21         else if find(number == w) < find(number == v) && isequal(w, u)
               == 0
22             Q(size(Q, 1) + 1, :) = [w, v];
23             end
24         end
25     end
26 end
27 end
28
29 %edge ordering
30 [~, I] = sort(number);
31 Q = I(Q);
32 [~, J] = sort(Q(:, 1));
```

```
33 Q = [Q(J, 1), Q(J, 2)];
34 edgenumber = [I(edgenumber); Q];
35
36 %Construct candidate sets for each edge
37 cand = cell(size(edgenumber, 1), 1);
38 for i = 1:size(edgenumber, 1)
39     cand{i} = candi(i);
40 end
41
42 %Definition of function candi(i)
43 function [c] = candi(i)
44
45 c = dlnode.empty;
46 for j = size(A):size(edgenumber, 1)
47     if edgenumber(i, 2) == edgenumber(j, 2) && edgenumber(j, 1) <=
        edgenumber(i, 1)
48         c(length(c)+ 1) = dlnode(j);
49         if length(c) > 1
50             c(length(c)).insertAfter(c(length(c)-1))
51         end
52     end
53 end
54 end
55 %Construct leave set
56 leave = dlnode.empty;
57 for i = 1:(size(A)-1)
```

```
    if ~isempty(cand{i})
        leave(length(leave)+1) = dlnode(i);
        if length(leave) > 1
            leave(length(leave)).insertAfter(leave(length(leave)-1))
        end
    end
end
end
```

```
function [inverses] = incidenceinverses(T0, E, T)
%Takes a depth first spanning tree T0 (vector of vertices in the order
   in which they were discovered) with edge set E (the first length(T0)
    - 1 of which are the edges of T0, the rest being edges of the full
   graph) and a list of edge additions and removals T that scan all
   spanning trees of the graph D from which we found T0, E and T (using
    DFSmethod and all_spanning_trees). This function is specific to
   PROBLEM ONE.

%construct inverse incidence matrix of T0.
I = zeros(length(T0) - 1); %We truncate the incidence matrix
for i = 1:length(I)
    for j = 1:length(I)
        I(i, j) = nnz(E(j, :) == i);
    end
end
I = inv(I);
```

```
12
13 %construct the set of vectors corresponding to the edges in E
14 E1 = cell(1, size(E, 1));
15 for i = 1:length(E1)
16     E1{i} = NaN(length(T0) - 1, 1);
17     for j = 1:(length(T0) - 1)
18         E1{i}(j) = nnz(T0(E(i, :)) == T0(j));
19     end
20 end
21
22 %produce 'inverses' set
23
24 inverses = cell.empty;
25 inverses{1} = I;
26
27 if ~isempty(T)
28     K = NaN(1, length(T) + 1);
29
30     for i = 1:length(T)
31         if T(i, 1) > 0
32             F = find(T(:, 1) == -T(i, 1) & T(:, 2) == -T(i, 2)); %finds
                   all of the rows of T that are equal to the negative of
                   row i
33             c = max(F(F < i))+1; %finds the most recent occurrence of
                   this, adds 1 because we will be using c as a marker in '
                   inverses' which has T0 added at the start
```

```
            inverses{i+1} = []; %dummy empty entry, deleted at the end
        else
            X = -E1{-T(i, 1)} + E1{T(i, 2)};
            if  (i == 1) || (T(i-1, 1) < 0)
                c = length(inverses);
                inverses{i+1} = invper(inverses{c}, X, -T(i, 1));
                K(i+1) = c;
            else
                inverses{i+1} = invper(inverses{K(c)}, X, -T(i, 1)); %K(
                    c) is the inverse that was used to compute inverses{
                    c}
                K(i+1) = K(c);
            end
        end
    end

    inverses = inverses(~cellfun('isempty', inverses));
else
    inverses = inverses(~cellfun('isempty', inverses));
end
end
```

```
function B = invper(A1, X, k)
%Takes as input an inverted matrix A^{-1}, the inverse of A, and a (0,
    1) column vector X. Returns the inverse of B = A + XY, where Y = kth
     standard basis vector. We take k as an input where the k-th edge (i
```

```
    .e. column) of A1 is being removed and another replacing it.
3
4 if length(A1) ~= length(X)
5     error('Dimensions do not match')
6 end
7
8 if k < 1 || k > length(A1)
9     error('k is outside range of matrix')
10 end
11
12 Y = zeros(1, size(A1, 1));
13 Y(k) = 1;
14
15 %Using the Sherman–Morrison formula
16 B = A1 - (1/(1+ Y*A1*X))*(A1*X*Y*A1);
17 end
```

A.2 Code pertaining to Chapter 5

```
1 function [table, clusters, bounds] = findcluster(T)
2 % finds clusters in a Markov chain whose transition matrix is T, by
    considering eigenvalues which are close to 1 - either real, or
    complex with real part close to 1 and imaginary part close to 0.
3
4 % OUTPUT:
```

```
5  % 'table' is a cell array where for each eigenvalue suff. close to 1, we
       have a table of results for each partitioning. Each partition
       corresponds to a row in the table, with the name of the partition,
       the index sets of the first and second blocks, and the lower bounds
       on the spectral radii of the corresponding matrix. If a hypothesis
       is not satisfied, this is noted.
6  % 'clusters' is a cell array where each cell contains the index set of a
       cluster detected by the algorithm
7  % 'bounds' is a cell array where each cell contains the lower bound
       produced by the algorithm on the spectral radius of the
       corresponding cluster in the 'clusters' cell array.
8  % These last two contain information given in the 'table' output, but
       they are isolated to make them easier to work with, and detected
       clusters for which the hypotheses do not hold are weeded out.
9
10
11
12
13 % CHECK THE EIGENVALUES
14 %   find the eigenvalues that are close to one
15
16 [V, D] = eig(T);
17 E = nonzeros(D);
18 one = max(real(E)); % this is to counteract any small inaccuracies with
       MATLAB — the largest won't be exactly 1, according to MATLAB
```

```
I = find(real(E) < one & real(E) >= 0.8); % index set of eigenvalues
    with real part close to 1
I = I((0 <= imag(E(I)) & imag(E(I)) < 0.2) | (imag(E(I))>= -eps & imag(E
    (I)) < 0)); %this is the index/indices of eigenvalues suff. close to
     one, with imaginary part greater than or equal to 0

% Set up output
if isempty(I)
    error('This matrix has no eigenvalue sufficiently close to 1');
else
    table = cell(0, 4, length(I));
    J = I(0==imag(E(I))); %J is the index set of real eigenvalues
    K = I(0~=imag(E(I))); %K is the index set of complex eigenvalues (
        nonreal)
    clusters = cell(1, 12*length(K)+2*length(J));
    bounds = cell(1, 12*length(K)+2*length(J));
end
c=1;


for m = 1:length(I) %for each eigenvalue that's 'close' to 1
    a = real(E(I(m)));
    b = imag(E(I(m))); %lambda = a + bi
    v = V(:, I(m));
    x = real(v);
    y = imag(v); % v = x + yi
```

```
41
42      if b==0 %if the imaginary part is zero, the eigenvalue is real; we
            use the approach in the IJC paper
43          S1 = find(x>0);
44          S2 = find(x<0);
45          table{1, 1, m} = 'real eigenvalue';
46          table{1, 2, m} = S1;
47          table{1, 3, m} = a;
48          table{1, 4, m} = S2;
49          table{1, 5, m} = a;
50          clusters{c} = S1;
51          bounds{c} = a;
52          c=c+1;
53          clusters{c} = S2;
54          bounds{c} = a;
55          c=c+1;
56
57      else % if the eigenvalue is complex, we use our new approach
58
59          %Partition with respect to where the vector x is positive, neg,
                and zero.
60          P = x > 0;
61          N = x < 0;
62          Z = x==0;
63
64          %sort and partition the vectors
```

```
65        x1 = x(P);
66        x2 = x(N);
67        x3 = x(Z);
68        y1 = y(P);
69        y2 = y(N);
70        y3 = y(Z);
71
72        %index sets for partitions
73        S1 = find(P);
74        S2 = find(N);
75        S3 = find(Z);
76
77        %Satisfying hypotheses
78        h1 = all(a*x1 - b*y1 > 0); %first hypothesis, to make sure lower
              bound of rho(A11) is positive
79        h2 = all(a*x2 - b*y2 < 0); %second hypothesis, to make sure
             lower bound of rho(A22) is positive
80
81        % We're going to do all the computations first, without
             accounting for the hypotheses. At the end, when we go to
             record the lower bounds in our output, I'm only going to
             record them if the appropriate hypothesis is satisfied. This
              is the easiest way.
82
83        % find lower bounds for spectral radius in this basic case,
             before optimising with t
```

```
84
85          lb1_tzero = a - b*max(y1./x1);
86          lb2_tzero = a - b*max(y2./x2);
87
88          %Output
89          table{1, 1, m} = 't zero';
90          table{1, 2, m} = S1;
91          table{1, 3, m} = lb1_tzero;
92          table{1, 4, m} = S2;
93          table{1, 5, m} = lb2_tzero;
94          if h1 == 0
95              table{1, 3, m} = 'cannot find lower bound for rho(A11):
                    hypothesis not satisfied';
96          end
97          if h2 == 0
98              table{1, 5, m} = 'cannot find lower bound for rho(A22):
                    hypothesis not satisfied';
99          end
100         clusters{c} = S1;
101         bounds{c} = table{1, 3, m};
102         c=c+1;
103         clusters{c} = S2;
104         bounds{c} = table{1, 5, m};
105         c=c+1;
106
107
```

```
108         %find where y3 is positive or negative, and repartition for
                when s =
109         %1, t > 0.
110         Ipos = find(y3 > 0);
111         Ineg = find(y3 < 0);
112         x1_tpos = [x1; x3(Ipos)];
113         y1_tpos = [y1; y3(Ipos)];
114         x2_tpos = [x2; x3(Ineg)];
115         y2_tpos = [y2; y3(Ineg)];
116         S1_tpos = [S1; S3(Ipos)];
117         S2_tpos = [S2; S3(Ineg)];
118
119         % if there are no neg entries of y1, t is unbounded and we take
                the limit
120         if ~isempty(find(y1_tpos < 0, 1))
121             tset_1 = (-x1_tpos(y1_tpos < 0)./y1_tpos(y1_tpos < 0));
122             tbound1 = min(tset_1);
123         else
124             tbound1 = Inf;
125         end
126         if ~isempty(find(y2_tpos > 0, 1)) % if there are no positive
                entries of y2, t is unbounded
127             tset_2 = (-x2_tpos(y2_tpos > 0)./y2_tpos(y2_tpos > 0));
128             tbound2 = min(tset_2);
129         else
130             tbound2 = Inf;
```

```
131         end
132         t = min(tbound1, tbound2);
133 
134         if t == Inf
135             lb1_tpos = a + b*min(x1_tpos./y1_tpos);
136             J = x2_tpos./y2_tpos;
137             for i = 1:length(J)
138                 if J(i) < -1/eps
139                     J(i) = Inf;
140                 end
141             end
142             lb2_tpos = a + b*min(J);
143         else if all(a*x1 + b*y1 > 0) && all(a*x2 + b*y2 < 0)
144                 J1 = (t*x1_tpos - y1_tpos)./(x1_tpos + t*y1_tpos);
145                 for i = 1:length(J1)
146                     if J1(i) < -1/eps
147                         J1(i) = Inf; %This just counteracts an issue
                                with Matlab dividing by 0 instead of taking
                                a limit
148                     end
149                 end
150                 lb1_tpos = a + b*min(J1);
151                 J2 = (t*x2_tpos - y2_tpos)./(x2_tpos + t*y2_tpos);
152                 for i = 1:length(J2)
153                     if J2(i) < -1/eps
154                         J2(i) = Inf;
```

```
155                 end
156             end
157             lb2_tpos = a + b*min(J2);
158         else
159             lb1_tpos = 'cannot find lower bound for rho(A11): no
                    such t';
160             lb2_tpos = 'cannot find lower bound for rho(A22): no
                    such t';
161         end
162     end
163
164     %Output
165     table{2, 1, m} = 't positive';
166     table{2, 2, m} = S1_tpos;
167     table{2, 3, m} = lb1_tpos;
168     table{2, 4, m} = S2_tpos;
169     table{2, 5, m} = lb2_tpos;
170     if h1 == 0
171         table{2, 3, m} = 'cannot find lower bound for rho(A11):
                hypothesis not satisfied';
172     end
173     if h2 == 0
174         table{2, 5, m} = 'cannot find lower bound for rho(A22):
                hypothesis not satisfied';
175     end
```

```
176         if all(abs(x1_tpos + t*y1_tpos) <= 0) % if they are linearly
                dependent
177             table{2, 3, m} = 'cannot find lower bound for rho(A11):
                    linearly dependent';
178         end
179         if all(abs(x2_tpos + t*y2_tpos) <= 0) % if they are linearly
                dependent
180             table{2, 5, m} = 'cannot find lower bound for rho(A22):
                    linearly dependent';
181         end
182         clusters{c} = S1_tpos;
183         bounds{c} = table{2, 3, m};
184         c=c+1;
185         clusters{c} = S2_tpos;
186         bounds{c} = table{2, 5, m};
187         c=c+1;
188
189
190
191
192         % s = 1, t negative
193         %repartitioning:
194         S1_tneg = [S1; S3(Ineg)];
195         S2_tneg = [S2; S3(Ipos)];
196         x1_tneg = [x1; x3(Ineg)];
197         y1_tneg = [y1; y3(Ineg)];
```

```
198         x2_tneg = [x2; x3(Ipos)];
199         y2_tneg = [y2; y3(Ipos)];
200
201         table{3, 1, m} = 't negative';
202         table{3, 2, m} = S1_tneg;
203         table{3, 3, m} = a-b*(max(y1_tneg./x1_tneg)); % because the
                lower bound is increasing in t, the best choice is t -> 0.
                This gives us the basic case, and we possibly get extra
                vertices for
                free.
204         table{3, 4, m} = S2_tneg;
205         table{3, 5, m} = a-b*(max(y2_tneg./x2_tneg));
206         if h1 == 0
207             table{3, 3, m} = 'cannot find lower bound for rho(A11):
                    hypothesis not satisfied';
208         end
209         if h2 == 0
210             table{3, 5, m} = 'cannot find lower bound for rho(A22):
                    hypothesis not satisfied';
211         end
212         clusters{c} = S1_tneg;
213         bounds{c} = table{3, 3, m};
214         c=c+1;
215         clusters{c} = S2_tneg;
216         bounds{c} = table{3, 5, m};
217         c=c+1;
```

```
218
219
220
221         % t = 1, s zero
222
223         %Partition with respect to where the vector y is positive, neg,
                and
224         %zero.
225         P = y > 0;
226         N = y < 0;
227         Z = y==0;
228
229         %sort and partition the vector and matrix
230         x1 = x(P);
231         x2 = x(N);
232         x3 = x(Z);
233         y1 = y(P);
234         y2 = y(N);
235         y3 = y(Z);
236
237         %index sets for partitions
238
239         S1 = find(P);
240         S2 = find(N);
241         S3 = find(Z);
242
```

```
243         % Check new hypotheses:
244         H1 = all(a*y1 + b*x1 > 0);
245         H2 = all(a*y2 + b*x2 < 0);
246
247         % find lower bounds for spectral radius in this basic case,
                before optimising with s
248
249         lb1_szero = a + b*min(x1./y1);
250         lb2_szero = a + b*min(x2./y2);
251
252         table{4, 1, m} = 's zero';
253         table{4, 2, m} = S1;
254         table{4, 3, m} = lb1_szero;
255         table{4, 4, m} = S2;
256         table{4, 5, m} = lb2_szero;
257         if H1 == 0
258             table{4, 3, m} = 'cannot find lower bound for rho(A11):
                    hypothesis not satisfied';
259         end
260         if H2 == 0
261             table{4, 5, m} = 'cannot find lower bound for rho(A22):
                    hypothesis not satisfied';
262         end
263         clusters{c} = S1;
264         bounds{c} = table{4, 3, m};
265         c=c+1;
```

```
266         clusters{c} = S2;
267         bounds{c} = table{4, 5, m};
268         c=c+1;
269
270         % t = 1, s positive
271
272         Ipos = find(x3 > 0);
273         Ineg = find(x3 < 0);
274
275         S1_spos = [S1; S3(Ipos)];
276         S2_spos = [S2; S3(Ineg)];
277
278         table{5, 1, m} = 's positive';
279         table{5, 2, m} = S1_spos;
280         table{5, 3, m} = lb1_szero;
281         table{5, 4, m} = S2_spos;
282         table{5, 5, m} = lb2_szero; % another set of bounds we get for
               free
283         if H1 == 0
284             table{5, 3, m} = 'cannot find lower bound for rho(A11):
                   hypothesis not satisfied';
285         end
286         if H2 == 0
287             table{5, 5, m} = 'cannot find lower bound for rho(A22):
                   hypothesis not satisfied';
288         end
```

```
289         clusters{c} = S1_spos;
290         bounds{c} = table{5, 3, m};
291         c=c+1;
292         clusters{c} = S2_spos;
293         bounds{c} = table{5, 5, m};
294         c=c+1;
295
296         % t = 1, s negative
297
298         % repartition:
299         x1_sneg = [x1; x3(Ineg)];
300         y1_sneg = [y1; y3(Ineg)];
301         x2_sneg = [x2; x3(Ipos)];
302         y2_sneg = [y2; y3(Ipos)];
303         S1_sneg = [S1; S3(Ineg)];
304         S2_sneg = [S2; S3(Ipos)];
305
306
307         % if there are no pos entries of x1, s is unbounded and we take
                the limit
308         if ~isempty(find(x1_sneg > 0, 1))
309             sbound1 = max(-y1_sneg(x1_sneg > 0)./x1_sneg(x1_sneg > 0));
310         else
311             sbound1 = -Inf;
312         end
313         if ~isempty(find(x2_sneg < 0, 1))
```

```
314             sbound2 = max(-y2_sneg(x2_sneg < 0)./x2_sneg(x2_sneg < 0));
315         else
316             sbound2 = -Inf;
317         end
318         s = min(sbound1, sbound2);
319
320         if s == -Inf
321             lb1_sneg = a + b*min(-y1_sneg./x1_sneg);
322             lb2_sneg = a + b*min(-y2_sneg./x2_sneg);
323         else if all(a*x1 + b*y1 > 0) && all(a*x2 + b*y2 < 0)
324                 J1 = (x1_sneg - s*y1_sneg)./(s*x1_sneg + y1_sneg);
325                 for i = 1:length(J1)
326                     if J1(i) < -1/eps
327                         J1(i) = Inf; %This just counteracts an issue
                                with Matlab dividing by 0 instead of taking
                                a limit
328                     end
329                 end
330                 lb1_sneg = a + b*min(J1);
331                 J2 = (x2_sneg - s*y2_sneg)./(s*x2_sneg + y2_sneg);
332                 for i = 1:length(J2)
333                     if J2(i) < -1/eps
334                         J2(i) = Inf; %This just counteracts an issue
                                with Matlab dividing by 0 instead of taking
                                a limit
335                     end
```

```
336             end
337             lb2_sneg = a + b*min(J2);
338         else
339             lb1_sneg = 'cannot find lower bound for rho(A11): no
                    such s';
340             lb2_sneg = 'cannot find lower bound for rho(A22): no
                    such s';
341         end
342     end
343
344     table{6, 1, m} = 's negative';
345     table{6, 2, m} = S1_sneg;
346     table{6, 3, m} = lb1_sneg;
347     table{6, 4, m} = S2_sneg;
348     table{6, 5, m} = lb2_sneg;
349     if H1 == 0
350         table{6, 3, m} = 'cannot find lower bound for rho(A11):
                hypothesis not satisfied';
351     end
352     if H2 == 0
353         table{6, 5, m} = 'cannot find lower bound for rho(A22):
                hypothesis not satisfied';
354     end
355     if all(abs(x1_sneg + t*y1_sneg) <= 0) % if they are linearly
        dependent
```

```
356             table{6, 3, m} = 'cannot find lower bound for rho(A11):
                    linearly dependent';
357         end
358         if all(abs(x2_sneg + t*y2_sneg) <= 0) % if they are linearly
                dependent
359             table{6, 5, m} = 'cannot find lower bound for rho(A22):
                    linearly dependent';
360         end
361         clusters{c} = S1_sneg;
362         bounds{c} = table{6, 3, m};
363         c=c+1;
364         clusters{c} = S2_sneg;
365         bounds{c} = table{6, 5, m};
366         c=c+1;
367     end
368 end
```

```
1  function [T, lambda, const_clust, rhos, det_clust, bounds, bounds2, Eq,
       containing] = cluster_sims(n, m, p_fix, q_fix, lambda_fix, ni_fix)
2  % Produces m simulations of order n clustered matrices
3
4  % INPUT:
5  % If p_fix = true, the density of diagonal blocks is 0.7. If p_fix =
       false, density of clusters ranges from 0.2 to 0.8.
6  % If q_fix = true, the density of off-diagonal blocks is 0.4. If q_fix =
        false, density of off-diagonal blocks ranges from 0.2 to 0.8.
```

```
7  % If lambda_fix = true, we'll pick a random s and t but generate m
       matrices that have the same eigenvalue
8  % If ni_fix = true, we fix the sizes of the clusters. The first cluster
       will have order n/2, and the second n/3.
9
10 % OUTPUT:
11 % 'T': a cell array of m transition matrices of order n that are
       generated
12 % 'lambda': records the eigenvalue which is close to 1. Either a single
       value or an array of m values
13 % 'const_clust': gives the index sets of the constructed clusters
14 % 'rhos': calculates the actual spectral radii of the constructed
       clusters
15 % 'det_clust' is a cell array of index sets of clusters detected by the
       algorithm
16 % 'bounds' is a cell array that give lower bounds for the spectral radii
        of the detected clusters
17 % 'bounds2' is a cell array that (in the case of recovery) gives the
       best  lower bounds that the algorithm finds
18 % 'Eq' is a cell array which contains the information of which
       partitions produce index sets that are equal to the index sets of
       the clusters we constructed
19 % 'containing' is a cell array which contains the information of which
       partitions produce index sets which contain (nontrivially) the index
        sets of the constructed clusters.
20
```

```
%%%%%%%%%% Setting up outputs %%%%%%%%%%%
T = cell(1, m); %cell containing generated transition matrices
% If we fix the size of the clusters, the constructed clusters have
    fixed index sets. If not, then we will record the two index sets for
     each generated matrix T.
if ni_fix == 1
    const_clust = cell(1, 3);
    const_clust{1} = (1:(floor(n/2))).';
    const_clust{2} = ((floor(n/2)+1):(floor(n/2)+1+ceil(n/3))).';
    const_clust{3} = ((floor(n/2)+2+ceil(n/3)):n).';
else
    const_clust = cell(1, m);
end

if lambda_fix == 1
    rhos = zeros(1, 3);
else
    rhos = cell(1, m); % Every entry here will be 1x3 double, [rho(A11)
        rho(A22) rho(A33)]
end

%Fixing intracluster density
if p_fix == 1
    p = 0.7*ones(1,m);
else
    dp = (0.8-0.2)/(m-1);
```

```
    p = 0.2 + (0:m-1)*dp;
end

%Fixing intercluster density
if q_fix == 1
    q = 0.7*ones(1,m);
else
    dq = (0.8-0.2)/(m-1);
    q = 0.2 + (0:m-1)*dq;
end

if lambda_fix == 1
    %If we want to fix the eigenvalue, we choose s and t now and
       generate m matrices from the associated 3x3 matrix
    t = (sqrt(2)/6)*rand(1);
    A = [5/6 0 1/6; 3/4 1/6 1/12; (2/3 - 12*t^2) (1/3 + 12*t^2) 0];
    s = 0.2*rand(1);
    M = (1-s)*eye(3) + s*A;
    lambda = (1-s)+(s*t)*(1i);
    rhos(1) = M(1, 1);
    rhos(2) = M(2, 2);
    rhos(3) = M(3, 3);

    for k = 1:m
        if ni_fix == 1 %If we want to fix the size of the clusters
            n1 = floor(n/2); %size of first block
```

```
69            n2 = ceil(n/3); %size of second block
70            n3 = n - n1 - n2; %size of third block
71        else
72            n1 = randi([3,floor(n/2)], 1); %first diag block is smaller
                  than half the size of the matrix.
73            n2 = randi([3,(n - n1 - 3)], 1); %size of second diag block
74            n3 = n - n1 - n2;  %size of third diag block
75            const_clust{k} = cell(1, 3);
76            const_clust{k}{1} = (1:n1).';
77            const_clust{k}{2} = ((n1+1):(n1+n2)).';
78            const_clust{k}{3} = ((n1+n2+1):n).';
79        end
80        c=0;
81        while c == 0
82            A11 = randdir(n1, n1, p(k));
83            A22 = randdir(n2, n2, p(k));
84            A33 = randdir(n3, n3, p(k));
85
86            A12 = randdir(n1, n2, q(k));
87            A13 = randdir(n1, n3, q(k));
88            A21 = randdir(n2, n1, q(k));
89            A23 = randdir(n2, n3, q(k));
90            A31 = randdir(n3, n1, q(k));
91            A32 = randdir(n3, n2, q(k)); % this sets up the zero/nonzero
                  pattern of the matrix. It is 'random' in that edges are
                  chosen to be present with probability q
```

```
92
93              S11 = randstochD(A11);
94              S22 = randstochD(A22);
95              S33 = randstochD(A33);
96
97              S12 = randstochD(A12);
98              S13 = randstochD(A13);
99              S21 = randstochD(A21);
100             S23 = randstochD(A23);
101             S31 = randstochD(A31);
102             S32 = randstochD(A32);
103
104             %This is our m^th transition matrix
105             d=0;
106             while d == 0
107                 T{k} = [M(1, 1)*S11 M(1, 2)*S12 M(1, 3)*S13;
108                             M(2, 1)*S21 M(2, 2)*S22 M(2, 3)*S23;
109                             M(3, 1)*S31 M(3, 2)*S32 M(3, 3)*S33];
110                 for i = 1:n
111                     T{k}(i, :) = T{k}(i, :)/sum(T{k}(i, :));
112                 end
113                 if ~any(any(isnan(T{k}))) && ~any(any(isinf(T{k})))
114                     d=1;
115                 end
116             end
117             %Sometimes something goes wrong with the construction and we
```

```
                don't get the eigenvalue we want. This removes those
                cases.
118             [~, D] = eig(T{k});
119             E = nonzeros(D);
120             one = max(real(E)); % this is to counteract any small
                    inaccuracies with MATLAB - the largest won't be exactly
                    1, according to MATLAB
121             I = find(real(E) < one & real(E) >= 0.8); % index set of
                    eigenvalues with real part close to 1
122             I = I((0 <= imag(E(I)) & imag(E(I)) < 0.2) | (imag(E(I))>= -
                    eps & imag(E(I)) < 0));
123             if isirred(T{k}) && ~isempty(I)
124                 c=1;
125             end
126         end
127     end
128 else
129     lambda = zeros(1, m);
130     for k = 1:m
131         t = (sqrt(2)/6)*rand(1);
132         A = [5/6 0 1/6; 3/4 1/6 1/12; (2/3 - 12*t^2) (1/3 + 12*t^2) 0];
133         s = 0.2*rand(1);
134         M = (1-s)*eye(3) + s*A;
135         lambda(k) = (1-s)+(s*t)*(1i);
136
137         if ni_fix == 1 %If we want to fix the size of the clusters
```

```
138             n1 = floor(n/2); %size of first block
139             n2 = ceil(n/3); %size of second block
140             n3 = n - n1 - n2; %size of third block
141         else
142             n1 = randi([3,floor(n/2)], 1); %first diag block is smaller
                    than half the size of the matrix.
143             n2 = randi([3,(n - n1 - 3)], 1); %size of second diag block
144             n3 = n - n1 - n2;  %size of third diag block
145             const_clust{k} = cell(1, 3);
146             const_clust{k}{1} = (1:n1).';
147             const_clust{k}{2} = ((n1+1):(n1+n2)).';
148             const_clust{k}{3} = ((n1+n2+1):n).';
149         end
150         % The following sets up the zero/nonzero pattern of the matrix.
               It is 'random' in that edges are chosen to be present with
               probability p or q
151         c=0;
152         while c == 0
153             A11 = randdir(n1, n1, p(k));
154             A22 = randdir(n2, n2, p(k));
155             A33 = randdir(n3, n3, p(k));
156
157             A12 = randdir(n1, n2, q(k));
158             A13 = randdir(n1, n3, q(k));
159             A21 = randdir(n2, n1, q(k));
160             A23 = randdir(n2, n3, q(k));
```

```
161             A31 = randdir(n3, n1, q(k));
162             A32 = randdir(n3, n2, q(k));
163
164             S11 = randstochD(A11);
165             S22 = randstochD(A22);
166             S33 = randstochD(A33);
167
168             S12 = randstochD(A12);
169             S13 = randstochD(A13);
170             S21 = randstochD(A21);
171             S23 = randstochD(A23);
172             S31 = randstochD(A31);
173             S32 = randstochD(A32);
174
175             %This is our m^th transition matrix
176             d=0;
177             while d == 0
178                 T{k} = [M(1, 1)*S11 M(1, 2)*S12 M(1, 3)*S13;
179                             M(2, 1)*S21 M(2, 2)*S22 M(2, 3)*S23;
180                             M(3, 1)*S31 M(3, 2)*S32 M(3, 3)*S33];
181                 for i = 1:n
182                     T{k}(i, :) = T{k}(i, :)/sum(T{k}(i, :));
183                 end
184                 if ~any(any(isnan(T{k}))) && ~any(any(isinf(T{k})))
185                     d=1;
186                 end
```

```
            end
            %Sometimes something goes wrong with the construction and we don't get the eigenvalue we want. This removes those cases.
            [~, D] = eig(T{k});
            E = nonzeros(D);
            one = max(real(E)); % this is to counteract any small inaccuracies with MATLAB - the largest won't be exactly 1, according to MATLAB
            I = find(real(E) < one & real(E) >= 0.8); % index set of eigenvalues with real part close to 1
            I = I((0 <= imag(E(I)) & imag(E(I)) < 0.2) | (imag(E(I))>= -eps & imag(E(I)) < 0));
            if isirred(T{k}) && ~isempty(I)
                c=1;
            end
        end
        rhos{k} = zeros(1, 3);
        rhos{k}(1) = M(1, 1);
        rhos{k}(2) = M(2, 2);
        rhos{k}(3) = M(3, 3);
    end
end %This ends the set up of the transition matrices.

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
% What follows is what is detected by our algorithm/method — the index sets of detected clusters and the bounds given that we may interpret as strongly/weakly clustered
det_clust = cell(1, m);
bounds = cell(1, m);
for k = 1:m
    [~, det_clust{k}, bounds{k}] = findcluster(T{k}, 0);
    % Next we disregard any index sets for which the hypotheses do not hold. These cases are referenced in the bounds cell array as a character string.
    bounds{k} = bounds{k}(~cellfun(@ischar,bounds{k}));
    det_clust{k} = det_clust{k}(~cellfun(@ischar,bounds{k}));
end

% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Here we determine the amount of times (in our m simulations) that the clusters constructed initially are recovered by the algorithm
bounds2 = cell(1, m);
Eq = cell(1, m);
containing = cell(1, m);
for k = 1:m
    l = length(det_clust{k});
    Eq{k} = cell(1, 3);
```

```
    Eq{k}{1} = NaN(1, l);
    Eq{k}{2} = NaN(1, l);
    Eq{k}{3} = NaN(1, l);
    containing{k} = cell(1, 3);
    containing{k}{1} = NaN(1, l);
    containing{k}{2} = NaN(1, l);
    containing{k}{3} = NaN(1, l);
    bounds2{k} = cell(1, 3);
    if ni_fix == 1
        for j = 1:l
            Eq{k}{1}(j) = isequal(const_clust{1}, det_clust{k}{j});
            Eq{k}{2}(j) = isequal(const_clust{2}, det_clust{k}{j});
            Eq{k}{3}(j) = isequal(const_clust{3}, det_clust{k}{j});
            %Note that we do not consider C2 found 'contained' in Si if
               C1 is also contained in Si, and vice versa
            containing{k}{1}(j) = (all(ismember(const_clust{1},
               det_clust{k}{j})));
            containing{k}{2}(j) = (all(ismember(const_clust{2},
               det_clust{k}{j})));
            containing{k}{3}(j) = (all(ismember(const_clust{3},
               det_clust{k}{j})));
        end
    else
        for j = 1:l
            Eq{k}{1}(j) = isequal(const_clust{k}{1}, det_clust{k}{j});
            Eq{k}{2}(j) = isequal(const_clust{k}{2}, det_clust{k}{j});
```

```
246             Eq{k}{3}(j) = isequal(const_clust{k}{3}, det_clust{k}{j});
247             containing{k}{1}(j) = all(ismember(const_clust{k}{1},
                    det_clust{k}{j}));
248             containing{k}{2}(j) = all(ismember(const_clust{k}{2},
                    det_clust{k}{j}));
249             containing{k}{3}(j) = all(ismember(const_clust{k}{3},
                    det_clust{k}{j}));
250         end
251     end
252     %determines maximum lower bound on spectral radius for detected
            cluster containing our constructed cluster
253     X = cell2mat(bounds{k});
254     bounds2{k}{1} = max(X(find(containing{k}{1})));
255     bounds2{k}{2} = max(X(find(containing{k}{2})));
256     bounds2{k}{3} = max(X(find(containing{k}{3})));
257     if isempty(bounds2{k}{1})
258         bounds2{k}{1} = 'first cluster not detected';
259     end
260     if isempty(bounds2{k}{2})
261         bounds2{k}{2} = 'second cluster not detected';
262     end
263     if isempty(bounds2{k}{3})
264         bounds2{k}{3} = 'third cluster not detected';
265     end
266 end
267
```

```
268
269 end
```

```
1  function M = randdir(n, m, p)
2  %'randomly' produces a {0, 1} nxm matrix M where each entry is 1 with
       prob p and 0 with prob 1-p
3
4  M = rand(n, m);
5  for i = 1:n
6      for j = 1:m
7          if M(i, j) <= p
8              M(i, j) = 1;
9          else
10             M(i, j) = 0;
11         end
12     end
13 end
14
15 end
```

```
1  function T = randstochD(A)
2  %Input: A is the adjacency matrix of a directed graph D. Returns a
       random stochastic matrix with directed graph D.
3
4  n = size(A, 1);
5  m = size(A, 2);
6
```

```
T = rand(n, m).*A;

for i = 1:n
    if sum(T(i, :)) ~= 0
        T(i, :) = T(i, :)/(sum(T(i, :)));
    end
end

end
```

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