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Markov Chain-Based Stochastic Strategies for Robotic Surveillance

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by

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To everyone who has shaped my life.

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Abstract

Markov Chain-Based Stochastic Strategies for Robotic Surveillance

by

Xiaoming Duan

This thesis contains two parts. In the first part, we discuss the robotic surveillance problems, with a focus on the Markov chain-based stochastic approaches. In chapter 2, we study the problem of maximizing the return time entropy of a Markov chain, subject to graph and stationary distribution constraints. We first obtain complete characterizations for the return time distribution and show its convergence. We then establish upper and lower bounds for the return time entropy. We also provide gradients of the truncated entropy function for computational purposes. Finally, we present the numerical comparisons between the proposed and existing Markov strategies.

In chapter 3, we analyze the meeting time between a pursuer and an evader. First, by analyzing multiple random walks on a common graph as a single random walk on the Kronecker product graph, we provide a closed-form expression for the expected meeting time. This novel expression leads to necessary and sufficient graph-theoretic conditions for the meeting time to be finite. Second, we study the minimization problem for the expected capture time for the pursuer. We finally report theoretical and numerical results on basic case studies.

In chapter 4, we study the problem where the mobile robot tries to capture a strategic intruder who knows the current location and the surveillance strategy of the mobile agent. We model the scenario by a Stackelberg game and study optimal and suboptimal surveillance strategies in star, complete and line graphs. We first derive a universal upper bound on the capture probability, which is shown to be tight in the complete graph

and provides suboptimality guarantees. For the star and line graphs, we characterize dominant strategies and rigorously prove the optimal surveillance plan.

In the second part, chapter 5, we study the graph-theoretic conditions for stability of positive monotone systems. We first establish necessary and sufficient conditions for the stability of linear positive systems described by Metzler matrices. Specifically, we derive two sets of stability conditions based on two forms of input-to-state stability gains, namely max-interconnection gains and sum-interconnection gains. We then extend our results to nonlinear monotone systems.

Contents

Curriculum Vitae	vii
Abstract	x
Part I Stochastic Strategies for Robotic Surveillance	1
1 Introduction	2
1.1 Deterministic strategy	3
1.2 Stochastic strategy	4
1.3 Notation and Preliminaries	7
2 Markov Chains with Maximum Return Time Entropy	12
2.1 Introduction	12
2.2 Problem formulation	16
2.3 Properties of the return time entropy	19
2.4 Truncated return time entropy and its optimization via gradient descent	33
2.5 Numerical results	40
2.6 Conclusion	51
3 The Meeting Time of Random Walks	53
3.1 Introduction	53
3.2 Meeting times of two randomly moving agents	57
3.3 Applications to Robotic Surveillance	62
3.4 Conclusions	71
4 Robotic Surveillance as Stackelberg Games	72
4.1 Introduction	72
4.2 Preliminaries	75
4.3 Problem formulation	76
4.4 Value of the game and suboptimal solution in complete graphs	80
4.5 Strategy dominance and optimal strategies in star and line graphs	84

4.6	Conclusion	98
4.7	Appendix	99
Part II Metzler Matrices and Monotone Systems		108
5	Graph-Theoretic Stability Conditions for Metzler Matrices and Monotone Systems	109
5.1	Introduction	109
5.2	Review of Metzler matrices	113
5.3	Review of ISS, interconnected systems and ISS gains	116
5.4	Graph-theoretic conditions for Hurwitzness of Metzler matrices	122
5.5	Graph-theoretic conditions for stability of nonlinear monotone systems .	138
5.6	Additional Concepts and proofs	143
5.7	Conclusion	145
5.8	Appendix	146
Bibliography		150

Part I

Stochastic Strategies for Robotic Surveillance

Chapter 1

Introduction

The first part of this thesis presents a stochastic approach for the design of robotic surveillance algorithms. We adopt Markov chains as the main algorithmic building block and discuss various properties relevant in surveillance applications. This approach leads to easily implementable and intrinsically unpredictable surveillance algorithms in which robots' visit frequency at different locations can be conveniently specified in a probabilistic fashion. In particular, the unpredictability of a random walk over a graph is a highly desirable characteristic for surveillance strategies in adversarial settings, because it makes it hard for potential intruders to take advantage of surveillance robots' motion patterns.

In persistent surveillance tasks, mobile robots patrol and visit sites of interest in the environment to collect sensing data, detect anomalies or intercept intrusions. Persistent surveillance is a key component in numerous applications such as environmental monitoring [1, 2], infrastructure inspection [3, 4] and urban security [5]. Different from traditional coverage or search and exploration problems, surveillance tasks require robots to repeatedly visit different locations and achieve continuous monitoring. Surveillance strategies specify in which order and how often the mobile robots should visit different

locations so that desirable performance is maintained. In this survey, we adopt a model where the physical environment is discretized and modeled by a connected graph: each node of the graph represents a location of interest in the environment and the edges in the graph represent the paths between locations. Scenarios where mobile robots move in continuous space are studied for example in [6, 7, 8, 9]. There are also works that consider (stochastic) dynamics at the locations of interest such as [10, 11, 12, 13].

1.1 Deterministic strategy

In the design of deterministic surveillance strategies, the performance criterion of typical interest is *idleness*, also known as refresh time or latency. At any given time instant, the idleness of a location is the time elapsed since the last time the location was visited by any surveillance robots. The *worst idleness* (respectively, *average idleness*) at that time instant is the largest (respectively, average) value of idleness for all locations. Then, one seeks a strategy that minimizes the largest worst (average) idleness over the entire (possibly infinite) surveillance period [14]. In the early work [15], the author shows that the cyclic strategy where a robot travels with the maximum speed on a shortest closed route through all locations is optimal in the sense that it minimizes the maximum worst idleness. The author also proposes a partition-based approach for the multi-robot case where the environment is partitioned into disjoint regions so that each robot patrols a single region. In [16], a multi-robot system composed of homogeneous robots is placed on a cyclic route in the environment, and a uniform visit frequency to all locations is achieved by carefully designing the displacements between robots. The authors of [17] study team strategies with minimum refresh time for the line, tree and cyclic graphs over a finite surveillance period; optimal and constant factor suboptimal strategies are obtained. When locations have different priorities, one can define the natural notion

of *weighted worst idleness*, whereby idleness is penalized proportionally to the location priority. Single-robot surveillance strategies that minimize the maximum weighted idleness are studied in [18]. The authors design two approximate algorithms to compute strategies whose costs are within factors of the optimal cost; these factors depend on the distribution of weights or the dimension of the graph. Given constraints on the weighted idleness at all locations, the authors in [19] propose an approximate algorithm to compute the minimum number of robots required to satisfy the idleness requirements. The recent work [20] proposes surveillance plans for a fixed number of robots that minimize the maximum weighted idleness. In summary, optimization problems concerning the idleness metrics and deterministic surveillance strategies are usually of combinatorial nature and, in most cases, approximation algorithms and suboptimal solutions are sought.

While clearly leaving any location of interest in the environment unattended for an extended period of time should be avoided, there are two main challenges for deterministic surveillance strategies: (i) as pointed out in [21], it is not always possible to assign an arbitrary visit frequency to different locations in the graph (see recent related work in [22]); (ii) deterministic strategies are fully predictable and can be easily exploited by potential intruders in adversarial settings. In this case, stochastic strategies become particularly appealing.

1.2 Stochastic strategy

In adversarial settings, potential intruders may be able to observe and learn the strategies of the surveillance robot and devise intrusion plans accordingly. For example, when surveillance robot adopts a deterministic strategy, the intruder can confidently attack a location immediately after the surveillance robot leaves that location, because it knows for certain that the robot will not return to that location for a deterministic known

duration of time. In such scenarios, robotic surveillance problems have to be tackled by resorting to randomized approaches. One popular technique in such approaches is to describe the surveillance strategy as a Markov chain. There are several advantages to using Markov chains as stochastic strategies, including: 1) the intrinsic stochasticity of Markov chains leads to more effective strategies against rational intruders; 2) the visit frequency to different locations can be easily assigned through the stationary distribution; and 3) Markov chains as routing algorithms are lightweight and require minimal amount of resources to implement and execute. Although high-order Markov chains are more versatile, their state space grows exponentially fast with the order (memory length), which results in high computational complexity or intractability. Therefore, first-order Markov chains are the default choices in the design. Depending on whether an intruder model is explicitly specified or not, there are two different common formulations in the literature. When no intruder model is assumed, stochastic strategies are designed based on performance metrics such as *speed* and *unpredictability*; when a specific intruder model is adopted, tailored strategies to the intruder behaviors are carefully constructed.

1.2.1 Metric-based design

Commonly-used design metrics for stochastic strategies in robotic surveillance include visit frequency, speed and unpredictability. In [23], the authors propose a Markov chain-based algorithm for a team of robots to achieve continuous coverage of an environment with a desirable visit frequency. Smart nodes deployed at different locations are responsible for recording the visits by robots and directing robots to the next site to be visited. To obtain fast strategies for the surveillance agent, the authors of [24] study Markov chains with the minimum weighted mean hitting time. Here, travel times between different locations are given as edge weights on the graph. The minimization

of the weighted mean hitting time is transcribed into a convex optimization problem for the special case where candidate Markov chains are assumed reversible. The problem also has a semidefinite reformulation and can be solved efficiently. A similar notion of mean hitting time for a multi-robot system is proposed and studied in [25]. To obtain maximally unpredictable surveillance strategies, the authors in [26] design Markov chains with maximum entropy rate: numerous properties of the maxentropic Markov chain are established and a fast algorithm to compute the optimal strategy is proposed. A new notion that quantifies unpredictability of surveillance strategies through the entropy in return time distributions has been recently introduced and characterized in [27]. This new concept is particularly relevant and useful in cases when only local observations are available to potential intruders. Similar studies on introducing randomness in return times also appeared in [28, 29], where the authors propose to insert random delays into the return times.

1.2.2 Intruder model-based design

In contrast to the metric-based designs where no explicit intruder behaviors are assumed, intruder model-based designs leverage available information on the intruder to achieve improved/guaranteed performance. In [30], a multi-robot perimeter patrol problem is proposed where a randomized strategy is used to defend against a strategic adversary. The adversary knows the surveillance strategy as well as the robots' locations on the perimeter, and it aims to maximize its probability of success by attacking the weakest spot along the perimeter. Coordinated sequential attacks in the multi-robot perimeter patrol problem are considered in [31]. The authors in [32] define a patrolling security game where a Markovian surveillance robot tries to capture an intruder that knows perfectly the location and the strategy of the surveillance agent. The intruder has

the freedom to choose where and when to attack so that the probability of being captured is minimized. Various intruder models that characterize different manners in which the intruders attack the locations are discussed in [33]. The authors design pattern search algorithms to solve for a Markov chain that minimizes the expected reward for the intruders. Variations of intruder models where intruders have limited observation time and varying attack duration are studied in [34] and [35], respectively. Many of the aforementioned models can be formalized as Stackelberg games. The Stackelberg game framework has been successfully applied in practical security domain applications [36]. However, only limited progress on efficient computational methods with optimality guarantees has been made.

1.3 Notation and Preliminaries

1.3.1 Notation

Let \mathbb{R} , \mathbb{R}^n and $\mathbb{R}^{m \times n}$ be the set of real numbers, real vectors of dimension n and real matrices of dimension m by n , respectively. The set of elementwise positive vectors and nonnegative matrices are denoted by $\mathbb{R}_{>0}^n$ and $\mathbb{R}_{\geq 0}^{m \times n}$. We denote the set of nonnegative and positive integers by $\mathbb{Z}_{\geq 0}$, and $\mathbb{Z}_{>0}$. Let $\mathbf{1}_n$ and $\mathbf{0}_n$ be column vectors in \mathbb{R}^n with all entries being 1 and 0, and \mathbf{e}_i be the i -th standard unit vector, whose dimension will be clear from the context. For a vector $v \in \mathbb{R}^n$, $\text{diag}(v) \in \mathbb{R}^{n \times n}$ is a diagonal matrix with diagonal elements being v ; for a matrix $S \in \mathbb{R}^{n \times n}$, $\text{diag}(S) \in \mathbb{R}^{n \times n}$ is a diagonal matrix with diagonal elements being the same as that of S . For a matrix $S \in \mathbb{R}^{m \times n}$, the vectorization $\text{vec}(S) \in \mathbb{R}^{mn}$ is constructed by stacking the columns of S on top of one another. The identity matrix is denoted by $I_n \in \mathbb{R}^{n \times n}$, and the indicator function is denoted by $\mathbf{1}_{\{\cdot\}}$.

1.3.2 Markov chains

A first-order discrete-time homogeneous Markov chain defined over the state space $\{1, \dots, n\}$ is a sequence of random variables X_k for $k \geq 0$ that satisfies the Markov property: $\mathbb{P}(X_{k+1} = i_{k+1} | X_k = i_k, \dots, X_0 = i_0) = \mathbb{P}(X_{k+1} = i_{k+1} | X_k = i_k)$ for all $k \geq 0$ and $i_0, \dots, i_{k+1} \in \{1, \dots, n\}$. The Markov chain $\{X_k\}_{k \geq 0}$ has an associated row-stochastic transition matrix $P \in \mathbb{R}^{n \times n}$ such that the (i, j) -th element $p_{ij} = \mathbb{P}(X_{k+1} = j | X_k = i)$ for $i, j \in \{1, \dots, n\}$. The transition diagram of a Markov chain is a directed graph $\mathcal{G} = (V, \mathcal{E})$, where $V = \{1, \dots, n\}$ is the set of nodes and $\mathcal{E} \subset V \times V$ is the set of edges, and $(i, j) \in \mathcal{E}$ if and only if $p_{ij} > 0$. A Markov chain is irreducible if its transition diagram is strongly connected. A walk of length ℓ exists from node i_1 to node $i_{\ell+1}$ for \mathcal{G} if there exists a sequence of nodes $i_1, i_2, \dots, i_{\ell+1}$ such that $p_{i_k i_{k+1}} > 0$ for $1 \leq k \leq \ell$. The period of a state i is defined as the greatest common divisor of all k in $\{k \geq 1 | \mathbb{P}(X_k = i | X_0 = i) \neq 0\}$. A state whose period is one is referred to as an aperiodic state, and a Markov chain is aperiodic if the greatest common divisor of all states' periods is one. The states in a communicating class (defined below) share the same period. For two states i and j of a Markov chain, state i communicates with j if $\mathbb{P}(X_k = j | X_0 = i) \neq 0$ for some $k > 0$. A subset of states $X \subset \{1, \dots, n\}$ forms a communicating class if for every state $i, j \in X$ the states communicate with each other, i.e., $\mathbb{P}(X_k = j | X_0 = i) \neq 0$ and $\mathbb{P}(X_{k'} = i | X_0 = j) \neq 0$ for some $k, k' > 0$. An absorbing class $C \subset \{1, \dots, n\}$ of a Markov chain is a communicating class such that the probability of escaping the set is zero, i.e., $\mathbb{P}(X_k = j | X_0 = i) = 0$ for all $k > 0$ and $i \in C, j \notin C$. A communicating class that is not absorbing is a transient class. A discrete-time Markov chain is said to be *ergodic* if it is irreducible and aperiodic. A finite-state irreducible Markov chain P has a unique stationary distribution $\boldsymbol{\pi} \in \mathbb{R}^n$ that satisfies $\boldsymbol{\pi}^\top P = \boldsymbol{\pi}^\top$ and $\pi_i > 0$ for $i \in \{1, \dots, n\}$. Moreover, the stationary distribution

π has the interpretation that regardless of the initial condition [37, Theorem 2.1],

$$\frac{1}{t+1} \sum_{k=0}^t \mathbf{1}_{\{X_k=i\}} \xrightarrow{\text{as } t \rightarrow \infty} \pi_i \quad \text{almost surely.} \quad (1.1)$$

We refer the readers to [38, 39] for more about Markov chains.

1.3.3 Hitting times of Markov chains

For a finite-state discrete-time Markov chain, the first hitting time from state i to state j is a random variable defined by

$$T_{ij} = \min\{k \mid X_0 = i, X_k = j, k \geq 1\}. \quad (1.2)$$

This notion can be extended to Markov chains defined over a weighted graph $\mathcal{G} = (V, \mathcal{E}, W)$, in which case the hitting time T_{ij} satisfies

$$T_{ij} = \min\left\{\sum_{\ell=0}^{k-1} w_{X_\ell, X_{\ell+1}} \mid X_0 = i, X_k = j, k \geq 1\right\}. \quad (1.3)$$

The computation of the hitting time distributions will be made clear when they are used in respective chapters.

1.3.4 Kronecker product and Kronecker graph

For two matrices $A \in \mathbb{R}^{n \times m}$ and $B \in \mathbb{R}^{q \times r}$, the Kronecker product $A \otimes B$ is an $nq \times mr$ matrix given by

$$A \otimes B = \begin{bmatrix} a_{1,1}B & \dots & a_{1,m}B \\ \vdots & \ddots & \vdots \\ a_{n,1}B & \ddots & a_{n,m}B \end{bmatrix}.$$

A few properties of the Kronecker product and vectorization of matrices are summarized in the following lemma.

Lemma 1.3.4.1 (Kronecker product and vectorization identities) *Given matrices A, B, C and D of appropriate dimensions, the following identities hold:*

1. $(A \otimes B)(C \otimes D) = (AC) \otimes (BD),$
2. $(B^\top \otimes A) \text{vec}(C) = \text{vec}(ACB).$

Given two graphs $\mathcal{G}_1 = (V_1, \mathcal{E}_1)$ and $\mathcal{G}_2 = (V_2, \mathcal{E}_2)$, where V_i and \mathcal{E}_i are the set of vertices and edges for $i \in \{1, 2\}$, the Kronecker graph of \mathcal{G}_1 and \mathcal{G}_2 is a graph $\mathcal{G} = (V_1 \times V_2, \mathcal{E})$ such that for any $i_1, j_1 \in V_1$ and $i_2, j_2 \in V_2$, the edge $((i_1, i_2), (j_1, j_2)) \in \mathcal{E}$ if $(i_1, j_1) \in \mathcal{E}_1$ and $(i_2, j_2) \in \mathcal{E}_2$.

1.3.5 Useful Lemmas

We collect a few lemmas that shall be used in the rest of the thesis.

Lemma 1.3.5.1 (Convergence of row-substochastic matrices [25, Lemma 2.2])

Any row-substochastic matrix $A \in \mathbb{R}^{n \times n}$ has spectral radius less than 1 if and only if for every node with row-sum 1 there exists a walk to a node with row-sum less than 1.

Lemma 1.3.5.2 (*A uniform bound for stable matrices [40, Proposition D.3.1]*) Assume the matrix subset $\mathcal{A} \subset \mathbb{R}^{n \times n}$ is compact and satisfies

$$\rho_{\mathcal{A}} := \max_{A \in \mathcal{A}} \rho(A) < 1,$$

where $\rho(A)$ is the spectral radius of the matrix A . Then for any $\lambda \in (\rho_{\mathcal{A}}, 1)$ and for any induced matrix norm $\|\cdot\|$, there exists $c > 0$ such that

$$\|A^k\| \leq c\lambda^k, \quad \text{for all } A \in \mathcal{A} \text{ and } k \in \mathbb{Z}_{\geq 0}.$$

Lemma 1.3.5.3 (*Weierstrass M-test [41, Theorem 7.10]*) Given a set \mathcal{X} , consider the sequence of functions $\{f_k : \mathcal{X} \rightarrow \mathbb{R}\}_{k \in \mathbb{Z}_{>0}}$. If there exists a sequence of scalars $\{M_k \in \mathbb{R}\}_{k \in \mathbb{Z}_{>0}}$ satisfying $\sum_{k=1}^{\infty} M_k < \infty$ and

$$|f_k(x)| \leq M_k, \quad \text{for all } x \in \mathcal{X}, k \in \mathbb{Z}_{>0},$$

then $\sum_{k=1}^{\infty} f_k$ converges uniformly on \mathcal{X} .

Lemma 1.3.5.4 (*Geometric distribution generates maximum entropy [42]*) Among all discrete random variables $Y \in \mathbb{Z}_{>0}$ with $\mathbb{E}[Y] = \mu \geq 1$, the probability distribution with maximum entropy is

$$\mathbb{P}(Y = k) = \left(1 - \frac{1}{\mu}\right)^{k-1} \frac{1}{\mu}, \quad k \in \mathbb{Z}_{>0},$$

with entropy

$$\mathbb{H}(Y) = \mu \log \mu - (\mu - 1) \log(\mu - 1). \quad (1.4)$$

Chapter 2

Markov Chains with Maximum Return Time Entropy

2.1 Introduction

2.1.1 Problem description and motivation

Given a Markov chain, the first return time of a given node is the first time that the random walker returns to the starting node; this is a discrete random variable with infinite support, whose randomness is measured by its entropy. In this chapter, given a strongly connected directed graph with integer-valued travel times (weights) and a prescribed stationary distribution, we study Markov chains with maximum return time entropy. Here the return time entropy of a Markov chain is a weighted average of the entropy of different states' return times with weights equal to the stationary distribution.

This optimization problem is motivated by robotic applications. We design stochastic surveillance strategies with an entropy maximization objective in order to thwart intruders who plan their attacks based on observations of the surveillance agent. The

randomness in the first return time is desirable because an intelligent intruder observing the inter-visit times of the surveillance agent is confronted with a maximally unpredictable return pattern by the surveillance agent. The advantages of formulating an entropy maximization problem are fourfold: a) entropy is a well-established fundamental concept that characterizes the randomness of a probability distribution (unpredictability in the surveillance strategy in our case); b) if the surveillance agent is highly entropic, it is hard for the intruders to learn the patterns in the behavior of the agent; c) since the behaviors of the intruders may not be exactly known/modelled in any case, optimizing the surveillance strategies against certain intruder behaviors may not be generally wise; d) as we demonstrate in the simulation section, the Markov chain with maximum return time entropy works well under a rational intruder model.

2.1.2 Literature review

Ekroot *et al.* studied the entropy of Markov trajectories in [43], i.e., the entropy of paths with specified initial and final states. The authors establish an equivalence relationship between the entropy of return Markov trajectories (paths with the same initial and final states) and the entropy rate of the Markov chains. Compared with [43], we study here the return time random variable, by lumping return trajectories with the same length. Importantly, our formulation incorporates travel times, as motivated by robotic applications.

The problem of designing robotic surveillance strategies has been widely studied [44, 18, 45, 11]. Stochastic surveillance strategies, which emphasize the unpredictability of the movement of the patroller, are desirable since they are capable of defending against intelligent intruders who aim to avoid detection/capture. One of the main approaches to the design of robotic stochastic surveillance strategies is to adopt Markov chains; e.g.,

see the early reference [46] and the more recent references [47, 48, 23, 49]. Srivastava *et al.* [21] justified the Markov chain-based stochastic surveillance strategy by showing that for the deterministic strategies, in addition to predictability, it is also hard to specify the visit frequency. However, for the finite state irreducible Markov chains, the visit frequency is embedded naturally in the stationary distribution. Patel *et al.* [24] studied the Markov chains with minimum weighted mean hitting time where weights are travel times on edges. For the class of reversible Markov chains, they formulated the problem as a convex optimization problem. An extension of the mean hitting time to the multi-agent case was studied in [25]. Asghar *et al.* [33] introduced different intruder models and designed a pattern search-based algorithm to solve for a Markov chain that minimizes the expected reward of the intruders. Recently, George *et al.* [26] studied and quantified the unpredictability of the Markov chains and designed the maximal entropy surveillance strategies by maximizing the entropy rate of Markov chains [50, 51]. Compared with [26], our problem formulation features a new notion of entropy, a directed graph topology, and travel times; these three features render the results potentially more widely applicable and more relevant (see also the performance comparison among multiple Markov chains later in the chapter).

2.1.3 Statement of Contributions

In this chapter, we propose a new metric that measures the unpredictability of the Markov chains over a directed graph with travel times. This novel formulation is of interest in the general study of Markov chains as well as for its applications to the robotic surveillance. Specifically, the notion of return time entropy is extremely relevant in the natural setting where the intruder hides near a location, collects inter-visit data of the surveillance agent, learns the return statistics/patterns and plans an attack with

the lowest chance of being detected. The main contributions of this chapter are sixfold. First, we introduce and analyze a discrete-time delayed linear system for the return time probabilities of the Markov chains. This system incorporates integer-valued travel times on the directed graph. Second, we propose to characterize the unpredictability of a Markov chain by the return time entropy and formulate an entropy maximization problem. Third, we prove the well-posedness of the return time entropy maximization problem, i.e., the objective function is continuous over a compact set and thus admits a global maximum. For the case of unitary travel times, we derive an upper bound for the return time entropy and solve the problem analytically for the complete graph. Fourth, we compare the return time entropy with the entropy rate of Markov chains; specifically, we prove that the return time entropy is lower bounded by the entropy rate and upper bounded by the number of nodes times of the entropy rate. Fifth, in order to compute Markov chains with maximum return time entropy numerically, we truncate the return time entropy and show that the truncated entropy is asymptotically equivalent to both the original objective and the practically useful conditional return time entropy. We also characterize the gradient of the truncated return time entropy and use it to implement a gradient projection algorithm. Sixth, we apply our solution to different prototypical robotic surveillance scenarios and test cases and show that, for a model of rational intruder, the Markov chain with maximum return time entropy outperforms several existing Markov chains.

The main content of this chapter lead to one conference publication [52] and one journal publication [27].

2.1.4 Organization

This chapter is organized as follows. We formulate the return time entropy maxi-

mization problem in Section 2.2. We establish the properties of the return time entropy in Section 2.3. The approximation analysis and the gradient formulas are provided in Section 2.4. We present the simulation results regarding the robotic surveillance problem in Section 2.5. Section 2.6 concludes the chapter.

2.2 Problem formulation

2.2.1 Return time of random walks

In this chapter, we consider a strongly connected directed weighted graph $\mathcal{G} = (V, \mathcal{E}, W)$, where V denotes the set of n nodes $\{1, \dots, n\}$, $\mathcal{E} \subset V \times V$ denotes the set of edges, and $W \in \mathbb{Z}_{\geq 0}^{n \times n}$ is the integer-valued weight (travel time) matrix with w_{ij} being the one-hop travel time from node i to node j . If $(i, j) \notin \mathcal{E}$, then $w_{ij} = 0$; if $(i, j) \in \mathcal{E}$, then $w_{ij} \geq 1$. Let $w_{\max} = \max_{i,j} \{w_{ij}\}$ be the maximum travel time. The *return time* T_{ii} of node i is the first time the random walk returns to node i starting from node i . Let the (i, j) -th element of the *first hitting time probability matrix* F_k denote the probability that the random walk reaches node j for the first time in exactly k time units starting from node i , i.e., $F_k(i, j) = \mathbb{P}(T_{ij} = k)$.

2.2.2 Return time entropy of random walks

For an irreducible Markov chain, the return time T_{ii} of each state i is a well-defined random variable over $\mathbb{Z}_{>0}$. We define the *return time entropy of state i* by

$$\mathbb{H}(T_{ii}) = - \sum_{k=1}^{\infty} \mathbb{P}(T_{ii} = k) \log \mathbb{P}(T_{ii} = k) = - \sum_{k=1}^{\infty} F_k(i, i) \log F_k(i, i),$$

where the logarithm is the natural logarithm and $0 \log 0 = 0$.

We define the set of Markov chains we will be optimizing over in the following.

Definition 2.2.2.1 *(The set of Markov chains ϵ -conforming to a graph) Given a strongly connected directed weighted graph $\mathcal{G} = (V, \mathcal{E}, W)$ with n nodes and the stationary distribution $\boldsymbol{\pi} > 0$, pick a minimum transition probability $\epsilon > 0$, the set of Markov chains ϵ -conforming to \mathcal{G} is defined by*

$$\begin{aligned} \mathcal{P}_{\mathcal{G}, \boldsymbol{\pi}}^\epsilon &= \{P \in \mathbb{R}^{n \times n} \mid p_{ij} \geq \epsilon \text{ if } (i, j) \in \mathcal{E}, \\ &\quad p_{ij} = 0 \text{ if } (i, j) \notin \mathcal{E}, \\ &\quad P\mathbf{1}_n = \mathbf{1}_n, \boldsymbol{\pi}^\top P = \boldsymbol{\pi}^\top\}. \end{aligned}$$

Given the definition of $\mathcal{P}_{\mathcal{G}, \boldsymbol{\pi}}^\epsilon$, we are now ready to define the *return time entropy* function $\mathbb{J}(P)$ over the set $\mathcal{P}_{\mathcal{G}, \boldsymbol{\pi}}^\epsilon$.

Definition 2.2.2.2 *(Return time entropy) Given a set $\mathcal{P}_{\mathcal{G}, \boldsymbol{\pi}}^\epsilon$, define the return time entropy function $\mathbb{J} : \mathcal{P}_{\mathcal{G}, \boldsymbol{\pi}}^\epsilon \mapsto \mathbb{R}_{\geq 0}$ by*

$$\mathbb{J}(P) = \sum_{i=1}^n \pi_i \mathbb{H}(T_{ii}). \quad (2.1)$$

Remark 2.2.2.3 *(The expectation of the first return time) For an irreducible Markov chain defined over a weighted graph with travel times, [24, Theorem 6] states*

$$\mathbb{E}[T_{ii}] = \frac{\boldsymbol{\pi}^\top (P \circ W) \mathbf{1}_n}{\pi_i}, \quad (2.2)$$

where \circ is the Hadamard element-wise product. For unitary travel times, this formula reduces to the usual $\mathbb{E}[T_{ii}] = 1/\pi_i$. In both cases, the first return times expectations are inversely proportional to the entries of $\boldsymbol{\pi}$.

In general, it is difficult to obtain the closed-form expression for the return time entropy function.

Examples 2.2.2.4 *(Two special cases with unitary travel times) The elementary proofs of the following results are omitted in the interest of brevity.*

1. *(Two-node complete graph case) Given a two-node complete graph \mathcal{G} with unit weights, if the transition matrix $P \in \mathcal{P}_{\mathcal{G}, \pi}^e$ has the following form*

$$P = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix},$$

then the return time entropy function is

$$\mathbb{J}(P) = -2\pi_1 p_{11} \log(p_{11}) - 2\pi_2 p_{22} \log(p_{22}) - 2\pi_1 p_{12} \log(p_{12}) - 2\pi_2 p_{21} \log(p_{21}).$$

2. *(Complete graph case with special structure) Given an $n \geq 2$ -node complete graph \mathcal{G} with unit weights and the stationary distribution $\pi = \frac{1}{n}\mathbb{1}_n$, if the transition matrix $P \in \mathcal{P}_{\mathcal{G}, \pi}^e$ has the form*

$$P = (a - b)I_n + b\mathbb{1}_n\mathbb{1}_n^\top,$$

for any $a \geq 0$ and $b > 0$ satisfying $a + (n - 1)b = 1$, then the return time entropy function is

$$\mathbb{J}(P) = -a \log(a) - (n - 1)b \log((n - 1)b) - (n - 1)(1 - b) \log(1 - b).$$

In this chapter, we are interested in the following problem.

Problem 1 (*Maximization of the return time entropy*) Given a strongly connected directed weighted graph $\mathcal{G} = (V, \mathcal{E}, W)$ and the stationary distribution $\boldsymbol{\pi} > 0$, pick a minimum transition probability $\epsilon > 0$. Find $P \in \mathcal{P}_{\mathcal{G}, \boldsymbol{\pi}}^\epsilon$ which maximizes the return time entropy $\mathbb{J}(P)$, i.e., solve the following optimization problem:

$$\begin{aligned} & \text{maximize} \quad \mathbb{J}(P) \\ & \text{subject to} \quad P \in \mathcal{P}_{\mathcal{G}, \boldsymbol{\pi}}^\epsilon \end{aligned}$$

2.3 Properties of the return time entropy

2.3.1 Dynamical model for hitting time probabilities

In this subsection, we characterize a dynamical model for the first hitting time probabilities and establish several important properties of the model. This dynamical model will be used to prove the well-posedness of Problem 1, and it is also used to compute the hitting time probabilities and their gradients in later sections.

Theorem 2.3.1.1 (*Linear dynamics for the first hitting time probabilities*) Consider a transition matrix $P \in \mathbb{R}^{n \times n}$ that is nonnegative, row-stochastic and irreducible. Then

1. the hitting time probabilities F_k , $k \in \mathbb{Z}_{>0}$, satisfy the discrete-time delayed linear system with a finite number of impulse inputs:

$$\text{vec}(F_k) = \text{vec}(P \circ \mathbf{1}_{\{k\mathbf{1}_n \mathbf{1}_n^\top = W\}}) + \sum_{i=1}^n \sum_{j=1}^n p_{ij} (E_j \otimes \mathbf{e}_i \mathbf{e}_j^\top) \text{vec}(F_{k-w_{ij}}), \quad (2.3)$$

where $E_i = \text{diag}(\mathbf{1}_n - \mathbf{e}_i) \in \mathbb{R}^{n \times n}$, $\mathbf{1}_{\{\cdot\}}$ is the indicator function, and the initial conditions are $\text{vec}(F_k) = \mathbf{0}_{n^2 \times 1}$ for all $k \leq 0$;

2. if the weights are unitary, i.e., $w_{ij} \in \{0, 1\}$, then the hitting time probabilities

satisfy

$$\text{vec}(F_k) = (I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n))) \text{vec}(F_{k-1}), \quad (2.4)$$

where the initial condition is $F_1 = P$.

Proof: By the definition in (1.3), $F_k(i, j)$ satisfies the following recursive formula for $k \in \mathbb{Z}_{>0}$

$$F_k(i, j) = p_{ij} \mathbf{1}_{\{k=w_{ij}\}} + \sum_{h=1, h \neq j}^n p_{ih} F_{k-w_{ih}}(h, j), \quad (2.5)$$

where $F_k(i, j) = 0$ for all $k \leq 0$ and $i, j \in V$.

Let $D_k(i) \in \mathbb{R}^{n \times n}$ be a matrix associated with node i at time k that has the form

$$D_k(i) = \sum_{h \in \mathcal{N}_i} \mathbf{e}_h \mathbf{e}_h^\top F_{k-w_{ih}},$$

where \mathcal{N}_i is the set of out-going neighbors of node i . The matrix $D_k(i)$, serving as an intermediate variable, selects the rows from the matrices $F_{k-w_{ih}}$ used in (2.5), and the summation in (2.5) can be written as

$$\sum_{h=1, h \neq j}^n p_{ih} F_{k-w_{ih}}(h, j) = \mathbf{e}_i^\top P(D_k(i) - \text{diag}(D_k(i))) \mathbf{e}_j.$$

Then, (2.5) can be written in the following matrix form

$$F_k = P \circ \mathbf{1}_{\{k \mathbf{1}_n \mathbf{1}_n^\top = W\}} + \sum_{i=1}^n \mathbf{e}_i \mathbf{e}_i^\top P(D_k(i) - \text{diag}(D_k(i))). \quad (2.6)$$

Vectorizing both sides of (2.6), we have

$$\text{vec}(F_k) = \text{vec}(P \circ \mathbf{1}_{\{k \mathbf{1}_n \mathbf{1}_n^\top = W\}}) + \sum_{i=1}^n (I_n \otimes \mathbf{e}_i \mathbf{e}_i^\top P)(I_{n^2} - \text{diag}(\text{vec}(I_n))) \text{vec}(D_k(i)). \quad (2.7)$$

Note that in (2.7), by the definition of $D_k(i)$, we have

$$\text{vec}(D_k(i)) = \sum_{j \in \mathcal{N}_i} (I_n \otimes \mathbf{e}_j \mathbf{e}_j^\top) \text{vec}(F_{k-w_{ij}}),$$

and

$$(I_{n^2} - \text{diag}(\text{vec}(I_n)))(I_n \otimes \mathbf{e}_j \mathbf{e}_j^\top) = E_j \otimes \mathbf{e}_j \mathbf{e}_j^\top.$$

Therefore, the summation in (2.7) can be written as

$$\begin{aligned} & \sum_{i=1}^n (I_n \otimes \mathbf{e}_i \mathbf{e}_i^\top P)(I_{n^2} - \text{diag}(\text{vec}(I_n))) \text{vec}(D_k(i)) \\ &= \sum_{i=1}^n (I_n \otimes \mathbf{e}_i \mathbf{e}_i^\top P) \sum_{j \in \mathcal{N}_i} (E_j \otimes \mathbf{e}_j \mathbf{e}_j^\top) \text{vec}(F_{k-w_{ij}}) \\ &= \sum_{i=1}^n \sum_{j \in \mathcal{N}_i} (E_j \otimes \mathbf{e}_i \mathbf{e}_i^\top P \mathbf{e}_j \mathbf{e}_j^\top) \text{vec}(F_{k-w_{ij}}) \\ &= \sum_{i=1}^n \sum_{j=1}^n p_{ij} (E_j \otimes \mathbf{e}_i \mathbf{e}_j^\top) \text{vec}(F_{k-w_{ij}}). \end{aligned}$$

Thus, we have (2.3).

Moreover, if the travel times are unitary, then $F_1 = P$ and

$$\sum_{i=1}^n \sum_{j=1}^n p_{ij} (E_j \otimes \mathbf{e}_i \mathbf{e}_j^\top) = (I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n))). \quad (2.8)$$

Thus, equation (2.4) follows. ■

The dynamical system (2.3) can be transformed to an equivalent homogeneous linear system by restarting the system at $k = w_{\max}$ with same system matrices and appropriate initial conditions. Moreover, we can augment the system and obtain a discrete-time linear system without delays. This equivalent augmented system is useful for example in

studying stability properties. For $k \geq 1$, we have

$$\begin{bmatrix} \text{vec}(F_{k+w_{\max}}) \\ \text{vec}(F_{k+w_{\max}-1}) \\ \vdots \\ \text{vec}(F_{k+1}) \end{bmatrix} = \Psi \begin{bmatrix} \text{vec}(F_{k+w_{\max}-1}) \\ \text{vec}(F_{k+w_{\max}-2}) \\ \vdots \\ \text{vec}(F_k) \end{bmatrix}, \quad (2.9)$$

where

$$\Psi = \begin{bmatrix} \Phi_1 & \Phi_2 & \cdots & \cdots & \Phi_{w_{\max}} \\ I_{n^2} & \mathbb{O}_{n^2 \times n^2} & \cdots & \cdots & \mathbb{O}_{n^2 \times n^2} \\ \mathbb{O}_{n^2 \times n^2} & I_{n^2} & \cdots & \cdots & \mathbb{O}_{n^2 \times n^2} \\ \vdots & \vdots & \ddots & \cdots & \mathbb{O}_{n^2 \times n^2} \\ \mathbb{O}_{n^2 \times n^2} & \cdots & \cdots & I_{n^2} & \mathbb{O}_{n^2 \times n^2} \end{bmatrix}, \quad (2.10)$$

and for $h \in \{1, \dots, w_{\max}\}$,

$$\Phi_h = \sum_{i=1}^n \sum_{j=1}^n p_{ij}(E_j \otimes \mathbf{e}_i \mathbf{e}_j^\top) \mathbf{1}_{\{w_{ij}=h\}}. \quad (2.11)$$

The initial conditions for (2.9) can be computed using (2.3). For brevity, we denote $\left[\text{vec}(F_{k+w_{\max}-1})^\top \cdots \text{vec}(F_k)^\top \right]^\top$ by $\text{vec}(\tilde{F}_k)$.

Lemma 2.3.1.2 (*Properties of the linear dynamics for the first hitting time probabilities*)

If $P \in \mathbb{R}^{n \times n}$ is nonnegative, row-stochastic and irreducible, then

1. the matrix $(I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n)))$ is row-substochastic with the spectral radius $\rho((I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n)))) < 1$.
2. the delayed discrete-time linear system with a finite number of impulse inputs (2.3) is asymptotically stable;
3. $\text{vec}(F_k) \geq 0$ for $k \in \mathbb{Z}_{>0}$ and $\sum_{k=1}^{\infty} \text{vec}(F_k) = \mathbf{1}_{n^2 \times 1}$.

Proof: Regarding (i), note that the matrix $(I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n)))$ is block diagonal with the i -th block being PE_i . Since P is irreducible, PE_i 's are row-substochastic and so is $(I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n)))$. By Lemma 1.3.5.1, $\rho(PE_i) < 1$ for all $i \in \{1, \dots, n\}$ and $\rho((I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n)))) = \max_i \rho(PE_i) < 1$.

Regarding (ii), since we can rewrite (2.3) as (2.9) with appropriate initial conditions and Φ_i 's are nonnegative, by the stability criterion for delayed linear systems [53, Theorem 1], (2.3) is asymptotically stable if

$$\rho\left(\sum_{i=1}^{w_{\max}} \Phi_i\right) = \rho((I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n)))) < 1,$$

which is true by (i).

Regarding (iii), first note that all the system matrices are nonnegative, thus $\text{vec}(F_k) \geq 0$ for all $k \in \mathbb{Z}_{>0}$. Moreover, due to (ii), the delayed linear system (2.3) is asymptotically stable. Summing both sides of (2.3) over k , we have

$$\begin{aligned} \sum_{k=1}^{\infty} \text{vec}(F_k) &= \text{vec}(P) + \sum_{i=1}^n \sum_{j=1}^n p_{ij}(E_j \otimes \mathbf{e}_i \mathbf{e}_j^{\top}) \sum_{k=1}^{\infty} \text{vec}(F_k) \\ &= \text{vec}(P) + (I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n))) \sum_{k=1}^{\infty} \text{vec}(F_k). \end{aligned}$$

Note that $\sum_{k=1}^{\infty} \text{vec}(F_k) = \mathbf{1}_{n^2 \times 1}$ is a solution, and by the proof of (ii), we have $\rho((I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n)))) < 1$. Therefore, $I_{n^2} - (I_n \otimes P)(I_{n^2} - \text{diag}(\text{vec}(I_n)))$ is invertible, which implies that $\mathbf{1}_{n^2 \times 1}$ is the unique solution. ■

2.3.2 Well-posedness of the optimization problem

We here show that the function \mathbb{J} is continuous over the compact set $\mathcal{P}_{\mathcal{G}, \pi}^{\epsilon}$. Then, by the extreme value theorem, \mathbb{J} has a (possibly non-unique) maximum point in the set and

thus Problem 1 is well-posed.

Lemma 2.3.2.1 (*Continuity of the return time entropy function*) *Given the compact set $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$, the following statements hold:*

1. *there exist constants $\lambda_{\max} \in (0, 1)$ and $c > 0$ such that*

$$F_k(i, i) \leq c\lambda_{\max}^k, \quad \text{for all } k \in \mathbb{Z}_{>0}, i \in \{1, \dots, n\};$$

2. *the return time entropy functions $\mathbb{H}(T_{ii})$, $i \in \{1, \dots, n\}$, and $\mathbb{J}(P)$ are continuous on the compact set $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$; and*

3. *Problem 1 is well-posed in the sense that a global optimum exists.*

Proof: Regarding (i), for $k \geq w_{\max} + 1$, since the spectral radius $\rho(\Psi)$ is a continuous function of Ψ [54, Example 7.1.3], where Ψ is given in (2.10), and Ψ is a continuous function of P , $\rho(\Psi)$ is a continuous function of P . Hence, by Lemma 2.3.1.2(ii) and the extreme value theorem, there exists a $\rho_{\max} < 1$ such that

$$\rho_{\max} = \max_{P \in \mathcal{P}_{\mathcal{G},\pi}^\epsilon} \rho(\Psi) < 1.$$

Therefore, for $k \geq w_{\max} + 1$ and $i \in \{1, \dots, n\}$, by Lemma 1.3.5.2, there exist $c_1 > 0$ and $\rho_{\max} < \lambda_{\max} < 1$ such that

$$\begin{aligned} F_k(i, i) &\leq \|\text{vec}(\tilde{F}_{k-w_{\max}+1})\|_\infty \\ &= \|(\Psi)^{k-w_{\max}} \text{vec}(\tilde{F}_1)\|_\infty \\ &\leq \|(\Psi)^{k-w_{\max}}\|_\infty \|\text{vec}(\tilde{F}_1)\|_\infty \\ &\leq c_1 \lambda_{\max}^{k-w_{\max}} = \frac{c_1}{\lambda_{\max}^{w_{\max}}} \lambda_{\max}^k. \end{aligned}$$

Let $c = \max\{\frac{c_1}{\lambda_{\max}^{w_{\max}}}, \frac{1}{\lambda_{\max}^{w_{\max}}}\}$, then we have for $k \geq w_{\max} + 1$,

$$F_k(i, i) \leq \frac{c_1}{\lambda_{\max}^{w_{\max}}} \lambda_{\max}^k \leq c \lambda_{\max}^k.$$

For $k \leq w_{\max}$,

$$c \lambda_{\max}^k \geq c \lambda_{\max}^{w_{\max}} \geq 1 \geq F_k(i, i).$$

Therefore, we have (i).

Regarding (ii), due to (i), there exists a positive integer K that does not depend on the elements of $\mathcal{P}_{\mathcal{G}, \pi}^\epsilon$ such that when $k \geq K$, $c \lambda_{\max}^k \leq e^{-1}$. Since $x \mapsto -x \log x$ is an increasing function for $x \in [0, e^{-1}]$, when $k \geq K$,

$$-F_k(i, i) \log F_k(i, i) \leq -c \lambda_{\max}^k \log(c \lambda_{\max}^k) := M_k.$$

For $k < K$, $-F_k(i, i) \log F_k(i, i) \leq e^{-1} := M_k$. Then

$$\sum_{k=1}^{K-1} M_k = \frac{K-1}{e},$$

and

$$\begin{aligned} \sum_{k=K}^{\infty} M_k &= - \sum_{k=K}^{\infty} c \lambda_{\max}^k \log(c \lambda_{\max}^k) \\ &= -c \log c \sum_{k=K}^{\infty} \lambda_{\max}^k - c \log(\lambda_{\max}) \sum_{k=K}^{\infty} k \lambda_{\max}^k \\ &= -c \left(\frac{\lambda_{\max}^K}{1 - \lambda_{\max}} \log(c \lambda_{\max}^K) + \frac{\lambda_{\max}^{K+1}}{(1 - \lambda_{\max})^2} \log(\lambda_{\max}) \right). \end{aligned} \tag{2.12}$$

Hence,

$$\sum_{k=1}^{\infty} M_k = \sum_{k=1}^{K-1} M_k + \sum_{k=K}^{\infty} M_k < \infty,$$

which holds for any i and any transition matrix in the compact set $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$. By Lemma 1.3.5.3, the series $-\sum_{k=1}^{\infty} F_k(i, i) \log F_k(i, i)$ converges uniformly. Since the limit of a uniformly convergent series of continuous function is continuous [41, Theorem 7.12], $\mathbb{H}(T_{ii})$ is a continuous function on $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$. Finally, $\mathbb{J}(P)$ is a finite weighted sum of continuous functions $\mathbb{H}(T_{ii})$, thus $\mathbb{J}(P)$ is a continuous function.

Regarding (iii), because \mathbb{J} is a continuous function over the compact set $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$, the extreme value theorem ensures that Problem 1 admits a global optimum solution (possibly non-unique) and is therefore well-posed. ■

2.3.3 Optimal solution for complete graphs with unitary travel times

We here provide: 1) an upper bound for the return time entropy with unitary travel times based on the principle of maximum entropy and 2) the optimal solution to Problem 1 for the complete graph case with unitary travel times.

Lemma 2.3.3.1 (*Maximum achieved return time entropy in a complete graph with unitary weights*) Given a strongly connected graph \mathcal{G} with unitary weights and the compact set $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$,

1. the return time entropy function is upper bounded by

$$\mathbb{J}(P) \leq - \sum_{i=1}^n (\pi_i \log \pi_i + (1 - \pi_i) \log(1 - \pi_i));$$

2. when the graph \mathcal{G} is complete, the upper bound is achieved and the transition matrix that maximizes the return time entropy $\mathbb{J}(P)$ is given by $P = \mathbb{1}_n \boldsymbol{\pi}^\top$.

Proof: Regarding (i), by Remark 2.2.2.3, in the case of unitary travel times, we have $\mathbb{E}[T_{ii}] = 1/\pi_i$. Thus, T_{ii} is a discrete random variable over the set of positive integers with fixed expectation $1/\pi_i$, whose entropy is bounded as shown in Lemma 1.3.5.4. For any transition matrix $P \in \mathcal{P}_{\mathcal{G}, \boldsymbol{\pi}}^e$, the return time entropy function $\mathbb{J}(P)$ satisfies

$$\begin{aligned} \mathbb{J}(P) &= \sum_{i=1}^n \pi_i \mathbb{H}(T_{ii}) \leq \sum_{i=1}^n \pi_i \max_{T_{ii}} \{\mathbb{H}(T_{ii})\} \\ &= \sum_{i=1}^n \pi_i \left(\frac{1}{\pi_i} \log \frac{1}{\pi_i} - \left(\frac{1}{\pi_i} - 1 \right) \log \left(\frac{1}{\pi_i} - 1 \right) \right) \\ &= - \sum_{i=1}^n \left(\pi_i \log \pi_i + (1 - \pi_i) \log(1 - \pi_i) \right), \end{aligned}$$

where the second line uses (1.4).

Regarding (ii), when the graph is complete and $P = \mathbb{1}_n \boldsymbol{\pi}^\top$, the return time T_{ii} follows the geometric distribution:

$$\mathbb{P}(T_{ii} = k) = \pi_i (1 - \pi_i)^{k-1}.$$

Then by Lemma 1.3.5.4, we obtain the results. ■

2.3.4 Relations with the entropy rate of Markov chains

Given an irreducible Markov chain P with n nodes and stationary distribution $\boldsymbol{\pi}$, the *entropy rate* of P is given by

$$\mathbb{H}_{\text{rate}}(P) = - \sum_{i=1}^n \pi_i \sum_{j=1}^n p_{ij} \log p_{ij}.$$

We next study the relationship between the return time entropy \mathbb{J} with unitary travel times and the entropy rate \mathbb{H}_{rate} .

Theorem 2.3.4.1 (*Relations between the return time entropy with unitary travel times and the entropy rate*) For all P in the compact set $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$ where \mathcal{G} has unitary travel times, the return time entropy $\mathbb{J}(P)$ and the entropy rate $\mathbb{H}_{\text{rate}}(P)$ satisfy

$$\mathbb{H}_{\text{rate}}(P) \leq \mathbb{J}(P) \leq n\mathbb{H}_{\text{rate}}(P), \quad (2.13)$$

where n is the number of nodes in the graph \mathcal{G} .

Remark 2.3.4.2 Theorem 2.3.4.1 establishes a large gap, possibly of size $O(n)$, between $\mathbb{H}_{\text{rate}}(P)$ and $\mathbb{J}(P)$ and, thereby, optimizing \mathbb{H}_{rate} and \mathbb{J} are two different matters altogether.

The proof of Theorem 2.3.4.1 follows from Lemmas 2.3.4.4 and Lemma 2.3.4.6 below.

First, we show that the return time entropy is upper bounded by n times of the entropy rate. As in [43], we define a *Markov trajectory from state i to state j* to be a path with initial state i , final state j , and no intervening state equal to j . Let \mathcal{T}_{ij} be the set of all Markov trajectories from state i to state j . Let $\mathbb{P}(\ell)$ denote the probability of a Markov trajectory $\ell \in \mathcal{T}_{ij}$; clearly $\sum_{\ell \in \mathcal{T}_{ij}} \mathbb{P}(\ell) = 1$. Let L_{ij} be the Markov trajectory random variable that takes value ℓ in \mathcal{T}_{ij} with probability $\mathbb{P}(\ell)$. Finally, we define the entropy of L_{ij} by

$$\mathbb{H}(L_{ij}) = - \sum_{\ell \in \mathcal{T}_{ij}} \mathbb{P}(L_{ij} = \ell) \log \mathbb{P}(L_{ij} = \ell).$$

Lemma 2.3.4.3 (*Entropy of Markov trajectories [43, Theorem 1]*) For an irreducible Markov chain with transition matrix P , the entropy $\mathbb{H}(L_{ii})$ of the random Markov trajec-

tory from state i back to state i is given by

$$\mathbb{H}(L_{ii}) = \frac{\mathbb{H}_{\text{rate}}(P)}{\pi_i}.$$

Through the entropy of the Markov trajectories, we are able to establish the upper bound of the return time entropy in (2.13).

Lemma 2.3.4.4 (*Upper bound of the return time entropy by n times of the entropy rate*)

Given the compact set $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$,

1. the return time entropy is upper bounded by

$$\mathbb{J}(P) \leq n\mathbb{H}_{\text{rate}}(P), \quad \text{for all } P \in \mathcal{P}_{\mathcal{G},\pi}^\epsilon; \quad (2.14)$$

2. the equality in (2.14) holds if and only if any node of the graph \mathcal{G} has the property that all distinct first return paths have different length, i.e., the return paths are distinguishable by their lengths, and in this case,

$$\operatorname{argmax}_{P \in \mathcal{P}_{\mathcal{G},\pi}^\epsilon} \mathbb{J}(P) = \operatorname{argmax}_{P \in \mathcal{P}_{\mathcal{G},\pi}^\epsilon} \mathbb{H}_{\text{rate}}(P).$$

Proof: Regarding (i), the return time random variable T_{ii} is defined by lumping the trajectories in \mathcal{T}_{ii} with the same length,

$$\mathbb{P}(T_{ii} = k) = \sum_{\ell \in \mathcal{T}_{ii}, |\ell|=k} \mathbb{P}(L_{ii} = \ell), \quad (2.15)$$

where $|\ell|$ denotes the length of the path ℓ . Note that

$$\begin{aligned}
& -\mathbb{P}(T_{ii} = k) \log \mathbb{P}(T_{ii} = k) \\
&= -\left(\sum_{\ell \in \mathcal{T}_{ii}, |\ell|=k} \mathbb{P}(L_{ii} = \ell) \right) \log \left(\sum_{\ell \in \mathcal{T}_{ii}, |\ell|=k} \mathbb{P}(L_{ii} = \ell) \right) \\
&\leq - \sum_{\ell \in \mathcal{T}_{ii}, |\ell|=k} \mathbb{P}(L_{ii} = \ell) \log \mathbb{P}(L_{ii} = \ell),
\end{aligned} \tag{2.16}$$

where we used that $(x + y) \log(x + y) \geq x \log x + y \log y$ for $x, y \geq 0$. Since both the return time entropy and the entropy of Markov trajectories are absolutely convergent, we have

$$\begin{aligned}
\mathbb{H}(T_{ii}) &= - \sum_{k=1}^{\infty} \mathbb{P}(T_{ii} = k) \log \mathbb{P}(T_{ii} = k) \\
&\leq - \sum_{k=1}^{\infty} \sum_{\ell \in \mathcal{T}_{ii}, |\ell|=k} (\mathbb{P}(L_{ii} = \ell) \log \mathbb{P}(L_{ii} = \ell)) \\
&= \mathbb{H}(L_{ii}),
\end{aligned}$$

which along with Lemma 2.3.4.3 imply

$$\mathbb{J}(P) \leq n \mathbb{H}_{\text{rate}}(P).$$

Regarding (ii), the inequality in (2.14) comes from the inequality (2.16). If any node of the graph \mathcal{G} has the property that all distinct first return paths have different length, then the summation on the right hand side of (2.15) only has one term and the inequality in (2.16) becomes an equality. On the other hand, if for some node of \mathcal{G} , there are distinct return paths that have the same length, then one needs to lump the paths with the same length and the inequality in (2.16) becomes strict. Moreover, if the equality holds, then $\mathbb{J}(P)$ is a constant n times of $\mathbb{H}_{\text{rate}}(P)$ and thus they have the same maximizer. \blacksquare

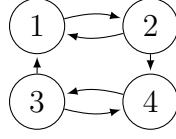


Figure 2.1: An example graph that satisfies the property in Lemma 2.3.4.4(ii)

Example 2.3.4.5 *For the two-node case in Examples 2.2.2.4(i), the return time entropy is twice the entropy rate. This is not a coincidence since the 2-node complete graph satisfies the property in Lemma 2.3.4.4(ii). Figure 2.1 illustrates a graph with 4 nodes that also satisfies the property in Lemma 2.3.4.4(ii).*

In the rest of this subsection, we show that the return time entropy is lower bounded by the entropy rate as shown in (2.13).

Lemma 2.3.4.6 *(Lower bound of the return time entropy by the entropy rate) Given the compact set $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$,*

1. *the return time entropy is lower bounded by*

$$\mathbb{J}(P) \geq \mathbb{H}_{\text{rate}}(P), \quad \text{for all } P \in \mathcal{P}_{\mathcal{G},\pi}^\epsilon; \quad (2.17)$$

2. *the equality in (2.17) holds if and only if P is a permutation matrix.*

Proof: Regarding (i), note that the first hitting time T_{ij} from state i to state j as defined in (1.3) is a random variable, whose entropy is $\mathbb{H}(T_{ij})$. Then by definition, we

have in the case of unitary travel times,

$$\begin{aligned}
\mathbb{H}(T_{ij}) &= - \sum_{k=1}^{\infty} \mathbb{P}(T_{ij} = k) \log \mathbb{P}(T_{ij} = k) \\
&= -p_{ij} \log p_{ij} - \left(\sum_{k_1 \neq j} p_{ik_1} p_{k_1 j} \right) \log \left(\sum_{k_1 \neq j} p_{ik_1} p_{k_1 j} \right) \\
&\quad - \left(\sum_{k_1, k_2 \neq j} p_{ik_1} p_{k_1 k_2} p_{k_2 j} \right) \log \left(\sum_{k_1, k_2 \neq j} p_{ik_1} p_{k_1 k_2} p_{k_2 j} \right) \\
&\quad - \cdots - \left(\sum_{k_1 \cdots k_m \neq j} p_{ik_1} \cdots p_{k_m j} \right) \log \left(\sum_{k_1 \cdots k_m \neq j} p_{ik_1} \cdots p_{k_m j} \right) - \cdots .
\end{aligned}$$

Since $x \mapsto -x \log x$ is a concave function, for $x_i \geq 0$ and for coefficients $\alpha_i \geq 0$ satisfying $\sum_{i=1}^n \alpha_i = 1$, we have

$$- \left(\sum_{i=1}^n \alpha_i x_i \right) \log \left(\sum_{i=1}^n \alpha_i x_i \right) \geq - \sum_{i=1}^n \alpha_i (x_i \log x_i). \quad (2.18)$$

Thus, for $m \geq 1$,

$$\begin{aligned}
&- \mathbb{P}(T_{ij} = m+1) \log \mathbb{P}(T_{ij} = m+1) \\
&= - \left(\sum_{k_1 \cdots k_m \neq j} p_{ik_1} \cdots p_{k_m j} \right) \log \left(\sum_{k_1 \cdots k_m \neq j} p_{ik_1} \cdots p_{k_m j} \right) \\
&= - \left(\sum_{k_1 \neq j} p_{ik_1} \sum_{k_2 \cdots k_m \neq j} p_{k_1 k_2} \cdots p_{k_m j} + p_{ij} \cdot 0 \right) \cdot \log \left(\sum_{k_1 \neq j} p_{ik_1} \sum_{k_2 \cdots k_m \neq j} p_{k_1 k_2} \cdots p_{k_m j} + p_{ij} \cdot 0 \right) \\
&\geq - \sum_{k_1 \neq j} p_{ik_1} \left(\sum_{k_2 \cdots k_m \neq j} p_{k_1 k_2} \cdots p_{k_m j} \cdot \log \left(\sum_{k_2 \cdots k_m \neq j} p_{k_1 k_2} \cdots p_{k_m j} \right) \right) \\
&= - \sum_{k_1 \neq j} p_{ik_1} \mathbb{P}(T_{k_1 j} = m) \log \mathbb{P}(T_{k_1 j} = m),
\end{aligned} \quad (2.19)$$

where the inequality is due to equation (2.18). Summing both sides of (2.19) over m for

$m \geq 1$, we have

$$\begin{aligned}\mathbb{H}(T_{ij}) &\geq -p_{ij} \log p_{ij} + \sum_{k_1 \neq j} p_{ik_1} \mathbb{H}(T_{k_1 j}) \\ &= -p_{ij} \log p_{ij} + \sum_{k_1=1}^n p_{ik_1} \mathbb{H}(T_{k_1 j}) - p_{ij} \mathbb{H}(T_{jj}).\end{aligned}\tag{2.20}$$

Let $\mathbb{H}(T)$ be a matrix whose (i, j) -th element is $\mathbb{H}(T_{ij})$. Then equation (2.20) can be written in the matrix form

$$\mathbb{H}(T) \geq -P \circ \log P + P\mathbb{H}(T) - P\text{diag}(\mathbb{H}(T)),\tag{2.21}$$

where the inequality and the log function are entry-wise. Multiplying $\boldsymbol{\pi}^\top$ from the left and $\mathbb{1}_n$ from the right on both sides of (2.21), we have

$$\boldsymbol{\pi}^\top \text{diag}(\mathbb{H}(T)) \mathbb{1}_n \geq -\boldsymbol{\pi}^\top (P \circ \log P) \mathbb{1}_n,$$

which is $\mathbb{J}(P) \geq \mathbb{H}_{\text{rate}}(P)$.

Regarding (ii), if P is a permutation matrix, then $\mathbb{J}(P) = \mathbb{H}_{\text{rate}}(P) = 0$. On the other hand, if P is not a permutation matrix, then there exist 2 or more nonzero elements on at least one row of P . In this case, the inequality in (2.19) is strict for that row for some m , which carries over to (2.20). Thus, $\mathbb{J}(P) > \mathbb{H}_{\text{rate}}(P)$. ■

2.4 Truncated return time entropy and its optimization via gradient descent

We now introduce the truncated and conditional return time entropy and setup a gradient descent algorithm.

2.4.1 The truncated and conditional return time entropy

In practical applications, we may discard events occurring with extremely low probability. In what follows, we study the return time distribution and its entropy conditioned upon the event that the return time is upper bounded. We first introduce a *truncation accuracy* parameter $0 < \eta \ll 1$ that upper bounds the cumulative probabilities of very large return times and we define a *duration* $N_\eta \in \mathbb{Z}_{>0}$ by

$$N_\eta = \left\lceil \frac{w_{\max}}{\eta \pi_{\min}} \right\rceil - 1, \quad (2.22)$$

where $\pi_{\min} = \min_{i \in \{1, \dots, n\}} \{\pi_i\}$ and $\lceil \cdot \rceil$ is the ceiling function. It is an immediate consequence of the Markov's inequality that, given the fixed stationary distribution $\boldsymbol{\pi}$, for all $i \in \{1, \dots, n\}$,

$$\mathbb{P}(T_{ii} \geq N_\eta + 1) \leq \frac{\mathbb{E}[T_{ii}]}{N_\eta + 1} \leq \frac{w_{\max}}{\pi_i(N_\eta + 1)} \leq \eta,$$

where we used (2.2)

$$\mathbb{E}[T_{ii}] = \frac{\boldsymbol{\pi}^\top (P \circ W) \mathbf{1}_n}{\pi_i} \leq \frac{w_{\max}}{\pi_i}.$$

We now define the conditional return time and its entropy.

Definition 2.4.1.1 (*Conditional return time and its entropy*) Given $P \in \mathcal{P}_{\mathcal{G}, \boldsymbol{\pi}}^\epsilon$ and a duration N_η , the conditional return time $T_{ii} \mid T_{ii} \leq N_\eta$ of state i is defined by

$$T_{ii} \mid T_{ii} \leq N_\eta = \min \left\{ \sum_{k'=0}^{k-1} w_{X_{k'} X_{k'+1}} \mid \sum_{k'=0}^{k-1} w_{X_{k'} X_{k'+1}} \leq N_\eta, X_0 = i, X_k = i, k \geq 1 \right\}.$$

with probability mass function

$$\mathbb{P}(T_{ii} = k \mid T_{ii} \leq N_\eta) = \frac{F_k(i, i)}{\sum_{k=1}^{N_\eta} F_k(i, i)}.$$

Moreover, the conditional return time entropy function $\mathbb{J}_{\text{cond},\eta} : \mathcal{P}_{\mathcal{G},\pi}^\epsilon \mapsto \mathbb{R}_{\geq 0}$ is

$$\mathbb{J}_{\text{cond},\eta}(P) = \sum_{i=1}^n \pi_i \mathbb{H}(T_{ii} \mid T_{ii} \leq N_\eta) = - \sum_{i=1}^n \pi_i \sum_{k=1}^{N_\eta} \frac{F_k(i, i)}{\sum_{l=1}^{N_\eta} F_l(i, i)} \log \frac{F_k(i, i)}{\sum_{l=1}^{N_\eta} F_l(i, i)}.$$

Given the duration N_η , $\mathbb{J}_{\text{cond},\eta}(P)$ is a finite sum of continuously differentiable functions and thus more tractable than the original return time entropy function $\mathbb{J}(P)$. Next, we introduce a truncated entropy that is even simpler to evaluate.

Definition 2.4.1.2 (*Truncated return time entropy function*) Given a compact set $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$ and the duration N_η , define the truncated return time entropy function $\mathbb{J}_{\text{trunc},\eta} : \mathcal{P}_{\mathcal{G},\pi}^\epsilon \mapsto \mathbb{R}_{\geq 0}$ by

$$\mathbb{J}_{\text{trunc},\eta}(P) = - \sum_{i=1}^n \pi_i \sum_{k=1}^{N_\eta} F_k(i, i) \log F_k(i, i).$$

The following lemma shows that, for small η , the truncated return time entropy $\mathbb{J}_{\text{trunc},\eta}(P)$ is a good approximation for the conditional return time entropy $\mathbb{J}_{\text{cond},\eta}(P)$. Furthermore, when η is sufficiently small, the truncated return time entropy $\mathbb{J}_{\text{trunc},\eta}(P)$ is also a good approximation for the original return time entropy function $\mathbb{J}(P)$.

Lemma 2.4.1.3 (*Approximation bounds*) Given $P \in \mathcal{P}_{\mathcal{G},\pi}^\epsilon$ and the truncation accuracy η , we have

1. the conditional return time entropy is related to the truncated return time entropy by

$$\mathbb{J}_{\text{trunc},\eta}(P) + \log(1 - \eta) < \mathbb{J}_{\text{cond},\eta}(P) < \frac{\mathbb{J}_{\text{trunc},\eta}(P)}{1 - \eta}; \quad (2.23)$$

2. $\mathbb{J}(P) \geq \mathbb{J}_{\text{trunc},\eta}(P)$ holds trivially and if

$$\eta \leq \frac{w_{\max} \log \lambda_{\max}}{\pi_{\min}(\log \lambda_{\max} - \log c - 1)}, \quad (2.24)$$

then

$$\mathbb{J}(P) - \mathbb{J}_{\text{trunc},\eta}(P) \leq \frac{c \log(\lambda_{\max}^{-1})}{(1 - \lambda_{\max})^2} (1 + N_\eta) \lambda_{\max}^{N_\eta}, \quad (2.25)$$

where c and λ_{\max} are given as in Lemma 2.3.2.1(i);

$$3. \mathbb{J}(P) = \lim_{\eta \rightarrow 0^+} \mathbb{J}_{\text{cond},\eta}(P) = \lim_{\eta \rightarrow 0^+} \mathbb{J}_{\text{trunc},\eta}(P).$$

Proof: Regarding (i), for $\mathbb{J}_{\text{cond},\eta}(P)$, we have

$$\begin{aligned} \mathbb{J}_{\text{cond},\eta}(P) &= - \sum_{i=1}^n \pi_i \sum_{k=1}^{N_\eta} \frac{F_k(i, i)}{\sum_{l=1}^{N_\eta} F_l(i, i)} \log \frac{F_k(i, i)}{\sum_{l=1}^{N_\eta} F_l(i, i)} \\ &= - \sum_{i=1}^n \pi_i \left(\frac{\sum_{k=1}^{N_\eta} F_k(i, i) \log F_k(i, i)}{\sum_{k=1}^{N_\eta} F_k(i, i)} - \log \sum_{k=1}^{N_\eta} F_k(i, i) \right). \end{aligned}$$

On one hand,

$$\begin{aligned} \mathbb{J}_{\text{cond},\eta}(P) &> - \sum_{i=1}^n \pi_i \left(\sum_{k=1}^{N_\eta} F_k(i, i) \log F_k(i, i) - \log \sum_{k=1}^{N_\eta} F_k(i, i) \right) \\ &\geq - \sum_{i=1}^n \pi_i \sum_{k=1}^{N_\eta} F_k(i, i) \log F_k(i, i) + \log(1 - \eta). \end{aligned} \quad (2.26)$$

On the other hand,

$$\begin{aligned} \mathbb{J}_{\text{cond},\eta}(P) &< - \sum_{i=1}^n \pi_i \frac{1}{\sum_{l=1}^{N_\eta} F_l(i, i)} \sum_{k=1}^{N_\eta} F_k(i, i) \log F_k(i, i) \\ &\leq - \frac{1}{1 - \eta} \sum_{i=1}^n \pi_i \sum_{k=1}^{N_\eta} F_k(i, i) \log F_k(i, i). \end{aligned} \quad (2.27)$$

Combining (2.26) and (2.27), we have (2.23).

Regarding (ii), if η satisfies (2.24), we have $c \lambda_{\max}^{N_\eta} \leq e^{-1}$. Then, following the same

arguments as in the proof of Lemma 2.3.2.1(ii) and replacing K in (2.12) with N_η , we have

$$\begin{aligned}
\mathbb{J}(P) - \mathbb{J}_{\text{trunc},\eta}(P) &\leq -c \left(\frac{\lambda_{\max}^{N_\eta}}{1 - \lambda_{\max}} \log(c\lambda_{\max}^{N_\eta}) + \frac{\lambda_{\max}^{N_\eta+1}}{(1 - \lambda_{\max})^2} \log(\lambda_{\max}) \right) \\
&\leq -\frac{c\lambda_{\max}^{N_\eta}}{(1 - \lambda_{\max})^2} ((N_\eta + \lambda_{\max}) \log(\lambda_{\max}) + \log(c)) \\
&\leq -\frac{c\lambda_{\max}^{N_\eta}}{(1 - \lambda_{\max})^2} (N_\eta \log(\lambda_{\max}) + \log(\lambda_{\max})) \\
&= \frac{c \log(\lambda_{\max}^{-1})}{(1 - \lambda_{\max})^2} (1 + N_\eta) \lambda_{\max}^{N_\eta}.
\end{aligned} \tag{2.28}$$

Regarding (iii), the results follow from (2.23) and (2.28), respectively. Specifically, in (2.28), since $0 < \lambda_{\max} < 1$, the error $\mathbb{J}(P) - \mathbb{J}_{\text{trunc},\eta}(P)$ goes to 0 exponentially fast as η goes to 0 ($N_\eta \rightarrow \infty$). ■

2.4.2 The gradient of the truncated return time entropy

Lemma 2.4.1.3 establishes how $\mathbb{J}_{\text{trunc},\eta}(P)$ is a good approximation to both of $\mathbb{J}(P)$ and $\mathbb{J}_{\text{cond},\eta}(P)$. Since it is also easier to compute $\mathbb{J}_{\text{trunc},\eta}(P)$ than the other two quantities, we focus on optimizing $\mathbb{J}_{\text{trunc},\eta}(P)$ by computing its gradient.

For $k \in \mathbb{Z}_{>0}$, define $G_k = \frac{\partial \text{vec}(F_k)}{\partial \text{vec}(P)} \in \mathbb{R}^{n^2 \times n^2}$ and note

$$G_k = \begin{bmatrix} \frac{\partial \text{vec}(F_k)}{\partial p_{11}} & \frac{\partial \text{vec}(F_k)}{\partial p_{21}} & \dots & \frac{\partial \text{vec}(F_k)}{\partial p_{(n-1)n}} & \frac{\partial \text{vec}(F_k)}{\partial p_{nn}} \end{bmatrix}. \tag{2.29}$$

Lemma 2.4.2.1 (*Gradient of the truncated return time entropy function*) Given $P \in$

$\mathcal{P}_{\mathcal{G},\pi}^\epsilon$, the matrix sequence G_k in (2.29) satisfies the iteration for $k \in \mathbb{Z}_{>0}$,

$$\begin{aligned} G_k = & \text{diag}(\text{vec}(\mathbf{1}_{\{k\mathbf{1}_n\mathbf{1}_n^\top=W\}})) + \sum_{i=1}^{w_{\max}} \Phi_i G_{k-i} \\ & + \sum_{i=1}^n \sum_{j=1}^n (E_j F_{k-w_{ij}}^\top \otimes I_n) \text{diag}(\text{vec}(\mathbf{e}_i \mathbf{e}_j^\top)) \mathbf{1}_{\{w_{ij}>0\}}, \end{aligned} \quad (2.30)$$

where the initial conditions are $G_k = \mathbf{0}_{n^2 \times n^2}$ for $k \leq 0$. Moreover, the vectorization of the gradient of $\mathbb{J}_{\text{trunc},\eta}$ satisfies

$$\text{vec}\left(\frac{\partial \mathbb{J}_{\text{trunc},\eta}(P)}{\partial P}\right) = - \sum_{i=1}^n \pi_i \sum_{k=1}^{N_\eta} \frac{\partial (F_k(i, i) \log F_k(i, i))}{\partial F_k(i, i)} G_k^\top \mathbf{e}_{(i-1)n+i}, \quad (2.31)$$

where $\mathbf{e}_{(i-1)n+i} \in \mathbb{R}^{n^2}$ and

$$\frac{\partial F_k(i, i) \log F_k(i, i)}{\partial F_k(i, i)} = \begin{cases} 1 + \log(F_k(i, i)), & \text{if } F_k(i, i) > 0, \\ 0, & \text{if } F_k(i, i) = 0. \end{cases}$$

Proof: For $k \in \mathbb{Z}_{>0}$, according to (2.3), we have for $p_{uv} > 0$,

$$\begin{aligned} \frac{\partial \text{vec}(F_k)}{\partial p_{uv}} = & \text{vec}(\mathbf{e}_u \mathbf{e}_v^\top) \mathbf{1}_{\{k=w_{uv}\}} + (E_v \otimes \mathbf{e}_u \mathbf{e}_v^\top) \text{vec}(F_{k-w_{uv}}) \\ & + \sum_{i=1}^n \sum_{j=1}^n p_{ij} (E_j \otimes \mathbf{e}_i \mathbf{e}_j^\top) \frac{\partial \text{vec}(F_{k-w_{ij}})}{\partial p_{uv}}, \end{aligned}$$

where the second term on the right hand side satisfies

$$(E_v \otimes \mathbf{e}_u \mathbf{e}_v^\top) \text{vec}(F_{k-w_{uv}}) = \text{vec}(\mathbf{e}_u \mathbf{e}_v^\top F_{k-w_{uv}} E_v) = (E_v F_{k-w_{uv}}^\top \otimes I_n) \text{vec}(\mathbf{e}_u \mathbf{e}_v^\top).$$

Stacking $\frac{\partial \text{vec}(F_k)}{\partial p_{uv}}$'s in a matrix as (2.29), we obtain (2.30).

Since $\mathbb{J}_{\text{trunc},\eta}(P)$ only involves $F_k(i, i)$ for $i = \{1, \dots, n\}$, we only need the corre-

sponding columns in G_k^\top to compute the gradient, which is realized by multiplying the standard unit vector as in (2.31). ■

Remark 2.4.2.2 *Iteration (2.30) is an exponentially stable discrete-time delayed linear system subject to a finite number of impulse inputs and an exponentially vanishing input. Hence, the state $G_k \rightarrow 0$ exponentially fast as $k \rightarrow \infty$.*

2.4.3 Optimizing the truncated entropy via gradient projection

Motivated by the previous analysis, we consider the following problem.

Problem 2 *(Maximization of the truncated return time entropy) Given a strongly connected directed graph \mathcal{G} and the stationary distribution π , pick a minimum transition probability $\epsilon > 0$ and a truncation accurate parameter $\eta > 0$. Find $P \in \mathcal{P}_{\mathcal{G},\pi}^\epsilon$ which maximizes the truncated return time entropy $\mathbb{J}_{\text{trunc},\eta}(P)$, i.e., solve the following optimization problem:*

$$\begin{aligned} & \text{maximize} && \mathbb{J}_{\text{trunc},\eta}(P) \\ & \text{subject to} && P \in \mathcal{P}_{\mathcal{G},\pi}^\epsilon \end{aligned}$$

To solve numerically this nonlinear program, we exploit the results in Lemma 2.4.2.1 and adopt the gradient projection method as presented in [55, Chapter 2.3]:

- 1: select: minimum transition probability $\epsilon \ll 1$, truncation accuracy $\eta \ll 1$, and initial condition P_0 in $\mathcal{P}_{\mathcal{G},\pi}^\epsilon$
- 2: **for** iteration parameter $s = 0$: (number-of-steps) **do**
- 3: $\{G_k\}_{k \in \{1, \dots, N_\eta\}} :=$ solution to iteration (2.30) at P_s
- 4: $\Delta_s :=$ gradient of $\mathbb{J}_{\text{trunc},\eta}(P_s)$ via equation (2.31)
- 5: $P_{s+1} := \text{projection}_{\mathcal{P}_{\mathcal{G},\pi}^\epsilon}(P_s + (\text{step size}) \cdot \Delta_s)$
- 6: **end for**

We analyze the computational complexity of this algorithm. To compute step 3:, we need to evaluate the right-hand side of equation (2.30) by computing three terms. For the first term, we need to do m comparisons, where m is the number of edges in the graph (i.e., the number of variables in the transition matrix), and it takes $O(m)$ elementary operations. For the second term, note that the matrices $\Phi_i \in \mathbb{R}^{n^2 \times n^2}$ introduced in equation (2.11) can be precomputed and is block diagonal with n blocks of size $n \times n$. Also note that $G_k \in \mathbb{R}^{n^2 \times n^2}$ has only m nonzero columns. Thus, we need $O(w_{\max}mn^3)$ operations. For the third term, F_k is updated by equation (2.9), which requires $O(w_{\max}n^3)$ and is the main computational cost. Therefore, it takes $O(w_{\max}mn^3)$ to compute one update of iteration (2.30). Thus, it takes $O(N_\eta w_{\max}mn^3)$ elementary operations to complete step 3:. In step 5:, we need to solve a least square problem with linear equalities and inequalities constraints, which requires $O(m^3)$ [56].

Remark 2.4.3.1 (*Coprime travel times*) *The return time entropy of states does not change when we scale the travel times on all edges simultaneously by the same factor. Therefore, we could preprocess the travel times on the graph to make them coprime, and this helps reduce the computational cost.*

2.5 Numerical results

In this section, we provide numerical results on the computation of the maximum return time entropy chain (Subsection 2.5.1) and its application to robotic surveillance problems (Subsection 2.5.2). We compute and compare three chains:

1. the Markov chain that maximizes the return time entropy (solution of Problem 1), abbreviated as the *MaxReturnEntropy chain*. This chain may be computed for a directed graph with arbitrary integer-valued travel times. Since we do not have a

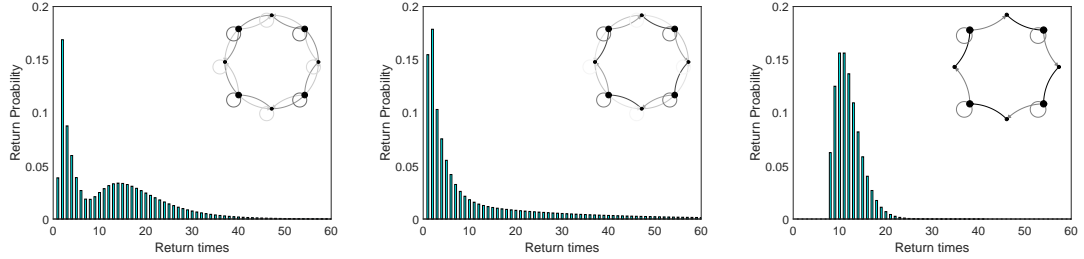
way to solve Problem 1 directly, the MaxReturnEntropy chain is approximated by the solution of Problem 2, which is obtained via the gradient projection algorithm. Unless otherwise stated, we choose the truncation accuracy $\eta = 0.1$. Note that (2.22) is quite conservative and the actual probabilities being discarded are much less than 0.1. In fact, the actual truncation error of all the MaxReturnEntropy chains computed in this section is less than 10^{-4} ;

2. the Markov chain that maximizes the entropy rate, abbreviated as the *MaxEntropyRate chain*. This chain can be computed for a directed graph with unitary weights via solving a convex program. Further, if the graph is undirected, the MaxEntropyRate chain can be computed efficiently using the method in [26];
3. the Markov chain that minimizes the (weighted) Kemeny constant, abbreviated as the *MinKemeny chain* [24]. The MinKemeny chain is obtained by solving the following optimization problem.

Problem 3 (*Minimization of the Kemeny constant*) *Given a strongly connected directed weighted graph $\mathcal{G} = (V, \mathcal{E}, W)$ and the stationary distribution $\boldsymbol{\pi} > 0$, the minimization of the Kemeny constant is as follows.*

$$\begin{aligned}
 & \text{minimize} && \sum_{i=1}^n \sum_{j=1}^n \pi_i \pi_j \mathbb{E}[T_{ij}] \\
 & \text{subject to} && p_{ij} \geq 0 \text{ if } (i, j) \in \mathcal{E}, \\
 & && p_{ij} = 0 \text{ if } (i, j) \notin \mathcal{E}, \\
 & && P \mathbf{1}_n = \mathbf{1}_n, \boldsymbol{\pi}^\top P = \boldsymbol{\pi}^\top.
 \end{aligned}$$

The MinKemeny chain has the minimum *mean first passage time* and travels on the graph quickly. This chain may be computed for a directed graph with arbitrary



(a) MaxReturnEntropy chain on ring graph (b) MaxEntropyRate chain on ring graph (c) MinKemeny chain on ring graph

Figure 2.2: Return time distributions of node 1 (i.e., top node) on an 8-node ring graph with stationary distribution $\pi = [1/12, 1/6, \dots, 1/12, 1/6]^\top$. Although the expectations of the first return time distributions in the figure are the same, the histogram is remarkably different for different chains. Specifically, for the nonreversible MaxReturnEntropy chain, the distribution is bimodal and generates more entropy. The node size is proportional to the stationary distribution.

travel times via solving a nonconvex program. We compute this chain using the solver implemented in the KNITRO/TOMLAB package.

2.5.1 Computation, comparison and intuitions

We divide this subsection into two parts. In the first part, we first compare 3 chains on graphs that have unitary travel times. We then summarize several observations in computing the MaxReturnEntropy chain. Finally, we visualize and plot the chains as well as the return time distributions. In the second part, we compare the MaxReturnEntropy chain with the MinKemeny chain on a realistic map taken from [18, Section 6.2] with travel times.

Chains on graphs with unitary travel times

Comparison: We consider 2 simple undirected graphs and solve for the MaxReturnEntropy chain, the MaxEntropyRate chain and the MinKemeny chain for each case. We compare the return time entropy, the entropy rate, and the Kemeny constant of

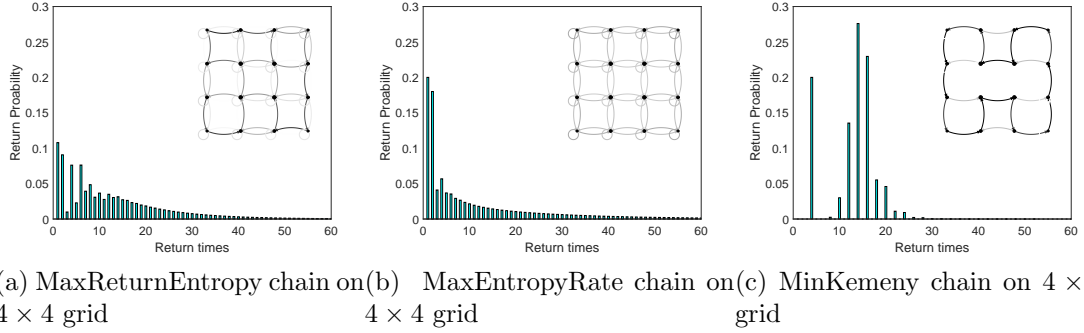


Figure 2.3: Return time distributions of node 6 (i.e., second node on the second row) on a 4×4 grid with stationary distribution π proportional to the node degree and unitary travel times. The node size is proportional to the stationary distribution.

these chains in Table 2.1. The stationary distribution of the ring graph is set to be $\pi = [1/12, 1/6, \dots, 1/12, 1/6]^\top$, and the stationary distribution of grid is proportional to the degree of nodes. To evaluate the value of $\mathbb{J}(P)$, we set $\eta = 10^{-2}$. From the table, we notice that the MaxReturnEntropy chain has the highest value of the return time entropy in both cases. It also has relatively good performance in terms of the entropy rate and the Kemeny constant, which indicates that the MaxReturnEntropy chain is potentially a good combination of speed (expected traversal time) and unpredictability. Furthermore, it is clear that (2.13), which characterizes the relationship between the entropy rate and the return time entropy, holds.

Table 2.1: Comparison between different chains on different graphs

Graph	Markov chains	$\mathbb{J}(P)$	$\mathbb{H}_{\text{rate}}(P)$	Kemeny constant
8-node ring	MaxReturnEntropy	2.4927	0.8698	10.0479
	MaxEntropyRate	2.3510	0.9883	19.5339
	MinKemeny	1.9641	0.4621	6.1667
4-by-4 grid	MaxReturnEntropy	3.6539	0.9491	16.3547
	MaxEntropyRate	3.2844	1.4021	30.8661
	MinKemeny	2.0990	0.2188	10.0938

Observations: In computing the MaxReturnEntropy chain, we observe some interest-

ing properties of our problem. First, when solving Problem 2 by the gradient projection method with different initial conditions, we find different optimal solutions, and they have slightly different optimal values. This suggests that Problem 1 is unlikely to be a convex problem. Secondly, the global optimal solution to Problem 1 is possibly not unique in general. For instance, for an undirected ring graph with even number of nodes and certain stationary distribution, exchanging the probability of going right and that of going left for all nodes does not change the return time entropy. Thirdly, the optimal solution to Problem 1 is likely to be nonreversible because none of the approximate optimal solutions we have encountered are reversible. This again indicates that the MaxReturnEntropy chain is a good combination of unpredictability and speed. Fourth, even if we set the minimum transition probability $\epsilon = 0$, the MaxReturnEntropy chain is always irreducible.

Intuitions: In order to provide intuitions for the maximization of the return time entropy, we compare and plot the chains as well as the return time distribution of a same node on the 8-node ring graph and the 4×4 grid graph in Fig. 2.2 and Fig. 2.3, respectively. Since the stationary distribution is fixed and identical for all chains in each case, the expectations of the probability mass functions in each figure are the same. From the figures, we note that for the MaxReturnEntropy chain, the return time distribution is reshaped so that the distribution spreads out and it is more difficult to predict the return time. In contrast, the return time distribution for the MinKemeny chain has a predictable pattern and the return time probability is constantly 0 for some time intervals. Moreover, from the visualization of the chains, we notice that the MaxReturnEntropy chain has a net flow on the graph, which again indicates its nonreversibility.

MaxReturnEntropy and MinKemeny on a realistic map

In this part, we compare the MaxReturnEntropy chain with the MinKemeny chain

on a realistic map with travel times. The problem data is taken from [18, Section 6.2]: a small area in San Francisco (SF) is modeled by a fully connected directed graph with 12 nodes and by-car travel times on edges measured in seconds. The map is shown in Fig. 2.4. The importance of the a location (node) is characterized by the the number of crimes recorded at that place during a specific period, and the surveillance agent should visit the places with higher crime rate more often. The visit frequency is set to be $[\frac{133}{866}, \frac{90}{866}, \frac{89}{866}, \frac{87}{866}, \frac{83}{866}, \frac{83}{866}, \frac{74}{866}, \frac{64}{866}, \frac{48}{866}, \frac{43}{866}, \frac{38}{866}, \frac{34}{866}]^T$.

For simplicity, we quantize the travel times by treating a minute as one unit of time, i.e., dividing the travel times by 60 and round the result to the smallest integer that is larger than it, and by doing so, we have $w_{\max} = 9$. The pairwise travel times are recorded in Table 2.2.

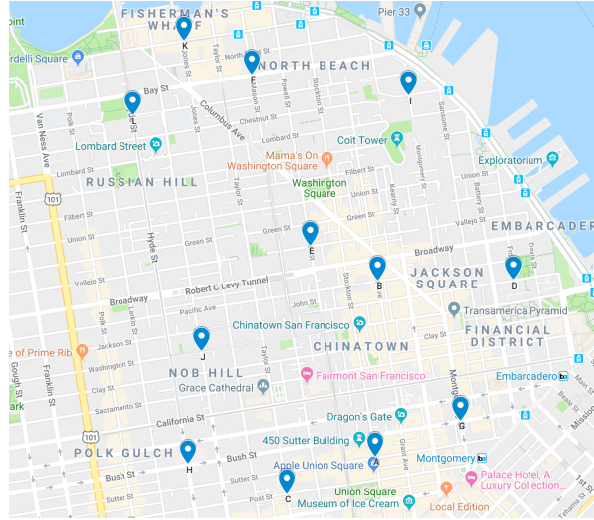


Figure 2.4: San Francisco (SF) crime map from [18, Section 6.2].

First, we compare three key metrics of the MaxReturnEntropy chain and MinKemeny chain. The results are reported in Table 2.3. It can be observed that the MaxReturnEntropy chain is much better than the MinKemeny chain regarding the return time entropy and the entropy rate. This better performance in terms of the unpredictability is

Table 2.2: The quantized pairwise by-car travel times on SF crime map

Location	A	B	C	D	E	F	G	H	I	J	K	L
A	1	3	3	5	4	6	3	5	7	4	6	6
B	3	1	5	4	2	4	4	5	5	3	5	5
C	3	5	1	7	6	8	3	4	9	4	8	7
D	6	4	7	1	5	6	4	7	5	6	6	7
E	4	3	6	5	1	3	5	5	6	3	4	4
F	6	4	8	5	3	1	6	7	3	6	2	3
G	2	5	3	5	6	7	1	5	7	5	7	8
H	3	5	2	7	6	7	3	1	9	3	7	5
I	8	6	9	4	6	4	6	9	1	8	5	7
J	4	3	4	6	3	5	5	3	7	1	5	3
K	6	4	8	6	4	2	6	6	4	5	1	3
L	6	4	6	6	3	3	6	4	5	3	2	1

obtained at the cost of being slower as indicated by the larger weighted Kemeny constant.

Table 2.3: Comparison between different chains on SF crime map

Markov chains	$\mathbb{J}(P)$	$\mathbb{H}_{\text{rate}}(P)$	Weighted Kemeny constant
MaxReturnEntropy	5.0078	1.7810	63.6007
MinKemeny	2.4678	0.6408	24.2824

We also plot the return time distribution of location A in Fig. 2.5. Apparently, the MaxReturnEntropy chain spreads the return time probabilities over the possible return times and it is hard to predict the exact time the surveillance agent comes back to the location. In contrast, the MinKemeny chain tries to achieve fast traversal on the graph and the return times distribute over a few intervals.

2.5.2 Application to the Robotic Surveillance Problem

In this subsection, we provide simulation results in the application of the robotic surveillance.

Setup: Consider the scenario where a single agent performs the surveillance task by

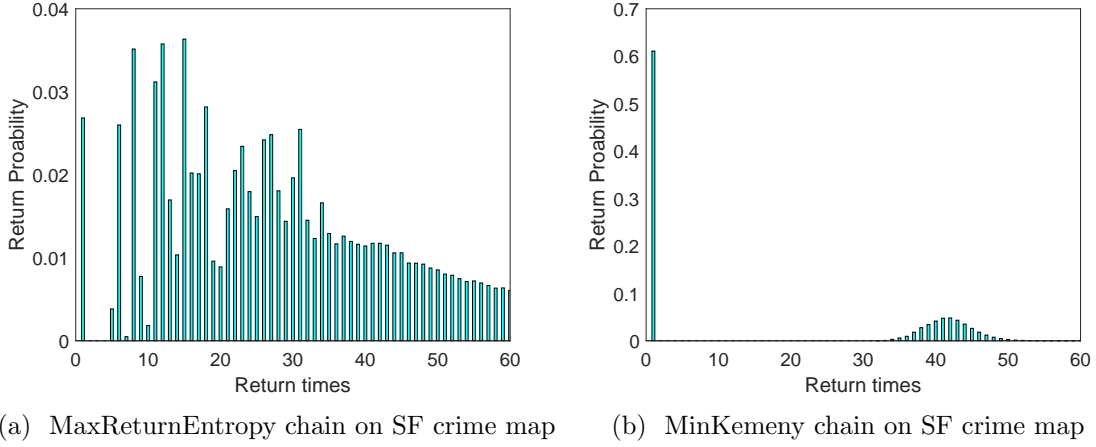


Figure 2.5: Return time distributions of location A on SF crime map. Note that the scales of the vertical axes are different in the two figures.

moving randomly according to a Markov chain on the road map. The intruder is able to observe the local behaviors of the surveillance agent, e.g., presence/absence and duration between visits, and he/she plans and decides the time of attack so as to avoid being captured. It takes a certain amount of time for the intruder to complete an attack, which is called the *attack duration* of the intruder. A successful detection/capture happens when the surveillance agent and the intruder are at the same location and the intruder is attacking.

Intruder model (success probability maximizer with bounded patience): Consider a rational intruder that exploits the return time statistics of the Markov chains and chooses an optimal attack time so as to minimize the probability of being captured. The intruder picks a node i to attack randomly according to the stationary distribution, and it collects and learns the probability distribution of node i 's first return time. Suppose the intruder and the surveillance agent are at the same node i at the beginning and the attack duration of the intruder is τ . If the intruder observes that the surveillance agent leaves the node and does not come back for s periods, he/she can attack with the probability of being

captured given by

$$\sum_{k=1}^{\tau} \mathbb{P}(T_{ii} = s + k \mid T_{ii} > s). \quad (2.32)$$

Mathematically speaking, (2.32) is the conditional cumulative return probability for the surveillance agent. Specifically for $s = 0$, (2.32) is the capture probability when the intruder attacks immediately after the agent leaves the node. Then, the optimal time of attack s_i for the intruder is given by

$$s_i = \operatorname{argmin}_{0 \leq s \leq S_i} \left\{ \sum_{k=1}^{\tau} \mathbb{P}(T_{ii} = s + k \mid T_{ii} > s) \right\}. \quad (2.33)$$

The reason there is an upper bound S_i on s is that the event $T_{ii} > s$ happens with very low probability when s is large, and the intruder may be unwilling to wait for such an event to happen. Let $\delta \in (0, 1)$ be the *degree of impatience* of the intruder, then S_i can be chosen as the minimal positive integer such that the following holds,

$$\mathbb{P}(T_{ii} \geq S_i) \leq \delta,$$

where a smaller δ implies a larger S_i and a more patient intruder. In other words, when δ is small, the intruder is willing to wait for a rare event to happen. Note that the value of S_i is also dependent on the node i that the intruder chooses to attack, and thus the argmin in (2.33) is over different ranges when the intruder attacks different nodes. In summary, the intruder is dictated by two parameters: the attack duration τ and the degree of impatience δ , and the strategy for the intruder is as follows: waits until the event that the surveillance agent leaves and does not come back for the first s_i steps happens, then attacks immediately.

From the surveillance point of view, the probability of capturing the rational intruder

when he/she attacks node i is

$$\mathbb{P}_i(\text{Capture}) = \sum_{k=1}^{\tau} \mathbb{P}(T_{ii} = s_i + k \mid T_{ii} > s_i),$$

and the performance of the Markov chains can be evaluated by the total probability of capture as follows

$$\mathbb{P}(\text{Capture}) = \sum_{i=1}^n \pi_i \mathbb{P}_i(\text{Capture}). \quad (2.34)$$

Simulation results: Designing an optimal defense mechanism for the rational intruder is an interesting yet challenging problem in its own. Instead, we use the MaxReturnEntropy chain as a heuristic solution and compare its performance with other chains. In the following, we consider two types of graphs: the grid graph and the SF crime map. The degree of impatience of the intruder is set to be $\delta = 0.1$ in this part.

We first consider a 4×4 grid and plot the probability of capture defined by (2.34) for the chains in comparison in Fig. 2.6. It can be observed that, when defending against the rational intruder described above, the MaxReturnEntropy chain outperforms all other chains when the attack duration of the intruder is small or moderate. The unpredictability in the return time prevents the rational intruder from taking advantage of the visit statistics learned from the observations. The MinKemeny chain, which emphasizes a faster traversal, has a hard time capturing the intruder when the attack duration of the intruder is small. This is because the agent moves in a relatively more predictable way, and the return time statistics may have a pattern that could be exploited. The MaxEntropyRate chain has the in-between performance.

For the SF crime map, we use the same problem data as described in Subsection 2.5.1. Since the MaxEntropyRate chain does not generalize to the case when there are travel times, we compare the performance of the MaxReturnEntropy chain and the MinKemny

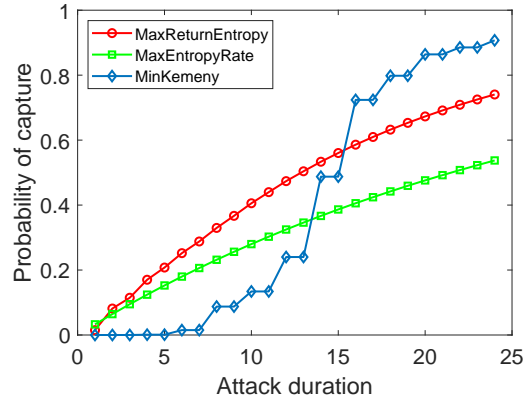


Figure 2.6: Performance of different chains on a 4×4 grid.

chain. Again, from Fig. 2.7, the MaxReturnEntropy chain outperforms the MinKemeny chain when the attack duration of the intruder is relatively small.

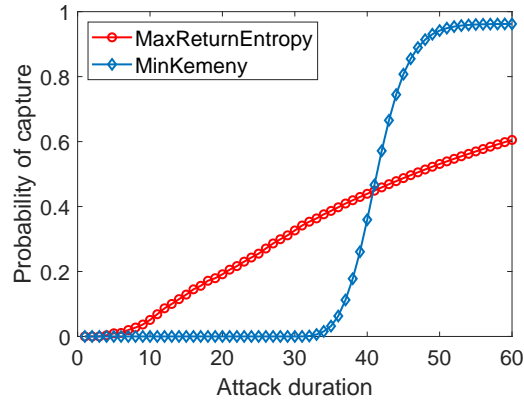


Figure 2.7: Performance of different chains on the SF crime map.

Summary: The simulation results presented in this subsection demonstrate that the MaxReturnEntropy chain is an effective strategy against the intruder with reasonable amount of knowledge and level of intelligence, particularly when the attack duration of the intruder is small or moderate. With the property of both unpredictability and speed, the MaxReturnEntropy chain should also work well in a much more broader range of

scenarios.

2.6 Conclusion

In this chapter, we proposed and optimized a new metric that quantifies the unpredictability of Markov chains over a directed strongly connected graph with travel times, i.e., the return time entropy. We characterized the return time probabilities and showed that optimizing the return time entropy is a well-posed problem. For the case of unitary travel times, we established an upper bound for the return time entropy by using the maximum entropy principle and obtained an analytic solution for the complete graph. We connected the return time entropy with the well-known entropy rate of Markov chains and showed that the return time entropy is lower bounded by the entropy rate and upper bounded by n times the entropy rate. In order to solve the optimization problem numerically, we approximated the return time entropy as well as a practically useful conditional return time entropy by the truncated return time entropy. We derived the gradient of the truncated return time entropy and proposed to solve the problem by the gradient projection method. We applied our results to the robotic surveillance problem and found that the chain with maximum return time entropy is a good trade-off between speed and unpredictability, and it performs better than several existing chains against a rational intruder.

A number of problems are still open. First of all, a simple closed-form expression for the return time entropy would enable us to establish more properties of the objective function and thus make the optimization problem more tractable. Second, it is interesting to design a best Markov chain directly that defends against the intruder model proposed in this chapter. Third, how to generalize the results to the case of multiple robots remains to be investigated. Fourth, we believe there are more application scenarios for Markov

chains where the return time entropy is an appropriate quantity to optimize.

Chapter 3

The Meeting Time of Random Walks

3.1 Introduction

3.1.1 Problem description and motivation

In this chapter, we examine the meeting time between two moving agents modeled by discrete-time Markov chains. This problem is motivated by a pursuer trying to intercept a moving evader. The meeting time, in the context of this chapter, describes the average time till a first encounter occurs between the pursuer and the evader given initial positions of the pursuer and the evader. This notion of two adversarial mobile agents wherein one of the agents is trying to intercept the other appears under several names: pursuit-evasion games [57], predator-prey interactions [58], cops and robbers games [59, 60] and princess-monster games [61]. Our primary motivation is the design of stochastic surveillance strategies for quickest detection of the mobile intruder. Single and multi-agent surveillance strategies appear in environmental monitoring [62], minimizing emergency

vehicle response times [63], traffic routing and border patrol [64]. More broadly, random walks on networks appear in many areas of research: they are used to describe effective resistance in electrical networks [65], for link-prediction and information propagation in social networks [66], and in designing search algorithms on networks [67]. Aside from our proposed application to stochastic surveillance, the meeting time has direct applications to information flow in distributed networks [68], self-stabilization of tokens [69] and measuring similarity of objects [70].

3.1.2 Literature review

Early interest in meeting times was motivated by applications to self-stabilizing token management schemes [71]. In a token management scheme, only one of the many processors on a distributed network is enabled to change state or perform a particular task, and this processor is said to possess the token. If two tokens meet then they collapse into a single token. Israeli and Jalfon suggest a scheme in which the token is passed randomly to a neighbor [69]. In a general connected undirected graph they were able to obtain an exponential bound for the meeting time of two tokens in terms of the maximum degree and the diameter of the graph. Coppersmith *et al.* [72] improved the bound to be polynomial in the number of nodes by bounding the meeting time in terms of the pairwise hitting time from the starting nodes of the tokens to hidden vertices. Bshouty *et al.* [73] obtain a bound on the meeting time of several such tokens in terms of the meeting time of two tokens. Bounds for meeting times of two identical independent continuous-time reversible Markov chains in terms of the pairwise hitting times of the chains are mentioned in [74].

Several metrics have been used to describe single and multiple random walks on graphs. One closely related metric is the hitting time which is the time taken by a single

random walker to travel between nodes of a graph. The hitting time of a finite irreducible Markov chain appeared in [75] and [38]. Several bounds have been obtained and many closed-form formulas exist to compute the hitting time for various graph topologies [76]. The authors in [25] obtain a closed-form solution for the hitting time of multiple random walkers. Another related notion is the coalescence time of multiple random walkers widely studied in the context of voter models [77]. Two random walks coalesce into one when they share the same node. Bounds for the coalescence time in terms of the worst case pairwise hitting times are discussed in [37]. More recently, Cooper *et al.* bounded the coalescence time using the second largest eigenvalue of the transition matrix [77].

Stochastic vehicle routing strategies have the desirable property that an intruder cannot predictably plan a path to avoid surveillance agents. The authors in [24, 26, 27] use Markov chains to design surveillance strategies. A novel convex optimization formulation is used to design strategies with minimum mean hitting time in [24]. In [78] the mean hitting time in conjunction with multiple parallel CUSUM algorithms at various nodes of interest in the graph are used to describe a policy which ensures quickest average time to the detection of anomalies. In the strategies mentioned in these works the intruder/anomaly is assumed to be stationary. The policies for surveillance derived in this chapter are for mobile intruders modeled by Markov chains.

3.1.3 Statement of Contributions

Given the above, there are several contributions in this chapter. First, we provide a set of necessary and sufficient conditions which characterize when the meeting times between a single pursuer and a single evader is finite for arbitrary Markov chains. The bounds on meeting times in the literature were usually obtained for meeting times between ergodic Markov chains where they are guaranteed to be finite. We extend the notion to

generic transition matrices as opposed to equal-neighbor models, and we discuss when the meeting times are finite based on the existence of walks of equal length to common nodes. Second, we provide a closed-form solution to the meeting times of two independent Markov chains by utilizing the Kronecker product of the transition matrices. Third, we use this closed-form expression to perform theoretical and simulation studies and design fast Markov chain strategies for the pursuer to capture, in minimum expected time, different moving evaders in different prototypical graphs. In particular, in ring and complete graphs, we rigorously show a few qualitative features of the design. For example, being fast for the pursuer is not always necessary and the mean capture time may be indifferent to the pursuer's strategy for certain evaders.

This chapter provides the first closed-form solutions for the computation of the meeting times between two agents moving on a graph according to discrete-time Markov chains. Two closely related references are as follows: first, a system of equations for computing meeting times for independent identical random walks on graphs with irreducible transition matrices, where the transition matrices are limited to equal-neighbor weights, were obtained using Laplace transform techniques in [79]. Second, Kronecker products and vectorization techniques have been used to compute the Simrank of information networks which has interpretations in terms of meeting times [80]. In contrast, we consider absolutely generic transition matrices which need not be identical.

3.1.4 Organization

This chapter is organized as follows. In Section 3.2, we derive formulas for the meeting times of pairs of Markov chains and obtain conditions on the finiteness of meeting times. In Section 3.3, we present simulation results on optimal Markov chain strategies for the mobile pursuer. Finally, we conclude the chapter in Section 3.4.

3.2 Meeting times of two randomly moving agents

In this section, we formulate the meeting time between a pursuer and an evader moving according to discrete-time Markov chains. We provide necessary and sufficient conditions for the finiteness of the meeting times given initial starting positions of the agents on the graph.

3.2.1 The meeting time of two Markov chains

Consider the pursuer and evader performing random walks on a strongly connected graph $\mathcal{G} = (V, \mathcal{E})$. The transition matrices P_p of the pursuer and P_e of the evader satisfy $p_{i,j}^{(p)}, p_{i,j}^{(e)} \geq 0$ if $(i, j) \in \mathcal{E}$ and $p_{i,j}^{(p)}, p_{i,j}^{(e)} = 0$ if $(i, j) \notin \mathcal{E}$.

Let $X_t^{(p)}, X_t^{(e)} \in \{1, \dots, n\}$ be the locations of the two agents at time $t \in \{0, 1, 2, \dots\}$, respectively. For any two starting nodes i and j , the *first meeting time from i and j* , denoted by $T_{i,j}$, is the first time that two random walkers meet at a common node when starting from nodes i and j . Formally,

$$T_{i,j} = \min\{t \geq 1 \mid X_t^{(p)} = X_t^{(e)}, X_0^{(p)} = i \text{ and } X_0^{(e)} = j\}.$$

Note that the first meeting time can be infinite and it is easy to construct examples in which the two agents never meet. Moreover, by definition, if the two agents are at the same location initially, i.e., $i = j$, then $T_{i,j}$ is the first time they meet again. Let $m_{i,j} = \mathbb{E}[T_{i,j}]$ be the expected first meeting time starting from nodes i and j . For brevity, we shall refer to the expected first meeting time as just the meeting time.

Theorem 3.2.1.1 (The meeting time of two Markov chains) *Consider two Markov chains with transition matrices P_p and P_e defined on a digraph $\mathcal{G} = (V, \mathcal{E})$ with the node set $V = \{1, \dots, n\}$. The following statements are equivalent:*

1. for each pair of nodes i, j , the meeting time $m_{i,j}$ from nodes i and j is finite;
2. for each pair of nodes i, j , there exists a node $k \in \{1, \dots, n\}$ and a length $\ell \geq 0$ such that a walk of length ℓ exists from i to k for P_p and a walk of length ℓ exists from j to k for P_e ;
3. for each pair of nodes i, j , there exists a walk for the stochastic matrix $P_e \otimes P_p$ from node (j, i) to a node (k, k) in the Kronecker graph, for some $k \in \{1, \dots, n\}$;
4. the row-substochastic matrix $(P_e \otimes P_p)E$ with $E = I_{n^2} - \text{diag}(\text{vec}(I_n))$ has spectral radius less than 1 and the vector of meeting times is given by

$$\text{vec}(M) = (I_{n^2} - (P_e \otimes P_p)E)^{-1} \mathbf{1}_{n^2}, \quad (3.1)$$

where $M = [m_{i,j}]$.

Proof: For the nodes i and j , the first meeting time satisfies the recursive formula

$$T_{i,j} = \begin{cases} 1, & \text{w.p. } \sum_k p_{i,k}^{(p)} p_{j,k}^{(e)}, \\ T_{k_1, h_1} + 1, & \text{w.p. } p_{i,k_1}^{(p)} p_{j,h_1}^{(e)}, k_1 \neq h_1. \end{cases}$$

Taking the expectation we have

$$\begin{aligned} m_{i,j} &= \sum_k p_{i,k}^{(p)} p_{j,k}^{(e)} + \sum_{k_1 \neq h_1} p_{i,k_1}^{(p)} p_{j,h_1}^{(e)} (m_{k_1, h_1} + 1), \\ &= \sum_{k_1} \sum_{h_1} p_{i,k_1}^{(p)} p_{j,h_1}^{(e)} + \sum_{k_1 \neq h_1} p_{i,k_1}^{(p)} p_{j,h_1}^{(e)} m_{k_1, h_1}, \\ &= 1 + \sum_{k_1 \neq h_1} p_{i,k_1}^{(p)} p_{j,h_1}^{(e)} m_{k_1, h_1} \\ &= 1 + \sum_{k_1, h_1} p_{i,k_1}^{(p)} m_{k_1, h_1} p_{j,h_1}^{(e)} - \sum_{k=1}^n p_{i,k}^{(p)} m_{k,k} p_{j,k}^{(e)}. \end{aligned} \quad (3.2)$$

We write (3.2) in matrix form as

$$M = \mathbb{1}_n \mathbb{1}_n^\top + P_p(M - \text{diag}(M)) P_e^\top, \quad (3.3)$$

where $\text{diag}(M) \in \mathbb{R}^{n \times n}$ is a diagonal matrix with only the diagonal elements of M .

Rewriting (3.3) in vector form and using properties in Lemma 1.3.4.1 lead to

$$\begin{aligned} \text{vec}(M) &= \mathbb{1}_{n^2} + (P_e \otimes P_p)(\text{vec}(M) - \text{vec}(\text{diag}(M))), \\ &= \mathbb{1}_{n^2} + (P_e \otimes P_p)(I_{n^2} - \text{diag}(\text{vec}(I_n))) \text{vec}(M), \\ &= \mathbb{1}_{n^2} + (P_e \otimes P_p) E \text{vec}(M). \end{aligned}$$

If the matrix $I_{n^2} - (P_e \otimes P_p)E$ is invertible, then we have a unique solution to the meeting times.

We shall now show that the finiteness of meeting times as in 1 is equivalent to the existence of walks of equal length to common nodes as mentioned in 2 and in 3, which guarantees invertibility of $I_{n^2} - (P_e \otimes P_p)E$ in 4.

We first prove that $1 \implies 2$ by contrapositive. Suppose there exists a pair of nodes i and j such that there exists no walk of equal length to any node in V , then the agents never meet and thus the meeting time cannot be finite. Therefore, we have $1 \implies 2$.

Next, we show that $2 \iff 3$. The Kronecker product of the transition matrices gives a joint transition matrix for the agents over the set of nodes $V \times V$. The entry in the matrix $P_e \otimes P_p$ corresponding to the node (j, i) represents the states $X^{(p)} = i$ and $X^{(e)} = j$ [81]. The statement 2 ensures the existence of a node k for every pair (j, i) which is reachable by a walk of equal length from i in P_p and j in P_e . This condition is equivalent to the node (k, k) being reachable from the pair (j, i) on the Kronecker product of the two Markov chains [82, Proposition 1].

Next, we show that $3 \implies 4$. The stochastic matrix $P_e \otimes P_p$ has a walk from any node (j, i) to some node (h_1, k_1) where $\mathbb{P}(X_1^{(e)} = k, X_1^{(p)} = k \mid X_0^{(e)} = h_1, X_0^{(p)} = k_1) \neq 0$ as there exists a walk from (j, i) to (k, k) for some k . Note that $(P_e \otimes P_p)E$ is obtained by setting the columns of $P_e \otimes P_p$ corresponding to nodes of the form (k, k) to 0. Therefore, the row corresponding to (h_1, k_1) has row-sum strictly less than 1. As a result, every node (j, i) has a walk to a node whose corresponding row-sum of the transition matrix is less than 1, which implies that the matrix $(P_e \otimes P_p)E$ has spectral radius less than 1 by virtue of Lemma 1.3.5.1. From this we obtain equation (3.1) since 3 guarantees the existence of $(I_{n^2} - (P_e \otimes P_p)E)^{-1}$.

Note that the existence of $\text{vec}(M)$ in 4 gives $4 \implies 1$. Thus we have shown that $1 \implies 2 \iff 3 \implies 4 \implies 1$. Hence the four statements are equivalent. \blacksquare

Remark 3.2.1.2 *The finiteness of meeting times is not guaranteed even if both P_p and P_e are irreducible, and a simple example is given in Fig. 3.1.*

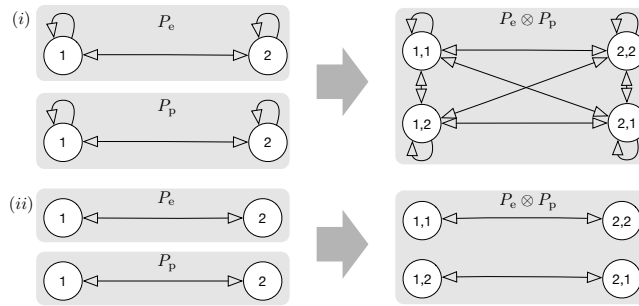


Figure 3.1: The pursuer-evader pair in (i) has finite meeting times as every node has a walk to the common nodes (1, 1) and (2, 2) in the Kronecker graph. However, in (ii) there exists no walks to common nodes from (1, 2) and (2, 1).

The necessary and sufficient conditions in Theorem 3.2.1.1 give the most general set of pairs of matrices for which finite meeting times exist. Moreover, the closed-form expression (3.1) for pairwise meeting times enables one to design the optimal strategy for

the surveillance agent to minimize the mean meeting time given the strategy of a moving evader.

3.2.2 Mean meeting time and relation to hitting times

In this subsection, we introduce the *mean meeting time* of two random walkers. We then show that the mean hitting time can be treated as a special case of mean meeting time where a mobile pursuer is faced with a stationary intruder.

Definition 3.2.2.1 (Mean meeting time) *Consider two transition matrices P_p and P_e with stationary distributions π_p and π_e , the mean meeting time $\mathcal{M}(P_p, P_e)$ is defined by*

$$\mathcal{M}(P_p, P_e) = \pi_p^\top M \pi_e = (\pi_e \otimes \pi_p)^\top \text{vec}(M), \quad (3.4)$$

where M is meeting time matrix of P_p and P_e .

The mean meeting time $\mathcal{M}(P_p, P_e)$ in (3.4) can also be written in element-wise form as follows,

$$\mathcal{M}(P_p, P_e) = \sum_i \sum_j \pi_p^{(i)} \pi_e^{(j)} m_{i,j},$$

where it is clear that the mean meeting time is the weighted sum of the pairwise meeting times with weights being the stationary distributions.

Remark 3.2.2.2 *In Definition 3.2.2.1, the uniqueness of the stationary distributions for P_p and P_e is not required. However, in order to compute the mean meeting time, one has to specify a stationary distribution consistent with the Markov chain for P_e and P_p , respectively.*

Our next result shows that the hitting times of a Markov chain are equal to the meeting times of the Markov chain and a stationary evader.

Corollary 3.2.2.3 (Connections with hitting times) *Consider a stationary evader with distribution π_e and a pursuer with an irreducible transition matrix P_p and stationary distribution π_p , then the following properties hold:*

1. *the meeting times between the stationary evader and the mobile pursuer are equal to the pairwise hitting times of P_p and are given by*

$$h_{i,j} = m_{i,j} = (\mathbf{e}_j \otimes \mathbf{e}_i)^\top (I_{n^2} - (I_n \otimes P_p)E)^{-1} \mathbf{1}_{n^2},$$

where $h_{i,j}$ is the expected time to travel from node i to node j for P_p and

2. *the mean meeting time between the stationary evader and the pursuer is given by*

$$\mathcal{M}_{\text{stationary}}(\pi_e, P_p) = (\pi_e \otimes \pi_p)^\top (I_{n^2} - (I_n \otimes P_p)E)^{-1} \mathbf{1}_{n^2}. \quad (3.5)$$

Proof: The conclusion follows by observing that a stationary evader can be described by the identity transition matrix I_n . ■

Remark 3.2.2.4 *When the stationary distribution of the evader π_e is equal to that of the pursuer π_p , the expression (3.5) for the meeting time is also identical to the mean first hitting time, also called Kemeny constant, of the Markov chain P_p [25, Theorem 2.3(i)].*

3.3 Applications to Robotic Surveillance

In this section, we numerically minimize the mean meeting time for the mobile pursuer given various strategies of the intruder in various prototypical graphs. The optimization problem we are interested in is as follows.

Problem 4 (*Minimization of the mean meeting time*) Given a strongly connected directed graph $\mathcal{G} = (V, \mathcal{E})$, an irreducible Markov chain P_e and the stationary distributions π_e and π_p . Find P_p which minimizes the mean meeting time $\mathcal{M}(P_p, P_e)$, i.e., solve the following optimization problem:

$$\begin{aligned} & \underset{P_p \in \mathbb{R}^{n \times n}}{\text{minimize}} && (\pi_e \otimes \pi_p)^\top \text{vec}(M) \\ & \text{subject to} && \pi_p^\top P_p = \pi_p^\top, \\ & && P_p \mathbf{1}_n = \mathbf{1}_n, \\ & && p_{i,j}^{(p)} \geq 0, \quad \forall (i, j) \in \mathcal{E}, \\ & && p_{i,j}^{(p)} = 0, \quad \forall (i, j) \notin \mathcal{E}. \end{aligned}$$

The mean meeting time measures in expectation how fast the pursuer is able to capture the evader when they start from different initial positions. By minimizing the mean meeting time, we obtain a fast pursuer given the strategy of the evader. Problem 4 is a nonconvex optimization problem with the Kemeny constant minimization problem as a special case. We conduct the numerical optimization using the KNITRO/TOMLAB package (with an implementation of the sequential quadratic programming algorithm), where the stationary distribution of P_p is set to be the same as that of P_e , i.e., $\pi_p = \pi_e$.

3.3.1 Evader models

We consider three different evaders, i.e., the random walk (RW) evader, the unpredictable evader using a Markov chain with maximum entropy rate, and the fast evader using a Markov chain with minimum Kemeny constant.

In the random walk model, the evader transitions from her current location to the neighboring locations (including the current location) with the same probability that

is equal to the reciprocal of the out-degree. The random walk has the maximum local uncertainty for the movement of the evader.

For the unpredictable evader, given the stationary distribution $\boldsymbol{\pi}_e$, the evader solves the following convex programming.

$$\begin{aligned}
& \underset{P_e \in \mathbb{R}^{n \times n}}{\text{maximize}} && - \sum_{i=1}^n \sum_{j=1}^n \pi_e^{(i)} p_{i,j}^{(e)} \log p_{i,j}^{(e)} \\
& \text{subject to} && \boldsymbol{\pi}_e^\top P_e = \boldsymbol{\pi}_e^\top, \\
& && P_e \mathbf{1}_n = \mathbf{1}_n, \\
& && p_{i,j}^{(e)} \geq 0, \quad \forall (i,j) \in \mathcal{E}, \\
& && p_{i,j}^{(e)} = 0, \quad \forall (i,j) \notin \mathcal{E}.
\end{aligned}$$

The unpredictable evader uses a Markov chain that has the maximum entropy rate with a given stationary distribution. The evader is unpredictable in terms of the sequence of locations that she visits [26].

For the fast evader, given the stationary distribution $\boldsymbol{\pi}_e$, the evader solves the following nonconvex optimization problem.

$$\begin{aligned}
& \underset{P_e \in \mathbb{R}^{n \times n}}{\text{minimize}} && \mathcal{M}_{\text{stationary}}(\boldsymbol{\pi}_e, P_e) \\
& \text{subject to} && \boldsymbol{\pi}_e^\top P_e = \boldsymbol{\pi}_e^\top, \\
& && P_e \mathbf{1}_n = \mathbf{1}_n, \\
& && p_{i,j}^{(e)} \geq 0, \quad \forall (i,j) \in \mathcal{E}, \\
& && p_{i,j}^{(e)} = 0, \quad \forall (i,j) \notin \mathcal{E},
\end{aligned}$$

where $\mathcal{M}_{\text{stationary}}(\boldsymbol{\pi}_e, P_e)$ is given in (3.5) with $\boldsymbol{\pi}_p = \boldsymbol{\pi}_e$. The fast evader uses a Markov chain that has minimum Kemeny constant. The evader is fast because the expected hitting time between pairs of locations on the graph is minimized [24].

3.3.2 Analysis and numerical results for different graphs

In this subsection, we consider different graph topology, i.e., ring, complete and grid, and solve for the best pursuer strategy P_p numerically. Since Problem 4 is in general a nonconvex optimization problem, we consider relatively small graph sizes $n = 5$ and $n = 6$ for the ring and complete, and $n = 9$ for the grid. In all the computations where a stationary distribution needs to be specified, we set the stationary distribution of the agents to be uniform, i.e., $\pi_p = \pi_e = \frac{1}{n}\mathbf{1}_n$.

Results for ring graphs: Note that ring graphs possess Hamiltonian tours (cycles in the graph that visit each vertex exactly once), which can be parameterized by Markov chains as permutation matrices with a uniform stationary distribution. Therefore, the fast evader on ring graphs follow Hamiltonian tours. However, depending on the number of nodes in the graph, the optimal strategies for the pursuer against the fast evader are different. When $n = 5$, the optimal strategy for the pursuer given by the solver is a Hamiltonian tour in the opposite direction from that of the evader. This coincides with our intuition because walking in a different direction for the pursuer should make it faster to catch the evader. However, it turns out that staying stationary for the pursuer is equally good as walking in the opposite direction. This happens because the pursuer may miss the evader when walking in an opposite direction. We formalize this observation as follows.

Lemma 3.3.2.1 (Strategies with same performance ring graphs) *In a ring graph with an odd number of nodes, if the evader adopts a Hamiltonian tour, then staying stationary and the Hamiltonian tour in the opposite direction have the same performance for a pursuer with a uniform stationary distribution.*

Proof: If the pursuer stays stationary with the distribution $\frac{1}{n}\mathbf{1}_n$, then the mean meeting time is the same as the Kemeny constant of the chain used by the fast evader,

which is $\frac{n+1}{2}$.

On the other hand, suppose the pursuer walks in the opposite direction from the evader. By symmetry, we can fix the initial condition of the evader to be $X_0^{(e)} = 1$ and vary the initial condition of the pursuer $X_0^{(p)}$. If $X_0^{(p)} = 1$, then the mean meeting time is n ; If $X_0^{(p)} > 1$ is odd, then the mean meeting time is $\frac{X_0^{(p)}-1}{2}$; If $X_0^{(p)}$ is even, then the mean meeting time is $\frac{n+X_0^{(p)}-1}{2}$. Therefore, the mean meeting time can be calculated as

$$\mathcal{M}(P_p, P_e) = \frac{1}{n} \left(\sum_{i=1}^{\frac{n-1}{2}} \frac{n+2i-1}{2} + \sum_{i=1}^{\frac{n-1}{2}} i + n \right) = \frac{n+1}{2},$$

which is the same as in the case of staying stationary. ■

When $n = 6$, the optimal strategy given by the solver is to stay stationary. Different from the case when the number of nodes is odd, walking in a different direction from the evader is bad because there are certain pairs of initial positions starting from which the pursuer and the evader never meet, i.e., the mean meeting time is infinite.

In the ring graph, the RW and unpredictable evader use the same chain where the evader moves to the neighbor nodes of her current position with equal probabilities. The optimal strategy for the pursuer given by the solver in these cases is a Hamiltonian tour regardless of the number of nodes in the graph. We summarize the results for ring graphs in Table 3.1.

Results for the complete graphs: Since complete graphs also possess Hamiltonian tours, the fast evader on complete graphs follow a Hamiltonian tour on the graph and the results for the fast evader in ring graphs carry over.

On the other hand, in complete graphs, the RW and unpredictable strategies are the same and equal to $\frac{1}{n} \mathbb{1}_n \mathbb{1}_n^\top$. The following result shows that if the evader adopts RW or unpredictable strategy in the complete graph, then the mean meeting time is n regardless of pursuer's strategy.

Table 3.1: Best Response for Pursuer in Ring Graphs

Evader strategy Number of nodes	Fast	RW/Unpredictable
n=5	stationary or P_e^\top	Hamiltonian tour
n=6	stationary	

When the number of nodes is odd, the best strategy for the pursuer against a fast evader is to either stay stationary or move fast in the opposite direction; when the number of nodes is even, staying stationary is the best. When the evader is unpredictable/slow, being fast is always good.

Lemma 3.3.2.2 (Strategy insensitivity in a complete graph) *If the evader's strategy on a complete graph is $\frac{1}{n}\mathbb{1}_n\mathbb{1}_n^\top$, then the mean meeting time between the evader and the pursuer is always n regardless of pursuer's strategy.*

Proof: If $P_e = \frac{1}{n}\mathbb{1}_n\mathbb{1}_n^\top$, then by (3.2) we have

$$m_{i,j} = 1 + \frac{1}{n} \sum_{k_1=1}^n p_{i,k_1}^{(p)} \sum_{h_1 \neq k_1} m_{k_1,h_1}.$$

Therefore, the meeting time $m_{i,j}$ does not depend on j . Let $\tilde{m}_i = m_{i,j}$, then we further have

$$\tilde{m}_i = 1 + \frac{n-1}{n} \sum_{k_1=1}^n p_{i,k_1}^{(p)} \tilde{m}_{k_1}.$$

Since the mean meeting time satisfies $\mathcal{M}(P_p, P_e) = \boldsymbol{\pi}_p^\top M \boldsymbol{\pi}_e = \boldsymbol{\pi}_p^\top \tilde{\mathbf{m}}$ in this case, we have

$$\mathcal{M} = 1 + \frac{n-1}{n} \mathcal{M},$$

and thus $\mathcal{M} = n$. ■

We summarize the results for complete graphs in Table 3.2.

Results for the grid: We plot the optimal strategies for the pursuer against an RW evader, an unpredictable evader, and a fast evader in Fig. 3.2, Fig. 3.3, and Fig. 3.4,

Table 3.2: Best Response for Pursuer in Complete Graphs

Evader strategy \ Number of nodes	Fast	RW/Unpredictable
n=5	stationary or P_e^\top	Arbitrary
n=6	stationary	

When the evader is fast, similar results as in ring graphs carry over. When the evader is unpredictable/slow, any strategy for the pursuer is optimal.

respectively. In all these figures, the size of the nodes indicates the magnitude of the stationary distribution, and the transparency of the edges indicates the magnitude of the transition probability.

From Fig. 3.2 and Fig. 3.3, we observe that when faced with an unpredictable and slow evader, the pursuer tends to travel fast in the graph. Note that the stationary distributions of the evaders and thus of the pursuers in these two cases are different (determined by the equal-neighbor model for RW and $\frac{1}{n}\mathbb{1}_n$ for the unpredictable chain). Specifically, the center node in Fig. 3.2 has a higher value in the stationary distribution than that in Fig. 3.3. Qualitatively, this difference forces the neighbor nodes of the center node to have positive transition probabilities to the center in the solution of the optimal pursuer in Fig. 3.2, whereas it is not the case in Fig. 3.3.

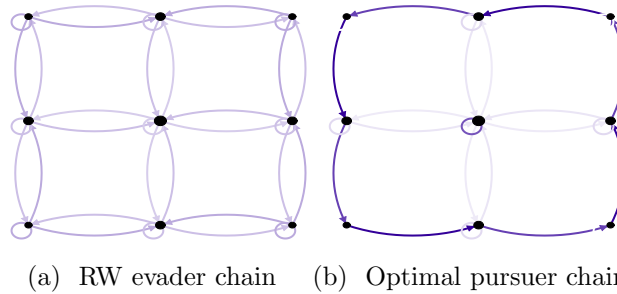


Figure 3.2: Random walk evader and optimal pursuer in grid

In contrast, when the evader moves fast enough, the optimal pursuer almost stays

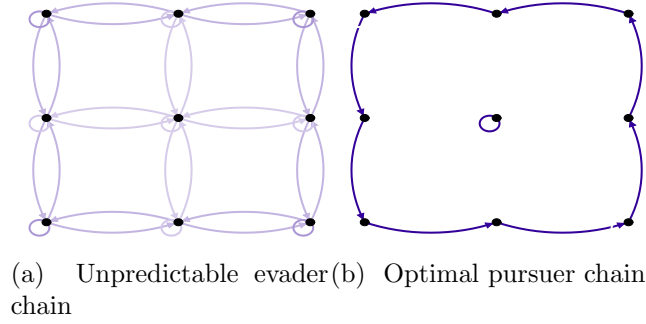


Figure 3.3: Unpredictable evader and optimal pursuer in grid

stationary and waits to be hit by the evader as shown in Fig. 3.4. The above observations in the grid graph are qualitatively consistent with those in the ring and complete graphs.

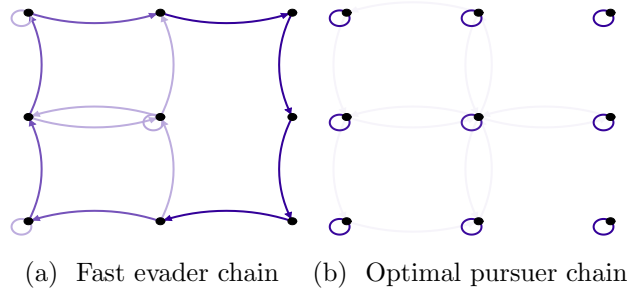


Figure 3.4: Fast evader and optimal pursuer in grid

3.3.3 Sensitivity analysis

In this subsection, we consider the case where the pursuer does not have a perfect estimate for the evader's strategy and investigate how sensitive Problem 4 is to this uncertainty. We consider two graph topologies: the 5-node ring graph and the 3×3 grid graph. The nominal evader's strategy P_e^0 that the pursuer optimizes against in these two cases is a random walk, i.e., the pursuer believes the evader walks randomly on the graph and runs the nonconvex programming in Problem 4 to solve for a best strategy P_p^0 for

herself (P_p^0 is a Hamiltonian tour in the ring graph and a strategy shown in Fig. 3.2(b) in the grid graph). However, in practice, the evader's strategy is not a standard random walk but a perturbed chain P_e^1 obtained by adding uniformly distributed perturbations over $[0, \delta]$ to each element of P_e^0 (we perform a normalization so that P_e^1 is a valid Markov chain). For the actual evader's strategy P_e^1 , there exists an optimal strategy P_p^1 against it, and the meeting time $\mathcal{M}(P_p^1, P_e^1)$ should be smaller than the meeting time $\mathcal{M}(P_p^0, P_e^1)$. We measure the relative performance degradation of P_p^0 with respect to P_p^1 by the following criterion

$$\text{Performance Degradation} = \frac{\mathcal{M}(P_p^0, P_e^1) - \mathcal{M}(P_p^1, P_e^1)}{\mathcal{M}(P_p^0, P_e^1)}.$$

In our simulation, we pick $\delta = 0.01, 0.05$, and 0.1 , and run the nonconvex programming for the ring and grid graph for 5000 and 1000 times, respectively. We report the empirical CDFs of the performance degradation in Fig. 3.5.

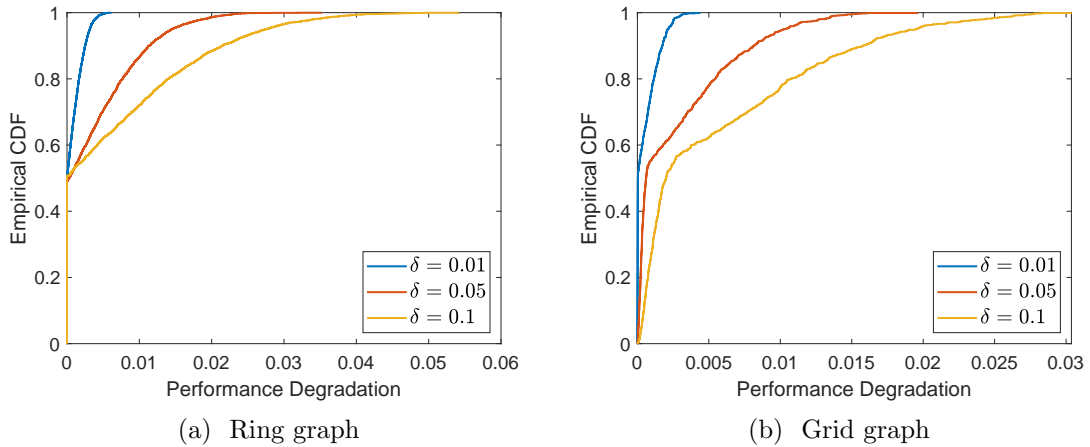


Figure 3.5: Performance degradation with uncertainty in evader strategy

From Fig. 3.5, we have the following two key observations. First, in most cases, the performance degradation is acceptable if not negligible. In particular, in the ring graph,

since P_p^0 is a fast Hamiltonian tour, it still performs very well when the evader's chain deviates slightly from the nominal random walk. Second, as the size of the perturbation increases, there are more cases with larger performance degradation, which is consistent with the intuition. A rigorous mathematical sensitivity analysis would be valuable but challenging; we leave it as our future work.

3.4 Conclusions

In this chapter, we studied the expected meeting time of a single pursuer and a single evader moving on a graph according to discrete-time Markov chains. We presented novel closed-form expressions for the meeting times and necessary and sufficient conditions for their finiteness. Then, we also discussed the connections with the hitting times of Markov chains. We finally formulated an optimization problem to obtain the optimal strategy for the pursuer faced with a mobile evader. Numerical examples were provided to explain the concepts and illustrate the results.

An interesting extension of the work discussed here would be to consider walkers moving with travel times similar to the cases studied in [27] and [24].

Chapter 4

Robotic Surveillance as Stackelberg Games

4.1 Introduction

Problem description and motivation

In a prototypical robotic surveillance scenario, mobile robots patrol and move among locations in an environment (usually modeled by a graph) with the goal of capturing potential intruders; see Fig. 4.1 for an illustration. Here, we consider a similar setup, where the patrolling robot is, in addition, facing an omniscient intruder. We model the strategic interactions between the mobile robot and the intruder as a Stackelberg game, where the optimal strategy for the surveillance agent is constructed under the assumption that the intruder acts optimally against her. This formulation captures the worst-case scenario for the surveillance agent when playing against the strongest possible opponent. The corresponding Stackelberg solution is meaningful and practical when little or no information is known about the intruder. Similar models have appeared in [32] and [33],

where heuristic algorithms without performance guarantees are provided. Instead, we analyze the problem from a mathematical perspective and obtain provably optimal or suboptimal solutions by considering three topologies: star, line and complete graph.

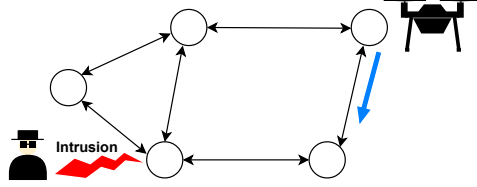


Figure 4.1: A surveillance scenario where a mobile robot patrols a graph with the goal of capturing potential intruders that attack certain locations.

Literature review

There have been continuing efforts to study robotic surveillance problems under various settings, formulations, and assumptions. The early work on designing deterministic surveillance strategies started in [15]. Recent deterministic extensions to cases where locations might have different importance, or to the coordination of multiple robots can be found in [16, 17, 6, 18, 19]. Unfortunately, deterministic strategies can be easily learned, and thus exploited in adversarial settings. In this respect, stochastic surveillance strategies are more appealing in that they are mostly unpredictable. One common approach to derive stochastic surveillance strategies is to model the motion of the surveillance agent as a first-order Markov chain [46, 23, 49]. Within this line of work, Patel *et al.* [24] studied minimum mean hitting time Markov chains for robotic surveillance with travel times on edges. They formulated a convex optimization problem by restricting attentions to the class of reversible Markov chains. More recently, George *et al.* [26] and Duan *et al.* [27] studied and quantified unpredictability of Markov chains and designed maxentropic surveillance strategies.

The aforementioned works do not explicitly describe the behavior of the malicious

intruders. On the other hand, when these models are available, they can be leveraged to design improved surveillance strategies. In order to model the interplay between the surveillance agent and the intruder, surveillance problems have also been studied under a game-theoretic lens. Stackelberg security games, where the defenders and intruders are modeled as strategic players with sequential plays, have been successfully applied in various real-world scenarios [36] such as checkpoints placement and patrolling at airports [83], coast guard surveillance [84] and wild life protection [85]. In these works, defenders allocate limited resources to a set of targets so as to optimize their objectives. The problems are formulated as matrix games and the topology of the environments are not explicitly taken into account. In [32], the authors introduce a patrolling game where a mobile robot moves on a graph to capture potential intruders who choose when and where to attack. Different intruder models were proposed and analyzed in [33], where the optimal Markov chain based stochastic strategy is computed via a pattern search algorithm. The authors in [34] consider an intruder with limited observation time and design a strategy that is both hard to learn and hard to attack. An intruder model where the intruder decides where, when and for how long it attacks is studied in [35], and it is found that increasing the randomness of the strategy helps reduce the intruder's reward. The authors in [86] study the impact of the graph topology on the maximization of the minimum expected hitting times. Finally, a sophisticated non-Markovian model was studied in [87] for the case of complete graphs.

While most of the existing works are concerned with the design of heuristics to compute suboptimal strategies without performance guarantees, in this chapter, we derive provably optimal/suboptimal strategies. Towards this goal, we adopt the model of [33] and focus on graphs that correspond to prototypical robotic roadmaps.

Statement of Contributions

In this chapter, we derive provably optimal and suboptimal strategies for surveillance agents in a Stackelberg game setting. We consider three prototypical robotic roadmaps are considered: star, complete and line graphs. Our problem formulation captures the worst-case scenario for the surveillance agent and thus the solution provides performance guarantees also in less pessimistic scenarios. Our main contributions are as follows.

1. We derive a universal upper bound for the capture probability, i.e., the maximum achievable performance for the surveillance agent facing an omniscient intruder;
2. We show that this upper bound is tight in the case of the complete graph, and further provide suboptimality guarantees for a natural strategy often referred to as a random walk;
3. We study dominant strategies for both the intruder and the surveillance agent. Leveraging these insights, we obtain optimal strategies in the star and line graphs.

Organization

We provide preliminaries on Markov chains and formulate the Stackelberg game problem in Section 4.2 and Section 4.3, respectively. An upper bound on the capture probability and a suboptimal solution in the case of complete graph are obtained in Section 4.4. We study dominant strategies for the players in Section 4.5, and optimal strategies for star and line graphs are given in the same section. The chapter is concluded in Section 4.6.

4.2 Preliminaries

In this chapter, we consider a strongly connected digraph $\mathcal{G} = (V, \mathcal{E})$, where V denotes the set of n nodes $\{1, \dots, n\}$ and $\mathcal{E} \subset V \times V$ denotes the set of edges. Given the graph

$\mathcal{G} = \{V, \mathcal{E}\}$, let $X_k \in \{1, \dots, n\}$ be the value of a Markov chain with transition diagram \mathcal{G} and transition matrix P at time $k \in \mathbb{Z}_{\geq 0}$. Let the (i, j) -th element of the *first hitting time probability matrix* F_k denote the probability that the Markov chain hits node j for the first time in exactly k time units starting from node i , i.e., $F_k(i, j) = \mathbb{P}(T_{ij} = k)$. It can be shown that the hitting time probabilities F_k for $k \geq 1$ satisfy the following recursive matrix equation [88, Chapter 5, Eq. (2.4)]

$$F_{k+1} = P(F_k - \text{diag}(F_k)), \quad (4.1)$$

where $F_1 = P$. The vectorized form of (4.1) can be written as

$$\text{vec}(F_{k+1}) = (I_n \otimes P)(I_{n^2} - E) \text{vec}(F_k), \quad (4.2)$$

where $E = \text{diag}(\text{vec}(I_n))$. Note that (4.1) can be generalized to the case where there are times on the graph \mathcal{G} [27].

4.3 Problem formulation

We consider a robotic surveillance problem where a mobile robot moves randomly between locations in a graph to perform surveillance tasks. Specifically, given a Markov chain strategy, the surveillance robot moves from the current node to a neighboring location according to the corresponding Markov chain transition matrix. An intruder attacks an unknown node in the graph by stationing at the given node for a certain period of time. The intruder is captured if the surveillance agent visits that node within the duration of the attack; see Fig. 4.1 for a pictorial representation. In this work, we study how the mobile robot should move on the graph in order to maximize the probability of capturing the intruder.

We model the strategic interactions between the surveillance robot and the intruder as a two-player Stackelberg game with a leader and a follower. The game proceeds as follows: the leader commits to a strategy first, and then the follower, based on the knowledge of the leader’s strategy, selects a strategy that optimizes her rewards. Having prior knowledge of the follower’s best-response, the leader commits to a strategy that ultimately maximizes her own objective. In our problem setting, the surveillance agent is the leader who chooses a Markov chain as surveillance strategy. This strategy is observed and learned by the intruder (follower) who then chooses the best time and location to attack so as to minimize the probability of being captured. We describe the intruder and surveillance models in the following subsections.

4.3.1 Intruder Model

An intruder aims to attack a location in the graph while the surveillance agent moves around with the goal of capturing her. The intruder requires τ units of time to complete the attack at any location in the graph. Once it commits to attacking a location, it stations at the location for that given period of time. We assume that the intruder is omniscient [32, 33], i.e., it knows or can learn the strategy (intended as a description of the Markov chain) as well as the current location of the surveillance agent perfectly. Given this information, the intruder decides when and where to attack so that it is least likely to be captured.

Given a Markov chain strategy for the surveillance agent, the intruder picks a pair of locations i and j so that the probability that the surveillance agent goes from location i to location j within the attack duration is minimized. Then, the intruder attacks location j whenever the surveillance agent is at location i . Formally, for a surveillance strategy parameterized by a Markov transition matrix P , an optimal strategy for the intruder

(i^*, j^*) is given by

$$(i^*, j^*) \in \operatorname{argmin}_{i,j} \{\mathbb{P}(T_{ij}(P) \leq \tau)\}. \quad (4.3)$$

Note that optimal strategies in (4.3) are not unique in general, and the intruder is free to pick any one of them.

4.3.2 Surveillance model and problem formulation

The surveillance agent, knowing that the intruder selects an optimal strategy according to (4.3), adopts a Markov chain P^* that maximizes the probability of capturing the intruder, i.e.,

$$P^* = \operatorname{argmax}_P \min_{i,j} \{\mathbb{P}(T_{ij}(P) \leq \tau)\}.$$

In this chapter, we are interested in finding an optimal strategy for the surveillance agent when playing against the omniscient intruder just described. That is, we are interested in solving the following optimization problem.

Problem 5 *Given a strongly connected digraph $\mathcal{G} = (V, \mathcal{E})$ and the attack duration $\tau \in \mathbb{Z}_{>0}$, find a Markov chain that conforms to the graph topology and maximizes the capture probability, i.e., solves the following optimization problem:*

$$\begin{aligned} & \underset{P \in \mathbb{R}^{n \times n}}{\text{maximize}} && \min_{i,j} \{\mathbb{P}(T_{ij}(P) \leq \tau)\} \\ & \text{subject to} && P \mathbf{1}_n = \mathbf{1}_n, \\ & && p_{ij} \geq 0, \quad \text{for all } (i, j) \in \mathcal{E}, \\ & && p_{ij} = 0, \quad \text{for all } (i, j) \notin \mathcal{E}. \end{aligned} \quad (4.4)$$

We let $\mathbb{V} \in [0, 1]$ denote the optimal value of Problem 5 and refer to it as the value of the game. Note that \mathbb{V} represents the capture probability obtained when the surveillance agent utilizes an optimal strategy against the omniscient intruder. As a consequence, \mathbb{V}

lower bounds the capture probability also in less pessimistic circumstances, e.g., in the case of a nonstrategic intruder.

Remark 4.3.2.1 (Impact of the attack duration) *Problem 5 is interesting only when the attack duration τ is in an appropriate range for a given graph topology. Specifically,*

1. *the attack duration should be greater than or equal to the diameter D of graph \mathcal{G} , i.e., $\tau \geq D$. Otherwise, the omniscient intruder always succeeds by attacking one end of the graph diameter when the surveillance agent is visiting the other. In this case, $\mathbb{V} = 0$ no matter what strategy the surveillance agent uses;*
2. *the attack duration should be smaller than the length of any closed path on the graph \mathcal{G} that has the same initial and final vertices and visits all locations at least once (e.g., a Hamiltonian tour of size n if it exists). Otherwise, the surveillance agent does not benefit from using a Markov chain as a randomized strategy, and the capture is guaranteed by following the deterministic closed path.*

We assume hereafter that the attack duration τ takes a nontrivial value as described in Remark 4.3.2.1.

Remark 4.3.2.2 (Irreducibility of optimal solutions) *No irreducibility constraint is imposed on the Markov chain in Problem 5. However, if τ takes nontrivial values, an optimal Markov chain is necessarily irreducible. As the transition diagrams of any reducible Markov chains is not strongly connected, there must exist a pair of locations i and j such that $\mathbb{P}(T_{ij} \leq \tau) = 0$, so that also $\mathbb{V} = 0$.*

Remark 4.3.2.3 (Graph dimension) *Without loss of generality, we consider graphs with more than 2 nodes in the rest of this chapter, i.e., $n \geq 3$. When $n = 2$, the only meaningful case is a complete graph, and the optimal solution to Problem 5 is $P = \frac{1}{2}\mathbb{1}_2\mathbb{1}_2^\top$*

with $\mathbb{V} = \frac{1}{2}$ if $\tau = 1$, and an irreducible permutation matrix (a Hamiltonian tour) with $\mathbb{V} = 1$ if $\tau \geq 2$.

4.4 Value of the game and suboptimal solution in complete graphs

In this section, we first derive a universal upper bound for the value of the game, which does not depend the graph topology. We then consider the case of complete graph and show that the upper bound can be tight. Further, we provide suboptimality guarantees for a Markov chain whose corresponding transition matrix has identical entries.

4.4.1 Upper bound of the value of the game

We introduce an auxiliary variable $\mu \in \mathbb{R}$ and exploit the iteration (4.1) to rewrite the optimization problem (4.4) as follows

$$\begin{aligned}
& \underset{\mu \in \mathbb{R}, P \in \mathbb{R}^{n \times n}}{\text{maximize}} && \mu \\
& \text{subject to} && \mu \mathbb{1}_n \mathbb{1}_n^\top \leq \sum_{k=1}^{\tau} F_k, \\
& && F_1 = P \\
& && F_{k+1} = P(F_k - \text{diag}(F_k)), \quad 1 \leq k \leq \tau - 1 \\
& && P \mathbb{1}_n = \mathbb{1}_n, \\
& && p_{ij} \geq 0, \quad \text{for all } (i, j) \in \mathcal{E}, \\
& && p_{ij} = 0, \quad \text{for all } (i, j) \notin \mathcal{E},
\end{aligned} \tag{4.5}$$

where the inequality in the first constraint is element-wise. Clearly, problem (4.5) is equivalent to (4.4), and the optimal value μ^* is the value of the game. The following theorem shows how to obtain a universal upper bound on μ^* .

Theorem 4.4.1.1 (Upper bound for the value of the game) *Given a strongly connected digraph $\mathcal{G} = (V, \mathcal{E})$ with n nodes and an attack duration τ that takes nontrivial values as in Remark 4.3.2.1, the value of the game satisfies $\mathbb{V} \leq \frac{\tau}{n}$.*

Proof: By Remark 4.3.2.2, an optimal solution P^* to problem (4.5) is irreducible and thus has a unique stationary distribution $\boldsymbol{\pi}$. We multiply $\boldsymbol{\pi}^\top$ from the left on both sides of (4.1) and obtain for $k \geq 1$,

$$\boldsymbol{\pi}^\top F_{k+1} = \boldsymbol{\pi}^\top (F_k - \text{diag}(F_k)) \leq \boldsymbol{\pi}^\top F_k. \quad (4.6)$$

By using (4.6) recursively, we have that for $k \geq 1$,

$$\boldsymbol{\pi}^\top F_k \leq \boldsymbol{\pi}^\top F_1 = \boldsymbol{\pi}^\top P^* = \boldsymbol{\pi}^\top. \quad (4.7)$$

Since (μ^*, P^*) is an optimal solution to problem (4.5), it satisfies the first constraint and thus

$$\mu^* \mathbf{1}_n \mathbf{1}_n^\top \leq \sum_{k=1}^{\tau} F_k. \quad (4.8)$$

Multiplying $\boldsymbol{\pi}^\top$ from the left on both sides of (4.8) and using (4.7), we obtain

$$\mu^* \mathbf{1}_n^\top \leq \sum_{k=1}^{\tau} \boldsymbol{\pi}^\top = \tau \boldsymbol{\pi}^\top.$$

Since $\boldsymbol{\pi}^\top \mathbf{1}_n = 1$, we must have $\min_{1 \leq i \leq n} \pi_i \leq \frac{1}{n}$. Therefore,

$$\mathbb{V} = \mu^* \leq \tau \min_{1 \leq i \leq n} \pi_i = \frac{\tau}{n}.$$

■

4.4.2 Suboptimal solution in complete digraphs

Next, we show that for complete digraphs the upper bound $\mathbb{V} \leq \frac{\tau}{n}$ can be achieved for certain combinations of n and τ .

Lemma 4.4.2.1 (Optimal solution in special complete digraph) *Given a complete digraph $\mathcal{G} = (V, \mathcal{E})$ with n nodes and the attack duration $\tau \leq n$, if τ divides n , then an optimal solution P^* is given by*

$$P^* = \Pi_0 \otimes \frac{\tau}{n} \mathbb{1}_{\frac{n}{\tau}} \mathbb{1}_{\frac{n}{\tau}}^\top,$$

where $\Pi_0 \in \mathbb{R}^{\tau \times \tau}$ is any irreducible permutation matrix that represents a Hamiltonian tour in \mathcal{G} . Moreover, the optimal strategy P^* achieves the upper bound of the value of the game.

Proof: By construction, the probability that a surveillance agent with P^* starting from any location i arrives at any location j within τ time steps is $\frac{\tau}{n}$. ■

The previous result holds only when the combination of n and τ is such that τ divides n . Nevertheless, leveraging Theorem 4.4.1.1 we are able to provide suboptimality guarantees for the natural choice of $P = \frac{1}{n} \mathbb{1}_n \mathbb{1}_n^\top$.

Lemma 4.4.2.2 (Constant factor optimality of random walk) *Given a complete digraph $\mathcal{G} = (V, \mathcal{E})$ with $n \geq 3$ nodes and the attack duration τ , the random walk strategy $P = \frac{1}{n} \mathbb{1}_n \mathbb{1}_n^\top$ achieves performance within*

$$\frac{n^\tau - (n-1)^\tau}{\tau n^{\tau-1}} \geq 1 - \frac{1}{e}$$

of optimality, where e is Euler's number.

Proof: First, note that the capture probability for the random walk surveillance policy $P = \frac{1}{n}\mathbb{1}_n\mathbb{1}_n^\top$ is $1 - (1 - \frac{1}{n})^\tau$. Therefore, the random walk achieves performance within

$$f(n, \tau) = \frac{n^\tau - (n-1)^\tau}{\tau n^{\tau-1}}$$

of optimality. Let n be fixed, and $g(\tau) = \frac{n^\tau - (n-1)^\tau}{\tau n^{\tau-1}}$. We relax τ to be a continuous variable and take derivative of $g(\tau)$ as

$$\begin{aligned} \frac{dg(\tau)}{d\tau} &= -\frac{n}{\tau^2} + \frac{n}{\tau^2}\left(1 - \frac{1}{n}\right)^\tau - \frac{n}{\tau}\left(1 - \frac{1}{n}\right)^\tau \log\left(1 - \frac{1}{n}\right) \\ &= \frac{n}{\tau^2}\left((1 - \tau \log(1 - \frac{1}{n}))\left(1 - \frac{1}{n}\right)^\tau - 1\right) \\ &\leq \frac{n}{\tau^2}\left((1 - \tau(1 - \frac{1}{1 - \frac{1}{n}}))\left(1 - \frac{1}{n}\right)^\tau - 1\right) \\ &= \frac{n}{\tau^2}\left((1 + \frac{\tau}{n-1})\left(1 - \frac{1}{n}\right)^\tau - 1\right) \leq 0, \end{aligned}$$

where we used the upper bound $\log x \geq 1 - \frac{1}{x}$ in the first inequality, and $\tau \leq n-1$ and $(1 - \frac{1}{n})^\tau \leq \frac{1}{2}$ in the second inequality. Therefore, for fixed n , $f(n, \tau)$ is a decreasing function in τ and

$$f(n, \tau) \geq f(n, n-1) = \frac{n}{n-1} - \left(1 - \frac{1}{n}\right)^{n-2} \triangleq h(n).$$

We relax n to be a continuous variable in this case and compute the derivative of $h(n)$

as

$$\begin{aligned}
\frac{dh(n)}{dn} &= -\frac{1}{(n-1)^2} + \left(1 - \frac{1}{n}\right)^{n-2} \left(\log \frac{n}{n-1} - \frac{n-2}{n^2-n}\right) \\
&\leq -\frac{1}{(n-1)^2} + \left(1 - \frac{1}{n}\right)^{n-2} \left(\frac{1}{n-1} - \frac{n-2}{n^2-n}\right) \\
&= -\frac{1}{(n-1)^2} + \left(1 - \frac{1}{n}\right)^{n-1} \frac{2}{(n-1)^2} \\
&\leq -\frac{1}{(n-1)^2} + \left(1 - \frac{1}{3}\right)^2 \frac{2}{(n-1)^2} \leq 0,
\end{aligned}$$

where we used the upper bound $\log(1+x) \leq x$ and the proved that $(1 - \frac{1}{n})^{n-1}$ is decreasing as n increases. Therefore, we have that $h(n)$ is a decreasing function. In summary, we have

$$f(n, \tau) \geq f(n, n-1) \geq \lim_{n \rightarrow \infty} h(n) = \lim_{n \rightarrow \infty} \left(\frac{n}{n-1} - \left(1 - \frac{1}{n}\right)^{n-2}\right) = 1 - \frac{1}{e}.$$

■

4.5 Strategy dominance and optimal strategies in star and line graphs

In this section, we first obtain dominated strategies for the intruder as well as the dominant strategies for the surveillance agent. Leveraging these result, we derive optimal strategies for the surveillance agent in star and line graphs.

4.5.1 Dominated strategies for the omniscient intruder

In this subsection, we present two lemmas characterizing dominated strategies for the omniscient intruder, i.e., strategies that intruder will never choose as they lead to a

higher probability of being captured.

Lemma 4.5.1.1 (Dominated strategy for the intruder) *Given a strongly connected digraph $\mathcal{G} = (V, \mathcal{E})$ and an irreducible Markov chain strategy P for the surveillance agent, attacking node $j \in V$ when the surveillance agent is at node $i \in V$, $i \neq j$, is not optimal for the omniscient intruder if:*

1. *there exists a node k such that any path from node k to node j contains node i ; or*
2. *there exists a node k such that any path from node i to node k contains node j .*

Moreover, in case 1 (resp. in case 2), attacking node j when the surveillance agent is at node k (resp. node i) is a better strategy for the omniscient intruder.

Proof: The probability that the surveillance agent visiting node i captures the intruder attacking node j is

$$\mathbb{P}(T_{ij} \leq \tau) = \sum_{t=1}^{\tau} \mathbb{P}(T_{ij} = t).$$

Regarding 1, we need to show that

$$\mathbb{P}(T_{kj} \leq \tau) \leq \mathbb{P}(T_{ij} \leq \tau).$$

Since any path from node k to node j contains node i , by definition of probability, and

the memoryless property of Markov chains, we have

$$\begin{aligned}
 \mathbb{P}(T_{kj} \leq \tau) &= \sum_{t=1}^{\tau-1} \mathbb{P}(T_{ki} = t) \mathbb{P}(T_{ij} \leq \tau - t) \\
 &\leq \max_{1 \leq t \leq \tau-1} \mathbb{P}(T_{ij} \leq \tau - t) \\
 &= \mathbb{P}(T_{ij} \leq \tau - 1) \\
 &\leq \mathbb{P}(T_{ij} \leq \tau),
 \end{aligned}$$

where we used that $\mathbb{P}(T_{ij} \leq \tau - t)$ is decreasing with t .

The proof for 2 follows a similar argument as in 1. ■

Lemma 4.5.1.2 (Dominated strategy on leaf nodes) *Given a strongly connected digraph $\mathcal{G} = (V, \mathcal{E})$ with $n \geq 3$ nodes and an irreducible Markov chain strategy P for the surveillance agent, if node $i \in V$ is a leaf node in \mathcal{G} , then attacking node i when the surveillance agent just leaves node i is not optimal for the omniscient intruder.*

Proof: The case of $\tau = 1$ is uninteresting here because the surveillance agent fails with probability 1 if the intruder attacks the leaf node i when the surveillance agent visits other nodes than node i and its neighbor. Therefore, we consider $\tau \geq 2$ in the following. Let node j be the neighbor node of the leaf node i , then

$$\mathbb{P}(T_{ii} \leq \tau) = p_{ii} + (1 - p_{ii})\mathbb{P}(T_{ji} \leq \tau - 1). \quad (4.9)$$

Moreover, for $k \in V$, $k \neq i$ and $k \neq j$,

$$\begin{aligned}
 \mathbb{P}(T_{ki} \leq \tau) &= \sum_{t=1}^{\tau-1} \mathbb{P}(T_{kj} = t) \mathbb{P}(T_{ji} \leq \tau - t) \\
 &\leq \max_{1 \leq t \leq \tau-1} \mathbb{P}(T_{ji} \leq \tau - t) \\
 &= \mathbb{P}(T_{ji} \leq \tau - 1).
 \end{aligned} \tag{4.10}$$

Therefore, by (4.9) and (4.10) we have

$$\begin{aligned}
 \mathbb{P}(T_{ii} \leq \tau) &\geq p_{ii} + (1 - p_{ii}) \mathbb{P}(T_{ki} \leq \tau) \\
 &\geq p_{ii} \mathbb{P}(T_{ki} \leq \tau) + (1 - p_{ii}) \mathbb{P}(T_{ki} \leq \tau) \\
 &= \mathbb{P}(T_{ki} \leq \tau),
 \end{aligned}$$

which implies that attacking node i when the surveillance agent is at node k is a better strategy. ■

4.5.2 Dominant strategies for the surveillance agent

In this subsection, we show that part of the optimal surveillance strategy can be determined readily when leaf nodes are present, where leaf nodes are nodes that have only one neighboring node.

Lemma 4.5.2.1 (Dominant strategy on leaf nodes) *Given a strongly connected digraph $\mathcal{G} = (V, \mathcal{E})$ with $n \geq 3$ nodes, if node $i \in V$ is a leaf node in \mathcal{G} with node $j \in V$ as its only neighbor, then the optimal strategy P^* satisfies*

$$P^*(i, i) = 0, \text{ and } P^*(i, j) = 1.$$

Proof: Without loss of generality, suppose that node 1 is a leaf node in \mathcal{G} and node 2 is its neighbor. Let P be a strategy that is the same as P^* except that $P(1,1) = p > 0$ and $P(1,2) = 1 - p < 1$. We prove that for all $i, j \in V$, the capture probability $\mathbb{P}(T_{ij}^* \leq \tau)$ for P^* is greater than or equal to $\min_{\{i,j \in V\}} \mathbb{P}(T_{ij} \leq \tau)$ for P , which leads to $\min_{\{i,j \in V\}} \mathbb{P}(T_{ij}^* \leq \tau) \geq \min_{\{i,j \in V\}} \mathbb{P}(T_{ij} \leq \tau)$.

Since P and P^* differ by only the first row and node 1 is a leaf node, we must have $\mathbb{P}(T_{i1}^* \leq \tau) = \mathbb{P}(T_{i1} \leq \tau)$ for all $i \in \{2, \dots, n\}$. Moreover, by Lemma 4.5.1.2, the strategy $(1,1)$ is a dominated strategy for the intruder, thus $\min_{\{i,j \in V\}} \mathbb{P}(T_{ij}^* \leq \tau)$ and $\min_{\{i,j \in V\}} \mathbb{P}(T_{ij} \leq \tau)$ do not attain minimum at $(1,1)$.

We next prove that $\mathbb{P}(T_{1j}^* \leq \tau) \geq \mathbb{P}(T_{1j} \leq \tau)$ for all $j \in \{2, \dots, n\}$ by induction. Let d_{1j} be the length of the shortest paths from node 1 to node j . The probabilities of these shortest paths are equal to the products of the edge probabilities along the paths, and for P and P^* they differ by a factor of $1-p$. Thus, we have that $\mathbb{P}(T_{1j}^* \leq d_{1j}) > \mathbb{P}(T_{1j} \leq d_{1j})$. Suppose when $\tau \leq t$ for $t \geq d_{1j}$, we have $\mathbb{P}(T_{1j}^* \leq \tau) > \mathbb{P}(T_{1j} \leq \tau)$ and let ℓ_{ij}^t be the set of paths from node i to node j that do not contain node 1 and have length less than or equal to t for $i \in \{2, \dots, n\}$, then for $\tau = t + 1$,

$$\begin{aligned}
\mathbb{P}(T_{1j}^* \leq t + 1) &= \mathbb{P}(T_{2j}^* \leq t) \\
&= \sum_{t_1=1}^t \mathbb{P}(T_{21}^* = t_1) \mathbb{P}(T_{1j}^* \leq t - t_1) + \mathbb{P}(\ell_{2j}^t) \\
&\geq \sum_{t_1=1}^t \mathbb{P}(T_{21} = t_1) \mathbb{P}(T_{1j} \leq t - t_1) + \mathbb{P}(\ell_{2j}^t) \\
&= \mathbb{P}(T_{2j} \leq t) \\
&\geq p \mathbb{P}(T_{1j} \leq t) + (1 - p) \mathbb{P}(T_{2j} \leq t) \\
&= \mathbb{P}(T_{1j} \leq t + 1),
\end{aligned}$$

where the first inequality follows from the induction hypothesis and the second inequality follows from Lemma 4.5.1.1.

Finally, for $i, j \in \{2, \dots, n\}$, we have

$$\begin{aligned} \mathbb{P}(T_{ij}^* \leq \tau) &= \sum_{t=1}^{\tau} \mathbb{P}(T_{i1}^* = t) \mathbb{P}(T_{1j}^* \leq \tau - t) + \mathbb{P}(\ell_{ij}^{\tau}) \\ &\geq \sum_{t=1}^{\tau} \mathbb{P}(T_{i1} = t) \mathbb{P}(T_{1j} \leq \tau - t) + \mathbb{P}(\ell_{ij}^{\tau}) \\ &= \mathbb{P}(T_{ij} \leq \tau). \end{aligned}$$

In summary, we have that $\min_{\{i,j \in V\}} \mathbb{P}(T_{ij}^* \leq \tau) \geq \min_{\{i,j \in V\}} \mathbb{P}(T_{ij} \leq \tau)$, which completes the proof. ■

4.5.3 Optimal solution for star graphs

In this subsection, we consider the star topology, which represents the abstraction of an environment where there is a corridor connecting multiple rooms. The optimal strategy for the surveillance agent is given in the following theorem.

Theorem 4.5.3.1 (Optimal solution in star graph) *Given a directed star graph $\mathcal{G} = (V, \mathcal{E})$ with $n \geq 3$ nodes and node 1 being the center, the optimal strategy P^* for the surveillance agent is given by*

$$P^* = \begin{bmatrix} 0 & \frac{1}{n-1} & \frac{1}{n-1} & \cdots & \frac{1}{n-1} \\ 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix}. \quad (4.11)$$

Moreover, the value of the game \mathbb{V} satisfies

$$\mathbb{V} = \begin{cases} 1 - \left(1 - \frac{1}{n-1}\right)^{\frac{\tau-1}{2}}, & \text{if } \tau \geq 2 \text{ is odd,} \\ 1 - \left(1 - \frac{1}{n-1}\right)^{\frac{\tau}{2}}, & \text{if } \tau \geq 2 \text{ is even.} \end{cases}$$

Proof: For the directed star graph \mathcal{G} , the Markov chain P corresponding to \mathcal{G} has the following general structure,

$$P = \begin{bmatrix} p_{11} & p_{12} & p_{13} & \cdots & p_{1n} \\ p_{21} & p_{22} & 0 & \cdots & 0 \\ p_{31} & 0 & p_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ p_{n1} & 0 & 0 & \cdots & p_{nn} \end{bmatrix}.$$

Since node 2 to node n are leaf nodes, by Lemma 4.5.2.1, the optimal Markov chain does not have self loops at these nodes and we can reduce P to

$$P = \begin{bmatrix} p_{11} & p_{12} & p_{13} & \cdots & p_{1n} \\ 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix}. \quad (4.12)$$

Note that the strategies $(1, j)$ are dominated for the intruder for all $j \in \{2, \dots, n\}$ by Lemma 4.5.1.1, and the capture probabilities $\mathbb{P}(T_{i1} \leq \tau) = 1$ for all $i \in \{1, \dots, n\}$ and $\tau \geq 2$. Therefore, we only need to find a P in (4.12) that maximizes $\min_{i,j \in \{2, \dots, n\}} \mathbb{P}(T_{ij} \leq \tau)$. We divide the rest of the proof into two parts. In the first part, we show that there is no self loop at the center node for the optimal solution, i.e., $p_{11} = 0$ in (4.12), and

further reduce P ; in the second part, we obtain the optimal solution.

No self loop at center We construct P_1 to be the same as P in (4.12) except for the first row where

$$P_1(1, 1) = 0, \quad P_1(1, j) = \frac{p_{1j}}{1 - p_{11}} \text{ for } j \in \{2, \dots, n\}.$$

We show that P_1 is a better strategy than P in (4.12) by induction on τ , i.e., for all $i, j \in \{2, \dots, n\}$, the capture probabilities $\mathbb{P}(T_{ij}^1 \leq \tau)$ for P_1 is greater than $\mathbb{P}(T_{ij} \leq \tau)$ of P . When $\tau = 2$, we have $\mathbb{P}(T_{ij}^1 \leq 2) = \frac{p_{1j}}{1 - p_{11}} > p_{1j} = \mathbb{P}(T_{ij} \leq 2)$. Suppose when $\tau \leq t$, we have $\mathbb{P}(T_{ij}^1 \leq \tau) > \mathbb{P}(T_{ij} \leq \tau)$, then for $\tau = t + 1$,

$$\begin{aligned} \mathbb{P}(T_{ij}^1 \leq t + 1) &= \mathbb{P}(T_{1j}^1 \leq t) \\ &= \frac{p_{1j}}{1 - p_{11}} + \sum_{k \notin \{1, j\}} \frac{p_{1k}}{1 - p_{11}} \mathbb{P}(T_{kj}^1 \leq t - 1) \\ &> \frac{p_{1j}}{1 - p_{11}} + \sum_{k \notin \{1, j\}} \frac{p_{1k}}{1 - p_{11}} \mathbb{P}(T_{kj} \leq t - 1) \\ &= \frac{1}{1 - p_{11}} (p_{1j} + \sum_{k \notin \{1, j\}} p_{1k} \mathbb{P}(T_{1j} \leq t - 1)) \\ &= \frac{1}{1 - p_{11}} (\mathbb{P}(T_{1j} \leq t) - p_{11} \mathbb{P}(T_{1j} \leq t - 1)) \\ &\geq \frac{1}{1 - p_{11}} (\mathbb{P}(T_{1j} \leq t) - p_{11} \mathbb{P}(T_{1j} \leq t)) \\ &= \mathbb{P}(T_{1j} \leq t) \\ &= \mathbb{P}(T_{ij} \leq t + 1), \end{aligned}$$

where the first inequality follows from the induction hypothesis and the second inequality follows from the fact that $\mathbb{P}(T_{1j} \leq t - 1) \leq \mathbb{P}(T_{1j} \leq t)$. Therefore, we conclude that the optimal strategy does not have a self loop at the center node.

Optimal solution Note that for any $\tau \geq 1$ and $j \in \{2, \dots, n\}$, we have that

$$\begin{aligned}
 \mathbb{P}(T_{1j} \leq \tau) &= p_{1j} + \sum_{k \notin \{1,j\}} p_{1k} \mathbb{P}(T_{kj} \leq \tau - 1) \\
 &= p_{1j} + \sum_{k \notin \{1,j\}} p_{1k} \mathbb{P}(T_{1j} \leq \tau - 2) \\
 &= p_{1j} + (1 - p_{1j}) \mathbb{P}(T_{1j} \leq \tau - 2),
 \end{aligned}$$

with the initial condition $\mathbb{P}(T_{1j} \leq 1) = \mathbb{P}(T_{1j} \leq 2) = p_{1j}$. Therefore, the capture probability $\mathbb{P}(T_{1j} \leq \tau)$ satisfies

$$\mathbb{P}(T_{1j} \leq \tau) = \begin{cases} 1 - (1 - p_{1j})^{\frac{\tau-1}{2}}, & \text{if } \tau \geq 2 \text{ is odd,} \\ 1 - (1 - p_{1j})^{\frac{\tau}{2}}, & \text{if } \tau \geq 2 \text{ is even.} \end{cases} \quad (4.13)$$

By (4.13), we have for odd $\tau \geq 2$,

$$\begin{aligned}
 \min_{i,j \in \{2, \dots, n\}} \mathbb{P}(T_{ij} \leq \tau) &= \min_{j \in \{2, \dots, n\}} \mathbb{P}(T_{1j} \leq \tau - 1) \\
 &= \min_{j \in \{2, \dots, n\}} 1 - (1 - p_{1j})^{\frac{\tau-1}{2}} \\
 &= 1 - \max_{j \in \{2, \dots, n\}} (1 - p_{1j})^{\frac{\tau-1}{2}} \\
 &= 1 - (1 - \min_{j \in \{2, \dots, n\}} p_{1j})^{\frac{\tau-1}{2}},
 \end{aligned}$$

which along with the fact that $\sum_{j=2}^n p_{1j} = 1$ implies that (4.11) is the optimal solution for the directed star graph. ■

4.5.4 Optimal solution for line graphs

In this subsection, we derive the optimal surveillance strategy for directed line graphs. In an n -node line graph, Problem 5 is interesting only when the attack duration τ satisfies $n - 1 \leq \tau \leq 2n - 3$. If $\tau < n - 1$, the omniscient intruder always succeeds by attacking an end node when the surveillance agent is at the other end; if $\tau > 2n - 3$, the surveillance agent who walks back and forth between two ends of the line graph (a deterministic sweeping) captures the omniscient intruder no matter how it attacks. Therefore, we consider only cases when $n - 1 \leq \tau \leq 2n - 3$. Note that a sweeping strategy fails as long as $\tau < 2n - 3$, because the intruder could attack an end node immediately after the surveillance agent just leaves that node and it succeeds with probability 1. We label the nodes in an n -node line graph successively from left to right by $(1, \dots, n)$. We need the following conjecture to establish our main result.

Conjecture 1 (Uniqueness of the optimal strategy) *Given a directed line graph $\mathcal{G} = (V, \mathcal{E})$ with $n \geq 3$ nodes, the optimal solution to Problem 5 is unique.*

We provide evidence for Conjecture 1 in Remark 4.5.4.2.

Theorem 4.5.4.1 (Optimal solution in line graph) *Given a directed line graph $\mathcal{G} = (V, \mathcal{E})$ with $n \geq 3$ nodes, if Conjecture 1 holds true, then the optimal strategy P^* is given by*

$$P^* = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0.5 & 0 & 0.5 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0.5 & 0 & 0.5 \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix}. \quad (4.14)$$

Proof: We divide the proof into three parts. In the first part, we show that in the line graph, the optimal strategy for the intruder is to attack one end of the graph when

the surveillance agent is at the other, in which case the objective function in Problem 5 becomes $\min\{\mathbb{P}(T_{1n} \leq \tau), \mathbb{P}(T_{n1} \leq \tau)\}$. In the second part, we show that there are no self loops at any locations in the optimal surveillance strategy. In the last part, we obtain the optimal strategy by using Conjecture 1 and a symmetry argument.

Attack the end nodes For $i, j \in V$ and $i < j$, by Lemma 4.5.1.1, we know that $\mathbb{P}(T_{ij} \leq \tau) \geq \mathbb{P}(T_{1j} \leq \tau) \geq \mathbb{P}(T_{1n} \leq \tau)$; on the other hand, for $i > j$, we have $\mathbb{P}(T_{ij} \leq \tau) \geq \mathbb{P}(T_{nj} \leq \tau) \geq \mathbb{P}(T_{n1} \leq \tau)$. Therefore, attacking any location in the middle while the surveillance agent is at another location in the middle is not optimal for the intruder. Since node 1 and n are leaf nodes, by Lemma 4.5.1.2, it is not optimal for the intruder to attack node 1 or n immediately after the surveillance agent leaves that node. Next, we show that attacking any node $i \in \{2, \dots, n-1\}$ immediately when the surveillance agent leaves node i is dominated by attacking an end node when the surveillance agent is visiting the other. For $i \in \{2, \dots, n-1\}$,

$$\begin{aligned} \mathbb{P}(T_{ii} \leq \tau) &= p_{ii} + p_{i,i+1}\mathbb{P}(T_{i+1,i} \leq \tau - 1) + p_{i,i-1}\mathbb{P}(T_{i-1,i} \leq \tau - 1) \\ &\geq p_{ii} + p_{i,i+1}\mathbb{P}(T_{n1} \leq \tau) + p_{i,i-1}\mathbb{P}(T_{1n} \leq \tau) \\ &\geq \min\{1, \mathbb{P}(T_{n1} \leq \tau), \mathbb{P}(T_{1n} \leq \tau)\} \\ &= \min\{\mathbb{P}(T_{n1} \leq \tau), \mathbb{P}(T_{1n} \leq \tau)\}, \end{aligned}$$

where the first inequality follows from the facts that

$$\mathbb{P}(T_{n1} \leq \tau) = \sum_{t_1, t_2} \mathbb{P}(T_{n,i+1} = t_1) \mathbb{P}(T_{i+1,i} \leq \tau - t_1 - t_2) \mathbb{P}(T_{i1} = t_2) \leq \mathbb{P}(T_{i+1,i} \leq \tau - 1),$$

and

$$\mathbb{P}(T_{1n} \leq \tau) = \sum_{t_1, t_2} \mathbb{P}(T_{1,i} = t_1) \mathbb{P}(T_{i,i+1} \leq \tau - t_1 - t_2) \mathbb{P}(T_{i+1,n} = t_2) \leq \mathbb{P}(T_{i,i+1} \leq \tau - 1).$$

Therefore, the best strategy for the omniscient intruder is to attack an end node when the surveillance agent is at the other. Problem 5 becomes $\max_P \min\{\mathbb{P}(T_{1n} \leq \tau), \mathbb{P}(T_{n1} \leq \tau)\}$.

No self loop at any location First, by Lemma 4.5.2.1, since nodes 1 and n are leaf nodes, the optimal strategy P^* for the surveillance agent must satisfy $P^*(1, 1) = 0$, $P^*(1, 2) = 1$, $P^*(n, n) = 0$ and $P^*(n, n-1) = 1$. Next, we focus on $i \in \{2, \dots, n-1\}$. Let P be any Markov chain strategy corresponding to the line graph with $p_{ii} > 0$, and P_1 is the same as P except for the i -th row where

$$P_1(i, i) = 0, \quad P_1(i, i+1) = \frac{p_{i,i+1}}{1 - p_{ii}}, \quad P_1(i, i-1) = \frac{p_{i,i-1}}{1 - p_{ii}}.$$

Note that

$$\begin{aligned} \mathbb{P}(T_{1n} \leq \tau) &= \sum_{t_1=i-1}^{\tau} \mathbb{P}(T_{1i} = t_1) \mathbb{P}(T_{in} \leq \tau - t_1), \\ \mathbb{P}(T_{n1} \leq \tau) &= \sum_{t_1=n-i}^{\tau} \mathbb{P}(T_{ni} = t_1) \mathbb{P}(T_{i1} \leq \tau - t_1). \end{aligned} \tag{4.15}$$

Since P and P_1 differ only by row i , their first hitting time probabilities satisfy $\mathbb{P}(T_{1i} = t_1) = \mathbb{P}(T_{1i}^1 = t_1)$ and $\mathbb{P}(T_{ni} = t_1) = \mathbb{P}(T_{ni}^1 = t_1)$ for all $t_1 \geq 1$. We first prove that $\mathbb{P}(T_{in} \leq \tau) \leq \mathbb{P}(T_{in}^1 \leq \tau)$ for all τ by induction. When $\tau = n-i$, since $P_1(i, i+1) > p_{i,i+1}$, we have $\mathbb{P}(T_{in} \leq n-i) \leq \mathbb{P}(T_{in}^1 \leq n-i)$. Suppose for all $\tau \leq t$, we have $\mathbb{P}(T_{in} \leq t) \leq \mathbb{P}(T_{in}^1 \leq t)$. Then, when $\tau = t+1$,

$$\begin{aligned}
\mathbb{P}(T_{in}^1 \leq t+1) &= \frac{p_{i,i-1}}{1-p_{ii}} \mathbb{P}(T_{i-1,n}^1 \leq t) + \frac{p_{i,i+1}}{1-p_{ii}} \mathbb{P}(T_{i+1,n}^1 \leq t), \\
&\geq \frac{p_{i,i-1}}{1-p_{ii}} \mathbb{P}(T_{i-1,n} \leq t) + \frac{p_{i,i+1}}{1-p_{ii}} \mathbb{P}(T_{i+1,n} \leq t) \\
&= \frac{1}{1-p_{ii}} (\mathbb{P}(T_{in} \leq t+1) - p_{ii} \mathbb{P}(T_{in} \leq t)) \\
&\geq \frac{1}{1-p_{ii}} (\mathbb{P}(T_{in} \leq t+1) - p_{ii} \mathbb{P}(T_{in} \leq t+1)) \\
&= \mathbb{P}(T_{in} \leq t+1),
\end{aligned}$$

where the first inequality follows from the hypothesis induction. A similar proof by induction shows that $\mathbb{P}(T_{ni} \leq \tau) \leq \mathbb{P}(T_{ni}^1 \leq \tau)$ for all τ . Then, by (4.15), we have that $\mathbb{P}(T_{n1} \leq \tau) \leq \mathbb{P}(T_{n1}^1 \leq \tau)$ and $\mathbb{P}(T_{1n} \leq \tau) \leq \mathbb{P}(T_{1n}^1 \leq \tau)$ and therefore P_1 is a better strategy than P . In summary, we have that the optimal surveillance strategy does not have self loop at any location.

Optimal solution By the first two parts, we conclude that the optimal strategy for the surveillance agent has the following general structure,

$$P = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1-x_1 & 0 & x_1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1-x_{n-2} & 0 & x_{n-2} \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix}, \quad (4.16)$$

and thus the objective function in Problem 5 can be parameterized by $0 < x_1 < 1, \dots, 0 < x_{n-2} < 1$. Let

$$f(x_1, \dots, x_{n-2}) = \min_{x_1, \dots, x_{n-2}} \{\mathbb{P}(T_{1n} \leq \tau), \mathbb{P}(T_{n1} \leq \tau)\}.$$

For the function f , following the proof in Appendix 4.7.1, we have

$$f(x_1, \dots, x_{n-2}) = f(1 - x_1, \dots, 1 - x_{n-2}).$$

If Conjecture 1 holds, then at the optimal solution, we must have $x_i^* = 1 - x_i^*$ for all $i \in \{1, \dots, n-2\}$, which implies $x_i^* = \frac{1}{2}$. Therefore, the optimal solution is given by (4.14). ■

We prove a necessary condition for a strategy to be optimal in line graphs in Lemma 4.7.2.1 in Appendix 4.7.2, which says that the optimal strategy must satisfy $\mathbb{P}(T_{1n}^* \leq \tau) = \mathbb{P}(T_{n1}^* \leq \tau)$. We provide evidence for Conjecture 1 in the following remark.

Remark 4.5.4.2 (Evidence for conjecture 1) *We first consider two tractable cases: $n = 3$ and $\tau = n - 1$ or $\tau = n$. When $n = 3$, the line graph is also a star graph, and by Theorem 4.5.3.1, we have that the optimal solution is unique. The case $\tau = n$ is the same as that of $\tau = n - 1$ since the optimal Markov chain in the form (4.16) is periodic. For $\tau = n - 1$, we have*

$$\mathbb{P}(T_{1n} \leq n - 1) = p_{23}p_{34} \cdots p_{n-1,n},$$

$$\mathbb{P}(T_{n1} \leq n - 1) = p_{n-1,n-2}p_{n-2,n-3} \cdots p_{21},$$

and note that

$$\begin{aligned} \mathbb{P}(T_{1n} \leq n-1) \mathbb{P}(T_{n1} \leq n-1) &= (p_{21}p_{23}) \cdots (p_{n-1,n-2}p_{n-1,n}) \\ &\leq \left(\frac{p_{21} + p_{23}}{2}\right)^2 \cdots \left(\frac{p_{n-1,n-2} + p_{n-1,n}}{2}\right)^2 = \frac{1}{2^{2n-4}}. \end{aligned} \quad (4.17)$$

There is a unique strategy that achieves the upper bound in (4.17): $p_{i,i+1} = p_{i,i-1} = \frac{1}{2}$ for all $i \in \{2, \dots, n-1\}$. Moreover, this strategy satisfies the necessary condition in Lemma 4.7.2.1. Therefore, the optimal solution is unique.

As a second justification, following the Monte Carlo probability estimation method in [89, Remark V.1], we randomly pick 27000 different Markov chains with the structure (4.16) for $n = 5, \tau = 8$ and $n = 6, \tau = 8$. In all these cases, no chain has been found to have a better or same value as that of (4.14). Therefore, we have 99% confidence that the probability of (4.14) being optimal is at least 0.99 for these cases.

4.6 Conclusion

In this chapter, we studied a Stackelberg game formulation for the robotic surveillance problem, where the surveillance agent defends against an omniscient intruder who decides where and when to attack. We derived an upper bound on the performance of the surveillance agent and provided provably suboptimal solution in the complete graph. We derived dominant strategies and leveraged them to obtain optimal strategies for the star and the line topology. For future works, we will consider arbitrary graph topology and heterogeneous attack duration.

4.7 Appendix

4.7.1 Proof of a symmetry property

Let P_1 be a Markov chain of the form (4.16) and P_2 be

$$\begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ x_1 & 0 & 1 - x_1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & x_{n-2} & 0 & 1 - x_{n-2} \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix},$$

which is, in terms of the objective function, equivalent to

$$P_2 = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 - x_{n-2} & 0 & x_{n-2} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 - x_1 & 0 & x_1 \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix}. \quad (4.18)$$

We work with P_2 in (4.18) for the rest of the proof. Let $\mathbb{P}(T_{1n}^1 \leq \tau)$ and $\mathbb{P}(T_{1n}^2 \leq \tau)$ be the capture probabilities for P_1 and P_2 , respectively. We show that $\mathbb{P}(T_{1n}^1 \leq \tau) = \mathbb{P}(T_{1n}^2 \leq \tau)$, and a similar proof strategy works for the claim $\mathbb{P}(T_{n1}^1 \leq \tau) = \mathbb{P}(T_{n1}^2 \leq \tau)$. From (4.2),

we have that

$$\begin{aligned}
\mathbb{P}(T_{1n}^1 \leq \tau) &= \mathbf{e}_1^\top \sum_{t=1}^{\tau} (P_1 - P_1 \mathbf{e}_n \mathbf{e}_n^\top)^{t-1} P \mathbf{e}_n \\
&= \mathbf{e}_1^\top (I_n - (P_1 - P_1 \mathbf{e}_n \mathbf{e}_n^\top)^\tau) \cdot (I_n - (P_1 - P_1 \mathbf{e}_n \mathbf{e}_n^\top))^{-1} P \mathbf{e}_n \\
&= \mathbf{e}_1^\top (I_{n-1} - A^\tau) (I_{n-1} - A)^{-1} b,
\end{aligned}$$

where $b = x_{n-2} \mathbf{e}_{n-1}$ and

$$A = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 - x_1 & 0 & x_1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 - x_{n-3} & 0 & x_{n-3} \\ 0 & \cdots & 0 & 1 - x_{n-2} & 0 \end{bmatrix}.$$

Note that $(I_{n-1} - A)\mathbf{1}_{n-1} = b$. Therefore, we have

$$\mathbb{P}(T_{1n}^1 \leq \tau) = \mathbf{e}_1^\top (I_{n-1} - A^\tau) \mathbf{1}_{n-1}. \tag{4.19}$$

Similarly, for P_2 , we have

$$\mathbb{P}(T_{1n}^2 \leq \tau) = \mathbf{e}_1^\top (I_{n-1} - B^\tau) \mathbf{1}_{n-1}, \tag{4.20}$$

where

$$B = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 - x_{n-2} & 0 & x_{n-2} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 - x_2 & 0 & x_2 \\ 0 & \cdots & 0 & 1 - x_1 & 0 \end{bmatrix}.$$

In order to show $\mathbb{P}(T_{1n}^1 \leq \tau) = \mathbb{P}(T_{1n}^2 \leq \tau)$, by (4.19) and (4.20), we only need to prove that for all $\tau \geq 1$,

$$\mathbf{e}_1^\top A^\tau \mathbf{1}_{n-1} = \mathbf{e}_1^\top B^\tau \mathbf{1}_{n-1}. \quad (4.21)$$

First, note that for all $\tau \leq n - 2$, we have

$$\mathbf{e}_1^\top A^\tau \mathbf{1}_{n-1} = \mathbf{e}_1^\top B^\tau \mathbf{1}_{n-1} = 1. \quad (4.22)$$

We next show that A and B have the same characteristic polynomials, and then by the Cayley-Hamilton and (4.22), we will have (4.21). Since both A and B are tridiagonal matrices, the characteristic polynomials of A and B can be generated as follows [90, equation (2.3)]. Note that A and B are of order $n - 1$. Let $g_0^{n-1}(\lambda) = h_0^{n-1}(\lambda) = 1$, $g_1^{n-1}(\lambda) = h_1^{n-1}(\lambda) = \lambda$, where the superscript indicates the order of the matrices, and for $k = 2, \dots, n - 1$,

$$\begin{aligned} g_k^{n-1}(\lambda) &= \lambda g_{k-1}^{n-1}(\lambda) - x_{k-2}(1 - x_{k-1})g_{k-2}^{n-1}(\lambda), \\ h_k^{n-1}(\lambda) &= \lambda h_{k-1}^{n-1}(\lambda) - x_k(1 - x_{k-1})h_{k-2}^{n-1}(\lambda), \end{aligned} \quad (4.23)$$

where $x_0 = x_{n-1} = 1$ and we obtain the recurrence h_k^{n-1} for B starting from the bottom right of B matrix. Then $g_{n-1}^{n-1}(\lambda)$ and $h_{n-1}^{n-1}(\lambda)$ are the characteristic polynomials for A

and B , respectively. Moreover, notice that

$$g_n^n = \begin{vmatrix} \lambda I_{n-1} - A & -x_{n-2}\mathfrak{e}_{n-1} \\ -(1-x_{n-1})\mathfrak{e}_{n-1}^\top & \lambda \end{vmatrix} = \lambda g_{n-1}^{n-1} - x_{n-2}(1-x_{n-1})g_{n-2}^{n-1},$$

and $g_{n-1}^n = g_{n-1}^{n-1}$. Thus,

$$\begin{bmatrix} g_n^n(\lambda) \\ g_{n-1}^n(\lambda) \end{bmatrix} = \begin{bmatrix} \lambda & -x_{n-2}(1-x_{n-1}) \\ 1 & 0 \end{bmatrix} \begin{bmatrix} g_{n-1}^{n-1}(\lambda) \\ g_{n-2}^{n-1}(\lambda) \end{bmatrix}. \quad (4.24)$$

At the same time, note that

$$\begin{aligned} h_{n-1}^n &= |\lambda I_{n-1} - B + (1-x_{n-1})\mathfrak{e}_1\mathfrak{e}_2^\top| \\ &= \lambda h_{n-2}^{n-1} - (1-x_{n-2})x_{n-1}h_{n-3}^{n-1}, \\ h_{n-2}^n &= h_{n-2}^{n-1}. \end{aligned} \quad (4.25)$$

Thus,

$$\begin{aligned}
\begin{bmatrix} h_n^n(\lambda) \\ h_{n-1}^n(\lambda) \end{bmatrix} &= \begin{bmatrix} \lambda & -(1-x_{n-1}) \\ 1 & 0 \end{bmatrix} \begin{bmatrix} h_{n-1}^n(\lambda) \\ h_{n-2}^n(\lambda) \end{bmatrix} \\
&= \begin{bmatrix} \lambda & -(1-x_{n-1}) \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \lambda & -x_{n-1}(1-x_{n-2}) \\ 1 & 0 \end{bmatrix} \begin{bmatrix} h_{n-2}^{n-1}(\lambda) \\ h_{n-3}^{n-1}(\lambda) \end{bmatrix} \\
&= \begin{bmatrix} \lambda & -(1-x_{n-1}) \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \lambda & -x_{n-1}(1-x_{n-2}) \\ 1 & 0 \end{bmatrix} \\
&\quad \cdot \begin{bmatrix} \lambda & -(1-x_{n-2}) \\ 1 & 0 \end{bmatrix}^{-1} \begin{bmatrix} h_{n-1}^{n-1}(\lambda) \\ h_{n-1}^{n-2}(\lambda) \end{bmatrix} \\
&= \begin{bmatrix} \lambda x_{n-1} & (\lambda^2 - 1)(1-x_{n-1}) \\ x_{n-1} & \lambda(1-x_{n-1}) \end{bmatrix} \begin{bmatrix} h_{n-1}^{n-1}(\lambda) \\ h_{n-2}^{n-1}(\lambda) \end{bmatrix}, \tag{4.26}
\end{aligned}$$

where the second and third equalities follow from (4.25) and (4.23), respectively.

In the following, we prove that

$$\begin{aligned}
g_{n-1}^{n-1}(\lambda) &= h_{n-1}^{n-1}(\lambda), \\
\lambda g_{n-1}^{n-1}(\lambda) &= x_{n-2} g_{n-2}^{n-1}(\lambda) + (\lambda^2 - 1) h_{n-2}^{n-1}, \tag{4.27}
\end{aligned}$$

by induction on n . When $n = 3$, by (4.23), we have

$$\begin{aligned}
g_2^2(\lambda) &= \lambda g_1^2(\lambda) - x_0(1-x_1)g_0^2(\lambda) = \lambda^2 - (1-x_1), \\
h_2^2(\lambda) &= \lambda h_1^2(\lambda) - x_2(1-x_1)h_0^2(\lambda) = \lambda^2 - (1-x_1),
\end{aligned}$$

and

$$\lambda g_2^2(\lambda) = \lambda^3 - \lambda(1 - x_1) = x_1 g_1^2(\lambda) + (\lambda^2 - 1)h_1^2.$$

Suppose (4.27) holds for $n = k$, then when $n = k + 1$,

$$\begin{aligned} g_k^k(\lambda) - h_k^k(\lambda) &= \lambda g_{k-1}^{k-1}(\lambda) - x_{k-2}(1 - x_{k-1})g_{k-2}^{k-1}(\lambda) \\ &\quad - \lambda x_{k-1}h_{k-1}^{k-1}(\lambda) - (\lambda^2 - 1)(1 - x_{k-1})h_{k-2}^{k-1}(\lambda) \\ &= x_{k-2}x_{k-1}g_{k-2}^{k-1}(\lambda) - \lambda x_{k-1}h_{k-1}^{k-1}(\lambda) + (\lambda^2 - 1)x_{k-1}h_{k-2}^{k-1}(\lambda) \\ &= \lambda x_{k-1}g_{k-1}^{k-1}(\lambda) - \lambda x_{k-1}h_{k-1}^{k-1}(\lambda) = 0, \end{aligned}$$

where the first equality follows from (4.24) and (4.26), the second and third follow from induction hypothesis. Moreover,

$$\begin{aligned} \lambda g_k^k(\lambda) - x_{k-1}g_{k-1}^k(\lambda) - (\lambda^2 - 1)h_{k-1}^k &= (\lambda^2 - x_{k-1})g_{k-1}^{k-1}(\lambda) - \lambda x_{k-2}(1 - x_{k-1})g_{k-2}^{k-1}(\lambda) \\ &\quad - (\lambda^2 - 1)(x_{k-1}h_{k-1}^{k-1}(\lambda) + \lambda(1 - x_{k-1})h_{k-2}^{k-1}(\lambda)) \\ &= (1 - x_{k-1})\lambda^2 g_{k-1}^{k-1}(\lambda) - \lambda^2(1 - x_{k-1})g_{k-1}^{k-1}(\lambda) = 0, \end{aligned}$$

where the first equality follows from (4.24) and (4.26), and the second follows from the induction hypothesis. The proof is completed.

4.7.2 Necessary optimality condition in line graphs

Lemma 4.7.2.1 (Necessary optimality condition in line graph) *Given a line graph $\mathcal{G} = (V, \mathcal{E})$ with $n \geq 3$ nodes, if the Markov chain strategy P^* is optimal for the surveillance agent, then it must satisfy $\mathbb{P}(T_{1n}^* \leq \tau) = \mathbb{P}(T_{n1}^* \leq \tau)$.*

Proof: We divide the proof into two parts. In the first part, we show a monotonicity

property of the hitting times $\mathbb{P}(T_{1n} \leq \tau)$ and $\mathbb{P}(T_{n1} \leq \tau)$. In the second part, we obtain the necessary condition.

Monotonicity of hitting times We claim that $\mathbb{P}(T_{1n} \leq \tau)$ is monotonically increasing (decreasing) with $p_{i,i+1}$ ($p_{i,i-1}$), and $\mathbb{P}(T_{n1} \leq \tau)$ is monotonically decreasing (increasing) with $p_{i,i+1}$ ($p_{i,i-1}$). We prove that $\mathbb{P}(T_{1n} \leq \tau)$ is monotonically increasing with $p_{i,i+1}$, and a similar proof works for the other cases. For any $i \in \{2, \dots, n-1\}$, let P^ϵ be a Markov chain that is the same as P except that $P^\epsilon(i, i+1) = P(i, i+1) + \epsilon$ and $P^\epsilon(i, i-1) = P(i, i-1) - \epsilon$, where $\epsilon > 0$ is small enough such that P^ϵ remains irreducible. We first show that for $i \in \{2, \dots, n-1\}$, we have $\mathbb{P}(T_{in}^\epsilon \leq \tau) \geq \mathbb{P}(T_{in} \leq \tau)$ by induction. When $\tau = n - i$,

$$\begin{aligned} \mathbb{P}(T_{in}^\epsilon \leq n - i) &= (\epsilon + p_{i,i+1})p_{i+1,i+2} \cdots p_{n-1,n} \\ &> p_{i,i+1}p_{i+1,i+2} \cdots p_{n-1,n} \\ &= \mathbb{P}(T_{in} \leq n - i). \end{aligned}$$

Suppose $\mathbb{P}(T_{in}^\epsilon \leq \tau) \geq \mathbb{P}(T_{in} \leq \tau)$ holds for $\tau \leq t$. For $i \in \{2, \dots, n-2\}$, let $\ell_{i+1,n}^t$ be the set of paths from node $i+1$ to node n that do not contain node i and have length

less than or equal to t . Then, when $\tau = t + 1$, for $i \in \{2, \dots, n - 2\}$,

$$\begin{aligned}
\mathbb{P}(T_{in}^\epsilon \leq t + 1) &= (p_{i,i-1} - \epsilon)\mathbb{P}(T_{i-1,n}^\epsilon \leq t) + p_{i,i}\mathbb{P}(T_{in}^\epsilon \leq t) + (p_{i,i+1} + \epsilon)\mathbb{P}(T_{i+1,n}^\epsilon \leq t) \\
&= (p_{i,i-1} - \epsilon) \sum_{t_1=1}^t \mathbb{P}(T_{i-1,i}^\epsilon = t_1) \mathbb{P}(T_{in}^\epsilon \leq t - t_1) \\
&\quad + p_{i,i}\mathbb{P}(T_{in}^\epsilon \leq t) + (p_{i,i+1} + \epsilon)\mathbb{P}(\ell_{i+1,n}^t) \\
&\quad + (p_{i,i+1} + \epsilon) \sum_{t_1=1}^t \mathbb{P}(T_{i+1,i}^\epsilon = t_1) \mathbb{P}(T_{in}^\epsilon \leq t - t_1) \\
&\geq (p_{i,i-1} - \epsilon)\mathbb{P}(T_{i-1,n}^\epsilon \leq t) + p_{i,i}\mathbb{P}(T_{in}^\epsilon \leq t) + (p_{i,i+1} + \epsilon)\mathbb{P}(T_{i+1,n}^\epsilon \leq t) \\
&\geq \mathbb{P}(T_{in}^\epsilon \leq t + 1),
\end{aligned} \tag{4.28}$$

where the first inequality follows from the induction hypothesis and the second inequality follows from the fact that $\mathbb{P}(T_{i+1,n}^\epsilon \leq t) \geq \mathbb{P}(T_{i-1,n}^\epsilon \leq t)$ by Lemma 4.5.1.1. Moreover, when $i = n - 1$, we equate $\mathbb{P}(T_{i+1,n}^\epsilon \leq t) = 1$ in the third line of (4.28), and a similar argument follows. Finally, we have

$$\begin{aligned}
\mathbb{P}(T_{1n}^\epsilon \leq \tau) &= \sum_{t_1=1}^{\tau} \mathbb{P}(T_{1i}^\epsilon = t_1) \mathbb{P}(T_{in}^\epsilon \leq \tau - t_1) \\
&\geq \sum_{t_1=1}^{\tau} \mathbb{P}(T_{1i}^\epsilon = t_1) \mathbb{P}(T_{in}^\epsilon \leq \tau - t_1) \\
&= \mathbb{P}(T_{1n}^\epsilon \leq \tau),
\end{aligned}$$

which completes the proof.

Necessary condition for optimality We prove by contradiction. Without loss of generality, suppose P^* is optimal and $\mathbb{P}(T_{1n}^* \leq \tau) < \mathbb{P}(T_{n1}^* \leq \tau)$. By the monotonicity properties in the first part, for $i \in \{2, n - 1\}$, if we increase $p_{i,i+1}^*$ and decrease $p_{i,i-1}^*$, then

$\mathbb{P}(T_{1n}^* \leq \tau)$ increases and $\mathbb{P}(T_{n1}^* \leq \tau)$ decreases continuously, which leads to an increase in the objective function $\min\{\mathbb{P}(T_{1n}^* \leq \tau), \mathbb{P}(T_{n1}^* \leq \tau)\}$. Therefore, the strategy P^* is not the optimal, which is a contradiction. ■

Part II

Metzler Matrices and Monotone Systems

Chapter 5

Graph-Theoretic Stability

Conditions for Metzler Matrices and Monotone Systems

5.1 Introduction

Problem description and motivation Much attention in recent years has been focused on multi-agent systems, but the majority of efforts has been devoted to averaging dynamics and consensus behavior. Much less attention has been drawn to dynamical flow systems, modeled as monotone or cooperative systems [91, 92]. Notable exceptions are a collection of recent papers motivated by applications to traffic and biological systems [93, 94] as well as the long-standing interest in positive systems [95, 96]. Despite these remarkable recent works, many open questions remain.

This chapter focuses on a key foundational question for linear monotone systems, i.e., positive systems modeled by Metzler matrices, and on its application to the study of nonlinear monotone systems: what are graph-theoretical conditions for the Hurwitzness

of a Metzler matrix? While a graph theoretical treatment is available for a subclass of Metzler matrices known as “compartmental matrices” [97], a general treatment is lacking. This is in stark contrast with the comprehensive understanding of the graph theoretical conditions guaranteeing convergence to consensus for row-stochastic matrices in averaging systems. Related to this open question is the work in [98]. The graph-theoretic conditions are particularly useful because they allow us to analyze stability based on the structural properties of the interconnection network given the existence of perturbations or uncertainties on the parameters.

For nonlinear monotone systems, much recent progress is documented in [99, 100], where a basic fundamental connection is built between monotone systems and contractive systems. A notable gap, however, remains, in explaining the relationship between the treatment of monotone contractive systems and the stability theory of network small gain developed in [101, 102].

In summary, we aim to develop an algebraic graph theory for monotone dynamical systems, starting with the linear case of Metzler matrices and continuing with the nonlinear setting and its connections with network small-gain theorems.

Literature review Monotone dynamical systems appear naturally in numerous applications and have many appealing properties. The mathematical theory of nonlinear monotone systems has been vastly studied in dynamical system literature [103, 91, 92]. In control community, the notion of monotonicity has been extended to systems with inputs and outputs, and properties of the interconnected monotone systems have been studied [93]. It is well known that linear monotone systems (also referred to as linear positive systems) are described by Metzler matrices. Conditions for stability of Metzler matrices have been studied extensively in the literature. Narendra and Shorten, *et al.* established an iterative method based on the Schur complement to check the Hurwitzness

of Metzler matrices in [104, 105]. A graph-theoretic characterization for diagonal stability of matrices whose underlying digraph is a cactus graph was proposed in [98]. Briat studied the sign stability of Metzler matrices and block Metzler matrices in [106]. Blanchini *et al.* studied switched Metzler systems and Hurwitz convex combinations in [107]. Stability of switched Metzler systems has also been studied in [108], where the authors provided guarantees for robustness with respect to delays. In [96], scalable methods for analysis and control of large-scale linear monotone systems have been studied. The admissibility, stability, and persistence of interconnected positive heterogeneous systems have been studied in [109]. For nonlinear monotone systems, using novel connections to the contraction theory, Coogan established sufficient conditions for global stability of monotone systems [99, 100]. The stability and properties of equilibria for homogeneous and subhomogeneous positive systems were investigated in [110, 111]. We refer the interested readers to [95] for a detailed study of linear positive systems and to the survey paper [112] for theoretical results and applications of interconnected monotone systems.

Small-gain theorems are arguably one of the fundamental results for stability of interconnected systems. Started with the works by Zames [113], the early classical studies on small-gain theorems mostly focused on stability analysis using linear gains [114]. Introduction of the notion of input-to-state stability (ISS) in the seminal paper [115] triggered a paradigm shift in the study of small-gain theorems. More recent works on small-gain theorems focused on the input-to-state framework and they provided results in terms of nonlinear notions of input-to-state gains [116, 101].

Statement of Contributions In this chapter, we study the graph-theoretic stability conditions for Metzler matrices. By using concepts from the small-gain theorems for interconnected systems, we obtain necessary and sufficient conditions for Hurwitzness of Metzler matrices in terms of the input-to-state gains, and we also extend our

results to the nonlinear monotone systems. Our main contributions are as follows. First, we characterize two types of input-to-state stability gains for linear Metzler systems, namely max-interconnection gains and sum-interconnection gains. Second, using the max-interconnection and the sum-interconnection gains, we obtain two main theorems on graph-theoretic characterizations for Hurwitzness of Metzler matrices. Our conditions highlight the role of cycles and cycle gains and provide valuable insights for connections between the network structure and network functions. In particular, our characterizations for Hurwitzness of Metzler matrices using the max-interconnection gains coincide with the well-known cyclic small gain theorem [102, Theorem 3.1], which becomes necessary and sufficient in our case; based on the sum-interconnection gains, in addition to necessary and sufficient cycle gain conditions that depend on the cycle structure of the interconnection graph, we also show that all cycle gains being less than 1 is a necessary condition and the sum of cycle gains being less than 1 is a sufficient condition. Finally, we extend our stability analysis using max-interconnection and sum-interconnection gains to nonlinear monotone systems. As a result, we provide two equivalent sufficient conditions for global stability of monotone nonlinear systems. The results in this chapter have the potential to be applied to the (local) stability analysis of epidemic propagation models [117], synchronization of diffusively coupled positive systems [118], and interconnection of large scale ISS systems [101].

Organization We review the known stability results for Metzler matrices in Section 5.2. The input-to-state stability and two forms of ISS gains are introduced in Section 5.3, where we also characterize different ISS gains for Metzler systems. The main results on graph-theoretic conditions for Hurwitzness of Metzler matrices are presented in Section 5.4. We extend the conditions to nonlinear monotone systems in Section 5.5. A few additional concepts and proofs are included in Section 5.6. We conclude the chapter

in Section 5.7.

5.2 Review of Metzler matrices

5.2.1 Notation and preliminaries

Let \mathbb{R} and $\mathbb{R}_{\geq 0}$ be the set of real and nonnegative real numbers, respectively. For a vector $v \in \mathbb{R}^n$, its Euclidean norm is denoted by $|v|$. In particular, if $v \in \mathbb{R}$, then $|v|$ is the absolute value of v . For a finite set S , $|S|$ is the cardinality. For $t \geq 0$ and a time-varying vector signal $x : [0, t] \rightarrow \mathbb{R}^n$, we define the norm

$$\|x\|_{[0,t]} = \operatorname{ess\,sup}_{s \in [0,t]} |x(s)|.$$

Moreover, for $x : \mathbb{R}_{\geq 0} \mapsto \mathbb{R}^n$, $\|x\|_{\infty} = \operatorname{ess\,sup}_{s \geq 0} |x(s)|$. A continuous function $\alpha : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}_{\geq 0}$ is a class \mathcal{K} function if it is strictly increasing and $\alpha(0) = 0$; it is a class \mathcal{K}_{∞} function if it is a class \mathcal{K} function and $\lim_{s \rightarrow \infty} \alpha(s) = \infty$. A continuous function $\beta : \mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}_{\geq 0}$ is a class \mathcal{KL} function if $\beta(s, t)$ is a class \mathcal{K} function of s for fixed t , and a decreasing function of t with $\lim_{t \rightarrow \infty} \beta(s, t) = 0$ for fixed s .

For a matrix $A \in \mathbb{R}^{n \times n}$, its associated graph $\mathcal{G}(A) = (V, \mathcal{E}, A)$ is a weighted digraph defined as follows: $V = \{1, \dots, n\}$ is the set of nodes, $\mathcal{E} = \{(j, i) \mid i, j \in V, a_{ij} \neq 0\}$ is the set of edges, and $A = \{a_{ij}\}$ is the weight matrix with a_{ij} being the weight on edge $(j, i) \in \mathcal{E}$. For $i \in V$, the neighbor set of node i is defined by $\mathcal{N}_i = \{j \in V \mid (j, i) \in \mathcal{E}\}$. A matrix $A \in \mathbb{R}^{n \times n}$ is irreducible if its associated digraph $\mathcal{G}(A)$ is strongly connected. A strongly connected component of a digraph \mathcal{G} is a strongly connected subgraph such that it is not strictly contained in any other strongly connected subgraph of \mathcal{G} .

In a digraph $\mathcal{G} = (V, \mathcal{E})$, a simple cycle c in \mathcal{G} is a directed path that starts and ends at the same node and has no repetitions other than the starting and ending nodes.

Two simple cycles c_1 and c_2 in \mathcal{G} intersect if they share at least one common node, i.e., $c_1 \cap c_2 \neq \emptyset$; c_1 is a subset of c_2 if all the nodes on c_1 are also on c_2 . Self loops are not considered as simple cycles in this chapter.

For a matrix $A \in \mathbb{R}^{n \times n}$, the leading principal submatrices of A are given by A_I , where $I = \{1, \dots, i\}$ is the set of indices for all $i \in \{1, \dots, n\}$. In particular, when $I = \{1, \dots, n\}$, we have $A_I = A$. A matrix $M \in \mathbb{R}^{n \times n}$ is Metzler if all its off-diagonal elements are nonnegative.

The following lemma will be useful later in the chapter.

Lemma 5.2.1.1 (Bounding sum by maximum) *Let $\{x_1, \dots, x_n\}$ and $\{\alpha_1, \dots, \alpha_n\}$ be a set of nonnegative and positive real numbers respectively. If $\sum_{i=1}^n \frac{1}{\alpha_i} \leq 1$, then*

$$\sum_{i=1}^n x_i \leq \max_{i \in \{1, \dots, n\}} \{\alpha_i x_i\}.$$

Proof: Let $s \in \{1, \dots, n\}$ satisfy $\alpha_i x_i \leq \alpha_s x_s$ for all $i \in \{1, \dots, n\}$. Then

$$\sum_{i=1}^n x_i \leq \sum_{i=1}^n \frac{\alpha_s x_s}{\alpha_i} \leq \alpha_s x_s = \max_{i \in \{1, \dots, n\}} \{\alpha_i x_i\}.$$

■

5.2.2 Algebraic conditions for Hurwitzness of Metzler matrices

We collect a few well-known equivalent conditions for the Hurwitzness of Metzler matrices in the following lemma.

Lemma 5.2.2.1 (Properties of Hurwitz Metzler matrices [119, Theorem 15.17], [95, Theorem 13]) *Let $M \in \mathbb{R}^{n \times n}$ be a Metzler matrix, then the following statements are equivalent:*

- (i) M is Hurwitz;
- (ii) M is invertible and $-M^{-1} \geq 0$;
- (iii) all leading principal minors of $-M$ are positive;
- (iv) there exists $\xi \in \mathbb{R}^n$ such that $\xi > \mathbb{0}_n$ and $M\xi < \mathbb{0}_n$;
- (v) there exists $\eta \in \mathbb{R}^n$ such that $\eta > \mathbb{0}_n$ and $\eta^\top M < \mathbb{0}_n^\top$;
- (vi) there exists a diagonal matrix $P \succ 0$ such that $M^\top P + PM \prec 0$.

The inequalities in (ii), (iv) and (v) of Lemma 5.2.2.1 are componentwise. The matrix inequalities in (vi) indicate positive/negative definiteness.

Remark 5.2.2.2 (Related stability notions)

1. Condition (iii) is also known as the Hicksian stability condition for general matrices in the classic economics literature [120]. To the best of our knowledge, the equivalence of parts (i) and (iii) in Lemma 5.2.2.1 for Hurwitz Metzler matrices has not been fully exploited in the literature, and we build one of our main results based on this equivalence.
2. Conditions (iv) and (v) are also referred to as quasi diagonal dominance condition in the literature [121].
3. If the Metzler matrices are symmetric, then the necessary and sufficient condition in Lemma 5.2.2.1(iii) is exactly the Sylvester's criterion for negative definiteness of general symmetric matrices.
4. The equivalence of parts (i) and (vi) in Lemma 5.2.2.1 implies that for Metzler matrices, the Hurwitzness and diagonal stability are equivalent. \triangle

Based on the Schur complement, Narendra *et al.* propose an iterative method to verify the Hurwitzness of a Metzler matrix [104]. Partition a Metzler matrix $M \in \mathbb{R}^{n \times n}$ as follows

$$M = \begin{bmatrix} M_{n-1} & b_{n-1} \\ c_{n-1}^\top & d_{n-1} \end{bmatrix}$$

where d_{n-1} is a scalar. The Schur complement of M with respect to d_{n-1} is given by $M[n-1] = M_{n-1} - \frac{b_{n-1}c_{n-1}^\top}{d_{n-1}}$. For $k \in \{1, \dots, n-1\}$, define $M[k]$ iteratively as the Schur complement of $M[k+1]$ with respect to d_k , where $M[n] = M$, then the following statement holds.

Lemma 5.2.2.3 (Necessary and sufficient condition based on the Schur complement [104]) *A Metzler matrix $M \in \mathbb{R}^{n \times n}$ is Hurwitz if and only if for all $k \in \{1, \dots, n\}$, all the diagonal elements of $M[k]$ are negative.*

By Lemma 5.2.2.3, we have the following necessary condition.

Corollary 5.2.2.4 (Negativity of diagonal elements [104]) *If a Metzler matrix $M \in \mathbb{R}^{n \times n}$ is Hurwitz, then all the diagonal elements of M are negative.*

5.3 Review of ISS, interconnected systems and ISS gains

We review the concepts of input-to-state stability and introduce the gain functions in two different forms for interconnected input-to-state stable systems [102, 101].

5.3.1 Input-to-state stability

Consider the system

$$\dot{x} = f(x, u), \tag{5.1}$$

where $x \in \mathbb{R}^N$ is the state, $u \in \mathbb{R}^m$ is the input, and $f : \mathbb{R}^N \times \mathbb{R}^m \mapsto \mathbb{R}^N$ is a locally Lipschitz function and satisfies $f(\mathbb{0}_N, \mathbb{0}_m) = \mathbb{0}_N$. Then, we have the following definition for input-to-state stability.

Definition 5.3.1.1 (Input-to-state stability [115, Definition 2.1]) *System (5.1) is input-to-state stable if there exist $\beta \in \mathcal{KL}$ and $\gamma \in \mathcal{K}$ such that for any initial state $x(0) = x_0$ and any measurable and locally essentially bounded input u , the solution $x(t)$ satisfies, for all $t \geq 0$,*

$$|x(t)| \leq \max\{\beta(|x_0|, t), \gamma(\|u\|_\infty)\}. \quad (5.2)$$

The class \mathcal{K} function γ in (5.2) is the *ISS gain* of the system.

Remark 5.3.1.2 (ISS Lyapunov function) *To verify ISS using Definition 5.3.1.1, we need to find an estimate for the trajectory of the system. In general this task is computationally hard, if not impossible. However, one can show that ISS is equivalent to the existence of an appropriate ISS Lyapunov function. We refer the interested readers to [122, Theorem 1].* \triangle

5.3.2 Interconnection, ISS gains, and cyclic small-gain theorem

In this subsection, we study input-to-state stability for networked interconnected systems. Suppose the interaction between subsystems is described by a directed graph $\mathcal{G} = (V, \mathcal{E})$, where $V = \{1, \dots, n\}$ is the set of nodes and for all $i, j \in V$ and $i \neq j$, $(j, i) \in \mathcal{E}$ if x_j is an input to subsystem i . We consider a network of n interconnected dynamical systems with the interconnection graph \mathcal{G} :

$$\dot{x}_i = f_i(x_i, x_{\mathcal{N}_i}, u_i), \quad \text{for all } i \in \{1, \dots, n\}, \quad (5.3)$$

where $x_i \in \mathbb{R}^{n_i}$ and $x_{\mathcal{N}_i} = \begin{bmatrix} x_{i_1}, \dots, x_{i_{k_i}} \end{bmatrix}^\top \in \mathbb{R}^{n_{\mathcal{N}_i}}$ with $\mathcal{N}_i = \{i_1, \dots, i_{k_i}\}$ and $n_{\mathcal{N}_i} = \sum_{j=1}^{k_i} n_{i_j}$. For every $i \in V$, the function $f_i : \mathbb{R}^{n_i + n_{\mathcal{N}_i} + m_i} \rightarrow \mathbb{R}^{n_i}$ is locally Lipschitz satisfying $f_i(\mathbb{0}_{n_i}, \mathbb{0}_{n_{\mathcal{N}_i}}, \mathbb{0}_{m_i}) = \mathbb{0}_{n_i}$. For the interconnected system (5.3), it is desirable to study ISS of the interconnection using the ISS of each subsystem. We first introduce componentwise ISS for network systems.

Definition 5.3.2.1 (Componentwise ISS) *An interconnected system (5.3) is componentwise ISS if every subsystem i is ISS for the input $\begin{bmatrix} x_{\mathcal{N}_i} & u_i \end{bmatrix}^\top \in \mathbb{R}^{n_{\mathcal{N}_i} + m_i}$.*

In other words, an interconnected network system is componentwise ISS if each subsystem, separated from the whole system, is ISS. In general, componentwise ISS does not guarantee ISS of the whole interconnected system, and conditions on the interconnection structure and composition of suitable gains are required to ensure ISS of the whole system. In the following, we introduce two notions of gains.

Definition 5.3.2.2 (Max-interconnection ISS gains) *Consider the interconnected system (5.3). The family of functions $\{\Psi_{ij}\} \in \mathcal{K} \cup \{0\}$ is a max-interconnection gain if, for every $i \in \{1, \dots, n\}$, there exists $\beta_i \in \mathcal{KL}$ and $\Psi_i \in \mathcal{K}$ such that for any initial state $x(0) = x_0$, and any measurable and locally essentially bounded inputs u_i , the solution $x_i(t)$ satisfies, for all $t \geq 0$,*

$$|x_i(t)| \leq \max_{j \in \mathcal{N}_i} \{\beta_i(|x_i(0)|, t), \Psi_{ij}(\|x_j\|_{[0,t]}), \Psi_i(\|u_i\|_\infty)\}.$$

Definition 5.3.2.3 (Sum-interconnection ISS gains) *Consider the interconnected system (5.3). The family of functions $\{\Gamma_{ij}\} \in \mathcal{K} \cup \{0\}$ is a sum-interconnection gain if, for every $i \in \{1, \dots, n\}$, there exists $\beta_i \in \mathcal{KL}$ and $\Gamma_i \in \mathcal{K}$ such that for any initial state $x(0) = x_0$, and any measurable and locally essentially bounded inputs u_i , the solution*

$x_i(t)$ satisfies, for all $t \geq 0$,

$$|x_i(t)| \leq \beta_i(|x_i(0)|, t) + \sum_{j \in \mathcal{N}_i} \Gamma_{ij}(\|x_j\|_{[0,t]}) + \Gamma_i(\|u_i\|_\infty).$$

The following lemma provides conditions on a set of max-interconnection ISS gains which guarantee ISS of the interconnected system (5.3).

Lemma 5.3.2.4 (Cyclic small-gain theorem [102, Theorem 3.2]) *Consider an interconnected system (5.3) where each subsystem i is componentwise ISS and has a family of max-interconnected gains $\{\Psi_{ij}\}$. The interconnected system (5.3) is ISS with x as the state and u as the input if, for every simple cycle $c = (i_1, i_2, \dots, i_k, i_1)$ in the interconnection graph \mathcal{G} and every $s > 0$,*

$$\Psi_{i_2 i_1} \circ \Psi_{i_3 i_2} \circ \dots \circ \Psi_{i_1 i_k}(s) < s, \quad (5.4)$$

where \circ is the function composition.

In the rest of this chapter, we consider the interconnection of scalar systems.

5.3.3 ISS gains for Metzler systems

In this subsection, we characterize the ISS gains for Metzler systems. Consider the continuous-time linear system

$$\dot{x} = Mx + u, \quad (5.5)$$

where $M \in \mathbb{R}^{n \times n}$ is a Metzler matrix and $u \in \mathbb{R}_{\geq 0}^n$ is the control input. The Metzler system (5.5) can be viewed as a network of n interconnected scalar systems, where the

interconnection is characterized by the digraph $\mathcal{G}(M)$. More specifically, one can write the Metzler system (5.5) in the interconnection form (5.3) as,

$$\dot{x}_i = m_{ii}x_i + \sum_{j \in \mathcal{N}_i} m_{ij}x_j + u_i, \quad \text{for all } i \in \{1, \dots, n\}. \quad (5.6)$$

We characterize the sum-interconnection and max-interconnection ISS gains for the Metzler system (5.5) in the following lemma. Some parts of Lemma 5.3.3.1 may be known in the literature, and we hereby provide self-contained proofs.

Lemma 5.3.3.1 (ISS Metzler systems) *The Metzler system (5.5) with interconnection digraph $\mathcal{G}(M) = (V, \mathcal{E}, M)$*

1. *is componentwise ISS if and only if*

$$m_{ii} < 0, \quad \text{for all } i \in \{1, \dots, n\};$$

2. *has sum-interconnection gains $\{s \mapsto \Gamma_{ij}(s) = \gamma_{ij}s\}$, if it is componentwise ISS and the set of scalars $\{\gamma_{ij}\}$ satisfies $\gamma_{ij} = 0$ for all $j \notin \mathcal{N}_i$ and*

$$\frac{m_{ij}}{-m_{ii}} \leq \gamma_{ij}, \quad \text{for all } i \in \{1, \dots, n\}, \quad j \in \mathcal{N}_i; \quad (5.7)$$

3. *has max-interconnection gains $\{s \mapsto \Psi_{ij}(s) = \psi_{ij}s\}$, if it is componentwise ISS and the set of scalars $\{\psi_{ij}\}$ satisfies $\psi_{ij} = 0$ for all $j \notin \mathcal{N}_i$ and*

$$\sum_{j \in \mathcal{N}_i} \left(\frac{m_{ij}}{-m_{ii}} \right) \psi_{ij}^{-1} < 1, \quad \text{for all } i \in \{1, \dots, n\}; \quad (5.8)$$

4. *is ISS if and only if M is Hurwitz.*

Proof: Regarding part 1, since the dynamics of the i th subsystem given by (5.6) is linear, it is ISS if and only if $m_{ii} < 0$ [102, Theorem 1.3]. Therefore, the Metzler system (5.5) is componentwise ISS if and only if, for every $i \in \{1, \dots, n\}$, we have $m_{ii} < 0$.

Regarding part 2, the state trajectory $x_i(t)$ satisfies

$$x_i(t) = e^{m_{ii}t}x_i(0) + \sum_{j \in \mathcal{N}_i} m_{ij} \int_0^t e^{m_{ii}(t-\tau)} x_j(\tau) d\tau + \int_0^t e^{m_{ii}(t-\tau)} u_i(\tau) d\tau,$$

which implies

$$\begin{aligned} |x_i(t)| &\leq e^{m_{ii}t}|x_i(0)| + \sum_{j \in \mathcal{N}_i} m_{ij} \int_0^t |e^{m_{ii}(t-\tau)} x_j(\tau)| d\tau + \int_0^t |e^{m_{ii}(t-\tau)} u_i(\tau)| d\tau \\ &\leq e^{m_{ii}t}|x_i(0)| + \sum_{j \in \mathcal{N}_i} m_{ij} \|x_j\|_{[0,t]} \int_0^t e^{m_{ii}(t-\tau)} d\tau + \|u_i\|_\infty \int_0^t e^{m_{ii}(t-\tau)} d\tau \quad (5.9) \\ &\leq e^{m_{ii}t}|x_i(0)| + \sum_{j \in \mathcal{N}_i} \frac{m_{ij}}{-m_{ii}} \|x_j\|_{[0,t]} + \frac{1}{-m_{ii}} \|u_i\|_\infty. \end{aligned}$$

Therefore, the Metzler system (5.5) has sum-interconnection ISS gains $\{s \mapsto \Gamma_{ij}(s) = \gamma_{ij}(s)\}$ if we have $\frac{m_{ij}}{-m_{ii}} \leq \gamma_{ij}$.

Regarding part 3, by Lemma 5.2.1.1 and (5.9), we have

$$|x_i(t)| \leq \max\{\alpha_1 e^{m_{ii}t}|x_i(0)|, \alpha_2 \sum_{j \in \mathcal{N}_i} \frac{m_{ij}}{-m_{ii}} \|x_j\|_{[0,t]}, \alpha_3 \frac{1}{-m_{ii}} \|u_i\|_\infty\}, \quad (5.10)$$

where $\alpha_1, \alpha_2, \alpha_3 > 0$ and $\sum_{i=1}^3 \frac{1}{\alpha_i} \leq 1$. If (5.8) holds, then by Lemma 5.2.1.1, we have

$$\sum_{j \in \mathcal{N}_i} \frac{m_{ij}}{-m_{ii}} \|x_j\|_{[0,t]} < \max_j \{\psi_{ij} \|x_j\|_{[0,t]}\}.$$

Therefore, we can pick $\alpha_2 > 1$ properly such that

$$\sum_{j \in \mathcal{N}_i} \frac{m_{ij}}{-m_{ii}} \|x_j\|_{[0,t]} \leq \frac{1}{\alpha_2} \max_j \{\psi_{ij} \|x_j\|_{[0,t]}\},$$

which combined with (5.10) imply that $\{\psi_{ij}\}$ are max-interconnection gains.

Regarding part 4, this is a straightforward application of [102, Theorem 1.3]. ■

5.4 Graph-theoretic conditions for Hurwitzness of Metzler matrices

In this section, we first show that we only need to consider irreducible Metzler matrices. Then, we show that different ISS gains result in different graph-theoretic conditions for the stability of Metzler systems. In particular, if we use the max-interconnection ISS gains, then the cycle condition (5.4) in Lemma 5.3.2.4 is a necessary and sufficient condition for the stability of Metzler systems. On the other hand, if we use the sum-interconnection ISS gains, then we can obtain new necessary and sufficient graph-theoretic conditions.

5.4.1 Metzler matrices with reducible graphs

The following lemma allows us to restrict our attention to irreducible Metzler matrices.

Lemma 5.4.1.1 (Hurwitzness and strongly connected components) *For a Metzler matrix $M \in \mathbb{R}^{n \times n}$, M is Hurwitz if and only if all the submatrices corresponding to the strongly connected components of $\mathcal{G}(M)$ are Hurwitz.*

Proof: If M is irreducible, then the statement holds true since there is only one strongly connected component in $\mathcal{G}(M)$, which is $\mathcal{G}(M)$ itself.

If M is reducible, then there exists a permutation matrix such that M can be brought into block upper triangular form where each block on the diagonal corresponds to a strongly connected component of $\mathcal{G}(M)$. Therefore, M is Hurwitz if and only if all the submatrices corresponding to the strongly connected components of $\mathcal{G}(M)$ are Hurwitz. ■

If $\mathcal{G}(M)$ is acyclic, then we have the following corollary.

Corollary 5.4.1.2 (Necessary and sufficient condition for acyclic graphs [106, Theorem 3.4]) *Consider a Metzler matrix $M \in \mathbb{R}^{n \times n}$ whose associated digraph is acyclic. The matrix M is Hurwitz if and only if all the diagonal elements of M are negative.*

Hereafter, we focus on irreducible Metzler matrices with negative diagonal elements.

5.4.2 Cycle gains and the case of a simple cycle

In this subsection, we define the sum-cycle gains and max-cycle gains for Metzler matrices, and we emphasize the importance of cycles through the case of a simple cycle. Note that self loops are not considered as simple cycles in this chapter.

Definition 5.4.2.1 (Cycle gains for Metzler matrices) *Let $M \in \mathbb{R}^{n \times n}$ be an irreducible Metzler matrix with negative diagonal elements and $c = (i_1, i_2, \dots, i_k, i_1)$ be a simple cycle in $\mathcal{G}(M)$. Then*

1. *a max-cycle gain of c is*

$$\psi_c = (\psi_{i_2 i_1}) (\psi_{i_3 i_2}) \cdots (\psi_{i_1 i_k}), \quad (5.11)$$

where the scalars $\{\psi_{i_j}\}$ satisfy (5.8); and

2. the sum-cycle gain of c is

$$\gamma_c = \left(\frac{m_{i_2 i_1}}{-m_{i_2 i_2}} \right) \left(\frac{m_{i_3 i_2}}{-m_{i_3 i_3}} \right) \cdots \left(\frac{m_{i_1 i_k}}{-m_{i_1 i_1}} \right). \quad (5.12)$$

Remark 5.4.2.2 (Uniqueness of cycle gains) *The max-interconnection gains and sum-interconnection gains as characterized in Lemma 5.3.3.1 are not unique. In Definition 5.4.2.1, the max-cycle gains as in (5.11) are not unique, and for every solution of (5.8), one can compute a set of max-cycle gains for simple cycles. However, the sum-cycle gains in (5.12) are uniquely defined for simple cycles in $\mathcal{G}(M)$ since we pick the natural lower bound for the sum-interconnection gains in (5.7). \triangle*

For an irreducible Metzler matrix $M \in \mathbb{R}^{n \times n}$ with negative diagonal elements, if the associated digraph $\mathcal{G}(M)$ is a simple cycle, i.e, M has the following structure,

$$M = \begin{bmatrix} m_{11} & m_{12} & 0 & \cdots & 0 \\ 0 & m_{22} & m_{23} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & m_{n-1,n-1} & m_{n-1,n} \\ m_{n1} & 0 & \cdots & 0 & m_{nn} \end{bmatrix},$$

then we have the following lemma.

Lemma 5.4.2.3 (Necessary and sufficient condition for simple cycles) *Let $M \in \mathbb{R}^{n \times n}$ be an irreducible Metzler matrix with negative diagonal elements whose associated digraph $\mathcal{G}(M)$ is a simple cycle $c = (1, n, \dots, 2, 1)$. Then the following statements are equivalent:*

1. M is Hurwitz;

2. $\gamma_c < 1$;

3. *there exists a solution to (5.8) such that $\psi_c < 1$.*

Proof: Regarding the equivalence between 1 and 2: by Lemma 5.2.2.1(iii), M is Hurwitz if and only if all the leading principal minors of $-M$ are positive. If $i < n$ and $I = \{1, \dots, i\}$, then the leading principal submatrices $(-M)_I$ of $-M$ are upper triangular with positive diagonal elements and thus $\det((-M)_I) > 0$. When $I = \{1, \dots, n\}$, we have

$$\det(-M) = \prod_{i=1}^n (-m_{ii}) - m_{n1} \prod_{i=1}^{n-1} m_{i,i+1}.$$

Then, $\det(-M) > 0$ if and only if

$$\prod_{i=1}^n (-m_{ii}) > m_{n1} \prod_{i=1}^{n-1} m_{i,i+1},$$

which is equivalent to $\gamma_c < 1$.

Regarding the equivalence between 2 and 3: notice that if we pick $\psi_{ij} = \frac{m_{ij}}{-m_{ii}} + \epsilon$ for sufficiently small $\epsilon > 0$, then (5.8) is satisfied and $\psi_c < 1$ is equivalent to $\gamma_c < 1$. ■

It is worth mentioning that the necessary and sufficient condition in Lemma 5.4.2.3 is a special case of a more general result in [98, Proposition 2] regarding diagonal stability.

Example 5.4.2.4 (A two by two Metzler matrix describing a flow system [119, Exercise 10.10]) *We apply Lemma 5.4.2.3 to a simple two by two case where the Metzler matrix describes a symmetric flow system $\dot{x} = Mx$. Suppose the Metzler matrix M has the following form*

$$M = \begin{bmatrix} g - f & f \\ f & -d - f \end{bmatrix},$$

where $f > 0$ is the flow rate between two nodes, $g > 0$ is the growth rate at node 1

and $d > 0$ is the decay rate at node 2. By Lemma 5.4.2.3, the flow system $\dot{x} = Mx$ is asymptotically stable if and only if

$$g - f < 0, \quad -d - f < 0, \quad \text{and} \quad \frac{f^2}{(f - g)(d + f)} < 1.$$

Equivalently, we have

$$d > g \quad \text{and} \quad f > \frac{dg}{d - g}.$$

This condition has a clear physical interpretation that in order for the two-node flow system $\dot{x} = Mx$ to be asymptotically stable, i.e., the flow does not accumulate in the system, the decay rate at one node must be larger than the growth rate at the other node and the flow rate between the nodes should be sufficiently large.

Lemma 5.4.2.3 states that a Metzler matrix whose associated digraph is a simple cycle is Hurwitz if and only if the cycle gain is less than 1. It turns out that, for irreducible Metzler matrices with general digraphs, the gains of the simple cycles play a central role in determining the Hurwitzness. Moreover, cycle gains in different forms (sum or max) lead to different graph-theoretic conditions.

5.4.3 Max-cycle gains and Hurwitz Metzler matrices

In this subsection, we use the max-cycle gains of the Metzler system (5.5) to characterize the Hurwitzness of a Metzler matrix, and the cyclic small gain theorem in Lemma 5.3.2.4 becomes necessary and sufficient in this case.

Theorem 5.4.3.1 (Max-interconnection characterization) *Let $M \in \mathbb{R}^{n \times n}$ be an irreducible Metzler matrix with negative diagonal elements, $\mathcal{G}(M) = (V, \mathcal{E}, M)$ be the associated digraph, and Φ be the set of simple cycles of $\mathcal{G}(M)$. Then the following conditions are equivalent:*

1. M is Hurwitz;
2. for every $i \in V$ and $j \in \mathcal{N}_i$, there exists $\psi_{ij} > 0$ such that

$$\sum_{j \in \mathcal{N}_i} \left(\frac{m_{ij}}{-m_{ii}} \right) \psi_{ij}^{-1} < 1, \quad \text{for all } i \in \{1, \dots, n\}, \quad (5.13)$$

$$\psi_c < 1, \quad \text{for all } c \in \Phi. \quad (5.14)$$

Proof: (i) \implies (ii): Suppose that M is Hurwitz, then by Lemma 5.2.2.1(iv) there exists $\xi > 0_n$ such that $M\xi < 0_n$. Therefore, $\text{diag}(\xi^{-1})M\text{diag}(\xi)$ is a Metzler matrix with negative row sums, which implies

$$\sum_{j \in \mathcal{N}_i} \left(\frac{m_{ij}}{-m_{ii}} \right) \frac{\xi_j}{\xi_i} < 1, \quad \text{for all } i \in \{1, \dots, n\}.$$

Note that, for every $(i_1, \dots, i_k, i_1) \in \Phi$, we have

$$\frac{\xi_{i_2}}{\xi_{i_1}} \dots \frac{\xi_{i_1}}{\xi_{i_k}} = 1.$$

Thus, we have

$$\begin{aligned} \sum_{j \in \mathcal{N}_i} \left(\frac{m_{ij}}{-m_{ii}} \right) \frac{\xi_j}{\xi_i} &< 1, & \text{for all } i \in \{1, \dots, n\}, \\ \frac{\xi_{i_2}}{\xi_{i_1}} \dots \frac{\xi_{i_1}}{\xi_{i_k}} &= 1, & \text{for all } (i_1, \dots, i_k, i_1) \in \Phi. \end{aligned}$$

By a straightforward continuity argument, one can show that, for every $i \in V$ and $j \in \mathcal{N}_i$, there exists $\psi_{ij} > 0$ such that

$$\begin{aligned} \sum_{j \in \mathcal{N}_i} \left(\frac{m_{ij}}{-m_{ii}} \right) \psi_{ij}^{-1} &< 1, & \text{for all } i \in \{1, \dots, n\}, \\ \psi_c &< 1, & \text{for all } c \in \Phi. \end{aligned}$$

(ii) \implies (i): Since the diagonal entries of M are negative, the Metzler system (5.5) is componentwise ISS by Lemma 5.3.3.11. By Lemma 5.3.3.13, there exist max-interconnection gains $\{\psi_{ij}\}$ such that

$$\sum_{j \in \mathcal{N}_i} \left(\frac{m_{ij}}{-m_{ii}} \right) \psi_{ij}^{-1} < 1, \quad \text{for all } i \in \{1, \dots, n\}.$$

Thus, the sufficient condition in Lemma 5.3.2.4 is equivalent to the existence of $\psi_{ij} > 0$, for $i \in V$ and $j \in \mathcal{N}_i$ such that

$$\begin{aligned} \sum_{j \in \mathcal{N}_i} \left(\frac{m_{ij}}{-m_{ii}} \right) \psi_{ij}^{-1} &< 1, & \text{for all } i \in \{1, \dots, n\}, \\ \psi_c &< 1, & \text{for all } c \in \Phi. \end{aligned}$$

Therefore, by Lemma 5.3.2.4, the Metzler system (5.5) is ISS and asymptotically stable, which implies that M is Hurwitz. This completes the proof. \blacksquare

By using Theorem 5.4.3.1, we can prove the following corollary.

Corollary 5.4.3.2 (Diagonal Stability and Hurwitzness of Metzler matrices)

Let $M \in \mathbb{R}^{n \times n}$ be an irreducible Metzler matrix with negative diagonal elements, $\mathcal{G}(M) = (V, \mathcal{E}, M)$ be the associated digraph, and Φ be the set of simple cycles of $\mathcal{G}(M)$. Assume that any two simple cycles of $\mathcal{G}(M)$ have at most one vertex in common, i.e., $\mathcal{G}(M)$ is

cactus. Then the following conditions are equivalent:

1. *M is Hurwitz;*
2. *for every $c \in \Phi$ and every node $i \in c$, there exists positive constant $\theta_i^c > 0$ such that*

$$\begin{aligned} \prod_{i \in c} \theta_i^c &> \gamma_c, \quad \text{for all } c \in \Phi, \\ \sum_{c \in \Phi} \theta_i^c &= 1, \quad \text{for all } i \in c, \end{aligned} \tag{5.15}$$

where γ_c is defined in equation (5.12).

Proof: We postpone the proof to Appendix 5.8.2. ■

Remark 5.4.3.3 1. *The condition in Corollary 5.4.3.22 for Metzler matrices is the same as conditions (11) and (12) in [98, Theorem 1] for the diagonal stability of arbitrary matrices with cactus graphs. Therefore, in the context of Metzler matrices, Theorem 5.4.3.1 is a generalization of [98, Theorem 1] to arbitrary topologies.*

2. *One can compute the positive constants ψ_{ij} in Theorem 5.4.3.12 by solving the following feasibility problem*

$$\begin{aligned} \text{Find} \quad & \xi \\ \text{subject to} \quad & \xi > \mathbb{0}_n, \\ & M\xi < \mathbb{0}_n. \end{aligned} \tag{5.16}$$

Then, for $i \in V$ and $j \in \mathcal{N}_i$, we can compute ψ_{ij} as

$$\psi_{ij} = \delta \frac{\xi_i}{\xi_j},$$

where $0 < \delta < 1$ is given by

$$\delta = \max_i \left\{ \sum_{j \in \mathcal{N}_i} \frac{m_{ij}}{-m_{ii}} \frac{\xi_j}{\xi_i} \right\}.$$

The problem (5.16) is not a linear programming due to the strict inequalities. However, one can easily transform it to the following linear programming.

$$\begin{aligned} &\text{Find} && \xi \\ &\text{subject to} && \xi \geq \mathbf{1}_n, \\ &&& M\xi \leq -\mathbf{1}_n. \end{aligned}$$

△

In order to check conditions (5.13) and (5.14), we need to compute the max-interconnection ISS gains using the method in Remark 5.4.3.32. This computation is essentially equivalent to the well-known condition in Lemma 5.2.2.1(iv).

5.4.4 Sum-cycle gains and Hurwitz Metzler matrices

In this subsection, we use sum-cycle gains to characterize the Hurwitzness of Metzler matrices. We first introduce the concept of *disjoint cycle sets*.

Definition 5.4.4.1 (Disjoint cycle sets) Let $M \in \mathbb{R}^{n \times n}$ be a Metzler matrix with the associated digraph $\mathcal{G}(M)$ and $\Phi = \{c_1, \dots, c_r\}$ be the set of simple cycles in $\mathcal{G}(M)$, the disjoint cycle sets K_ℓ^M for $\ell \in \{1, \dots, r\}$ are defined by

$$K_\ell^M = \{\{c_{i_1}, \dots, c_{i_\ell}\} \subset \Phi \mid c_{i_k} \cap c_{i_{k'}} = \emptyset, k \neq k' \text{ and } k, k' \in \{1, \dots, \ell\}\}.$$

Intuitively, the disjoint cycle sets K_ℓ^M are sets where each element is a set of ℓ cycles

that are mutually disjoint. We collect the graph-theoretic interpretations for the disjoint cycle sets in Section 5.6.1. With the disjoint cycle sets, we are ready to define the notion of total cycle gain of a Metzler matrix and its leading principal submatrices.

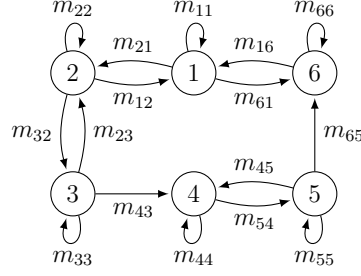
Definition 5.4.4.2 (Total cycle gain) *Let $M \in \mathbb{R}^{n \times n}$ be an irreducible Metzler matrix with negative diagonal elements. For $i = \{1, \dots, n\}$ and $I = \{1, \dots, i\}$, the leading principal submatrix M_I has the associated digraph $\mathcal{G}(M_I)$, set of simple cycles $\Phi_{M_I} = \{c_1, \dots, c_{r_{M_I}}\}$ and disjoint cycle sets $K_\ell^{M_I}$, $\ell \in \{1, \dots, r_{M_I}\}$, then the total cycle gain of M_I is defined by*

$$\gamma_{M_I} = \begin{cases} \sum_{\ell=1}^{r_{M_I}} \sum_{\{c_{i_1}, \dots, c_{i_\ell}\} \in K_\ell^{M_I}} (-1)^{\ell-1} \gamma_{c_{i_1}} \dots \gamma_{c_{i_\ell}}, & \text{if } \Phi_{M_I} \neq \emptyset, \\ 0, & \text{if } \Phi_{M_I} = \emptyset. \end{cases} \quad (5.17)$$

Example 5.4.4.3 (Disjoint cycle sets and total cycle gain) *We illustrate the definitions of the disjoint cycle sets and the total cycle gain in this example. Let $M \in \mathbb{R}^{6 \times 6}$ be an irreducible Metzler matrix with negative diagonal elements as follows*

$$M = \begin{bmatrix} m_{11} & m_{12} & 0 & 0 & 0 & m_{16} \\ m_{21} & m_{22} & m_{23} & 0 & 0 & 0 \\ 0 & m_{32} & m_{33} & 0 & 0 & 0 \\ 0 & 0 & m_{43} & m_{44} & m_{45} & 0 \\ 0 & 0 & 0 & m_{54} & m_{55} & 0 \\ m_{61} & 0 & 0 & 0 & m_{65} & m_{66} \end{bmatrix}.$$

The associated weighted digraph $\mathcal{G}(M)$ is shown in Fig. 5.1. There are five cycles in $\mathcal{G}(M)$, i.e., $c_1 = (1, 2, 1)$, $c_2 = (2, 3, 2)$, $c_3 = (4, 5, 4)$, $c_4 = (6, 1, 6)$, $c_5 = (1, 2, 3, 4, 5, 6, 1)$,

Figure 5.1: The associated weighted digraph $\mathcal{G}(M)$

and the disjoint cycle sets of M are:

$$\begin{aligned}
 K_1^M &= \{\{c_1\}, \{c_2\}, \{c_3\}, \{c_4\}, \{c_5\}\}, \\
 K_2^M &= \{\{c_1, c_3\}, \{c_2, c_3\}, \{c_2, c_4\}, \{c_3, c_4\}\}, \\
 K_3^M &= \{\{c_2, c_3, c_4\}\}, \\
 K_4^M &= K_5^M = \emptyset.
 \end{aligned} \tag{5.18}$$

According to (5.17), the total cycle gains of the leading principal submatrices are given by:

$$\begin{aligned}
 \gamma_{M_{\{1\}}} &= 0, & \gamma_{M_{\{1,2\}}} &= \gamma_{c_1}, \\
 \gamma_{M_{\{1,2,3\}}} &= \gamma_{c_1} + \gamma_{c_2}, & \gamma_{M_{\{1,2,3,4\}}} &= \gamma_{c_1} + \gamma_{c_2}, \\
 \gamma_{M_{\{1,2,3,4,5\}}} &= \gamma_{c_1} + \gamma_{c_2} + \gamma_{c_3} - \gamma_{c_1}\gamma_{c_3} - \gamma_{c_2}\gamma_{c_3}, \\
 \gamma_{M_{\{1,2,3,4,5,6\}}} &= \gamma_M = \gamma_{c_1} + \gamma_{c_2} + \gamma_{c_3} + \gamma_{c_4} + \gamma_{c_5} - \gamma_{c_1}\gamma_{c_3} - \gamma_{c_2}\gamma_{c_3} - \gamma_{c_2}\gamma_{c_4} \\
 &\quad - \gamma_{c_3}\gamma_{c_4} + \gamma_{c_2}\gamma_{c_3}\gamma_{c_4}.
 \end{aligned} \tag{5.19}$$

With the above definitions, we now present a useful lemma.

Lemma 5.4.4.4 (Determinant and total cycle gain) *Let $M \in \mathbb{R}^{n \times n}$ be an irreducible Metzler matrix with negative diagonal elements and let γ_{M_I} be the total cycle gain of M_I*

for $i \in \{1, \dots, n\}$ and $I = \{1, \dots, i\}$. Then

$$\det(M_I) = (1 - \gamma_{M_I}) \prod_{j=1}^i m_{jj}. \quad (5.20)$$

Proof: We postpone the proof to Appendix 5.8.1. ■

We are now ready to write the leading principal minor condition in Lemma 5.2.2.1(iii) in the graph-theoretic language.

Theorem 5.4.4.5 (Sum-interconnection characterization) *Let $M \in \mathbb{R}^{n \times n}$ be an irreducible Metzler matrix with negative diagonal elements, $\mathcal{G}(M) = (V, \mathcal{E}, M)$ be the associated digraph, and Φ be the set of simple cycles of $\mathcal{G}(M)$. Then the following statements hold:*

1. *(necessary and sufficient condition) M is Hurwitz if and only if, for all $i \in \{1, \dots, n\}$*

$$\gamma_{M_I} < 1, \quad I = \{1, \dots, i\};$$

2. *(sufficient condition) if*

$$\sum_{c \in \Phi} \gamma_c < 1,$$

then M is Hurwitz;

3. *(necessary condition) if M is Hurwitz then*

$$\gamma_c < 1, \quad \text{for all } c \in \Phi.$$

Proof: Regarding part 1, by Lemma 5.4.4.4, we have that for $i \in \{1, \dots, n\}$ and

$$I = \{1, \dots, i\},$$

$$\det((-M)_I) = \left(\prod_{j=1}^i (-m_{jj})\right)(1 - \gamma_{M_I}).$$

By Lemma 5.2.2.1(iii), M is Hurwitz if and only if for all $i \in \{1, \dots, n\}$ and $I = \{1, \dots, i\}$, $\det((-M)_I) > 0$, i.e.,

$$\left(\prod_{j=1}^i (-m_{jj})\right)(1 - \gamma_{M_I}) > 0,$$

which is equivalent to $\gamma_{M_I} < 1$.

Regarding part 2, we prove the result by showing that part 1 holds. For all $i \in \{1, \dots, n\}$ and $I = \{1, \dots, i\}$, the leading submatrix M_I only involves a subset of Φ . If Φ_{M_I} is empty, then $\gamma_{M_I} = 0 < 1$. Otherwise, from (5.17), we know that γ_{M_I} has the following form:

$$\begin{aligned} \gamma_{M_I} = & \sum_{\{c_{i_1}\} \in K_1^{M_I}} \gamma_{c_{i_1}} - \sum_{\{c_{i_1}, c_{i_2}\} \in K_2^{M_I}} \gamma_{c_{i_1}} \gamma_{c_{i_2}} + \sum_{\{c_{i_1}, c_{i_2}, c_{i_3}\} \in K_3^{M_I}} \gamma_{c_{i_1}} \gamma_{c_{i_2}} \gamma_{c_{i_3}} \\ & + \sum_{\ell=3}^{r_{M_I}} \sum_{\{c_{i_1}, \dots, c_{i_\ell}\} \in K_\ell^{M_I}} (-1)^{\ell-1} \gamma_{c_{i_1}} \dots \gamma_{c_{i_\ell}}. \end{aligned}$$

Since for all $c \in \Phi$, we have $\gamma_c > 0$ and $\sum_{c \in \Phi} \gamma_c < 1$ by assumption, then we have that $\gamma_c < 1$ for all $c \in \Phi$ and $\sum_{\{c_{i_1}\} \in K_1^{M_I}} \gamma_{c_{i_1}} < 1$. Note that by the definition of $K_\ell^{M_I}$, for any $\{c_{i_1}, \dots, c_{i_\ell}\} \in K_\ell^{M_I}$, we must have that all the subsets of $\{c_{i_1}, \dots, c_{i_\ell}\}$ with $\ell - 1$ elements are contained in $K_{\ell-1}^{M_I}$. Thus, we have that, for all $k \geq 1$,

$$\sum_{\ell=2k}^{2k+1} \sum_{\{c_{i_1}, \dots, c_{i_\ell}\} \in K_\ell^{M_I}} (-1)^{\ell-1} \gamma_{c_{i_1}} \dots \gamma_{c_{i_\ell}} < 0.$$

Hence, we have for all $i \in \{1, \dots, n\}$ and $I = \{1, \dots, i\}$, $\gamma_{M_I} < 1$, and by Theo-

rem 5.4.4.51, M is Hurwitz.

Regarding part 3, we postpone the proof to Section 5.6.2, where an expansion algorithm for $\mathcal{G}(M)$ is given so that all the simple cycles can be identified by the leading principal submatrices and a simple proof is constructed. ■

Remark 5.4.4.6 (Necessary and sufficient condition in special graphs) *The sufficient condition for Hurwitzness in Theorem 5.4.4.52 becomes necessary and sufficient when any two cycles share at least one common node in the digraph associated with the Metzler matrix.* △

We give two simple examples illustrating that the condition in Theorem 5.4.4.53 is not sufficient and the condition in Theorem 5.4.4.52 is not necessary.

Example 5.4.4.7 (Insufficiency of condition 3 in Theorem 5.4.4.5) *Consider an irreducible Metzler matrix $M \in \mathbb{R}^{3 \times 3}$ as follows*

$$M = \begin{bmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix}.$$

The associated weighted digraph $\mathcal{G}(M)$ is shown in Fig. 5.2. There are two cycles in $\mathcal{G}(M)$, i.e., $c_1 = (1, 2, 1)$ and $c_2 = (2, 3, 2)$, and the cycle gains are $\gamma_{c_1} = \gamma_{c_2} = \frac{1}{2}$. The cycle gains satisfy the condition in Theorem 5.4.4.53, but M is not Hurwitz since it has a zero eigenvalue.

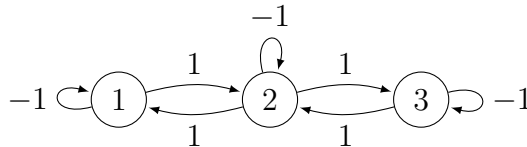


Figure 5.2: The associated weighted digraph of M

Example 5.4.4.8 (Lack of necessity of condition 2 in Theorem 5.4.4.5) Consider an irreducible Metzler matrix $M \in \mathbb{R}^{4 \times 4}$ as follows

$$M = \begin{bmatrix} -5 & 1 & 0 & 0 \\ 3 & -1 & 1 & 0 \\ 0 & 1 & -5 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix}.$$

The associated weighted digraph $\mathcal{G}(M)$ is shown in Fig. 5.3. There are three cycles in $\mathcal{G}(M)$, i.e., $c_1 = (1, 2, 1)$, $c_2 = (2, 3, 2)$ and $c_3 = (3, 4, 3)$, and the cycle gains are $\gamma_{c_1} = \frac{3}{5}$, $\gamma_{c_2} = \frac{1}{5}$ and $\gamma_{c_3} = \frac{1}{5}$. The cycle gains do not satisfy the sufficient condition in Theorem 5.4.4.52, but one can check that M is Hurwitz.

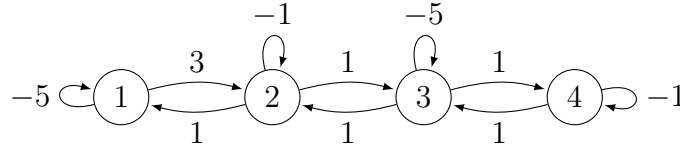


Figure 5.3: The associated weighted digraph of M

We give the Hurwitzness conditions for Example 5.4.4.3.

Example 5.4.4.9 (continues=exam:concepts) By Theorem 5.4.4.51 and (5.19), the necessary and sufficient conditions for M to be Hurwitz are given by

$$\begin{aligned} \gamma_{c_1} &< 1, & \gamma_{c_1} + \gamma_{c_2} &< 1, \\ \gamma_{c_1} + \gamma_{c_2} + \gamma_{c_3} - \gamma_{c_1}\gamma_{c_3} - \gamma_{c_2}\gamma_{c_3} &< 1, & \gamma_M &< 1, \end{aligned}$$

which are equivalent to

$$\gamma_{c_1} + \gamma_{c_2} < 1, \quad (5.21)$$

$$\gamma_{c_1} + \gamma_{c_2} + \gamma_{c_3} - \gamma_{c_1}\gamma_{c_3} - \gamma_{c_2}\gamma_{c_3} < 1, \quad (5.22)$$

$$\gamma_M < 1. \quad (5.23)$$

It is not obvious whether the necessary conditions in Theorem 5.4.4.53 hold in this example. We show that (5.21)-(5.23) imply those necessary conditions in the following. From (5.21), since the cycle gains are positive, we know that $\gamma_{c_1} < 1$ and $\gamma_{c_2} < 1$. We can rewrite (5.22) as follows

$$\gamma_{c_3}(1 - \gamma_{c_1} - \gamma_{c_2}) < 1 - \gamma_{c_1} - \gamma_{c_2},$$

which along with (5.21) imply that $\gamma_{c_3} < 1$. By using (5.19), we can rearrange (5.23) as follows

$$\gamma_{c_1}(1 - \gamma_{c_3}) + \gamma_{c_2} + \gamma_{c_3} - \gamma_{c_2}\gamma_{c_3} + \gamma_{c_5} + \gamma_{c_4}(1 - \gamma_{c_2})(1 - \gamma_{c_3}) < 1,$$

which is equivalent to

$$\gamma_{c_1}(1 - \gamma_{c_3}) + \gamma_{c_5} < (1 - \gamma_{c_4})(1 - \gamma_{c_2})(1 - \gamma_{c_3}). \quad (5.24)$$

Since all the terms on the left hand side of (5.24) are positive, and on the right hand side we have $\gamma_{c_2} < 1$ and $\gamma_{c_3} < 1$, thus we must have that $\gamma_{c_4} < 1$. At the same time, since the term on the right hand side of (5.24) is less than 1, we must have that $\gamma_{c_5} < 1$.

5.5 Graph-theoretic conditions for stability of nonlinear monotone systems

In this section, we extend our stability results to monotone nonlinear systems. We consider a network of n interconnected scalar dynamical systems with the interconnection graph \mathcal{G} :

$$\dot{x}_i = f_i(x_i, x_{\mathcal{N}_i}), \quad \text{for all } i \in \{1, \dots, n\}, \quad (5.25)$$

where $x_i \in \mathbb{R}$ and $x_{\mathcal{N}_i} = \begin{bmatrix} x_{i_1}, \dots, x_{i_{k_i}} \end{bmatrix}^\top \in \mathbb{R}^{|\mathcal{N}_i|}$ with $\mathcal{N}_i = \{i_1, \dots, i_{k_i}\}$. For every $i \in \{1, \dots, n\}$, the function $f_i : \mathbb{R}^{|\mathcal{N}_i|+1} \rightarrow \mathbb{R}$ is continuously differentiable. We assume that the interconnected system (5.25) is monotone, i.e., for every $x \in \mathbb{R}_{\geq 0}^n$, the Jacobian matrix $J(x)$ is Metzler. Moreover, we assume that $f(\mathbb{0}_n) = \mathbb{0}_n$. We show that our characterizations of stability for linear Metzler systems can be generalized to sufficient conditions for global stability of nonlinear monotone systems. In particular, we prove two global results for asymptotic stability of monotone interconnected networks based on the max-interconnection gains and the sum-interconnection gains.

Theorem 5.5.0.1 (Max-interconnection stability) *Consider an interconnected nonlinear system (5.25) evolving on the positive orthant $\mathbb{R}_{\geq 0}^n$ with the interconnection graph $\mathcal{G} = (V, \mathcal{E})$. Assume that $f(\mathbb{0}_n) = \mathbb{0}_n$, and for every $x \in \mathbb{R}_{\geq 0}^n$, the matrix $J(x)$ is Metzler with negative diagonal entries. Moreover, assume there exists a family of positive numbers $\{\psi_{ij}\}$ for $i \in V$ and $j \in \mathcal{N}_i$ such that:*

1. *for every $i \in \{1, \dots, n\}$,*

$$\sum_{j \in \mathcal{N}_i} \frac{J_{ij}(x)}{-J_{ii}(x)} \psi_{ij}^{-1} < 1, \quad \text{for all } x \in \mathbb{R}_{\geq 0}^n, \quad (5.26)$$

2. for every $c = (i_1, \dots, i_k, i_1) \in \Phi$,

$$\psi_{i_2 i_1} \dots \psi_{i_1 i_k} < 1.$$

Then \mathbb{O}_n is globally asymptotically stable for system (5.25).

Proof: Let $\kappa = \max \{ \max_{(i,j) \in \mathcal{E}} \psi_{ij}^{-1}, 1 \}$. Then, we always have $\kappa \geq 1$. Given $c > 0$, we define the set $B_i(c)$, for every $i \in \{1, \dots, n\}$, and the real number $\delta(c)$ as follows:

$$B_i(c) = \{x \in \mathbb{R}_{\geq 0}^n \mid x_j \leq \kappa c, \text{ for any } j \in \mathcal{N}_i \cup \{i\}\},$$

$$\delta(c) = \min_i \min_{x \in B_i(c)} \left(-J_{ii}(x) - \sum_{j \in \mathcal{N}_i} J_{ij}(x) \psi_{ij}^{-1} \right).$$

Note that $J_{ii}(x) + \sum_{j \in \mathcal{N}_i} J_{ij}(x) \psi_{ij}^{-1}$ only depends on x_k such that $k \in \mathcal{N}_i \cup \{i\}$. Therefore, using (5.26), we get $\delta(c) > 0$. Let $\beta : \mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0} \mapsto \mathbb{R}$ be a class \mathcal{KL} function given by $\beta(s, t) = s e^{-\delta(s)t}$, where $\delta(s) > 0$ is a nonincreasing function with respect to s (for $s_1 \leq s_2$, we have that $B_i(s_1) \subseteq B_i(s_2)$ and thus $\delta(s_1) \geq \delta(s_2)$). Consider the control system

$$\dot{x} = f(x) + \mathbb{O}_{n \times n} u, \quad (5.27)$$

where $u \in \mathbb{R}_{\geq 0}^n$. We first show that, for every $t \geq 0$ and every $i \in \{1, \dots, n\}$,

$$x_i(t) \leq \max_{j \in \mathcal{N}_i} \{ \beta(x_i(0), t), \psi_{ij} \|x_j\|_{[0,t]}, \|u_i\|_{\infty} \}. \quad (5.28)$$

We prove (5.28) by contradiction. Suppose that the statement (5.28) is not true. Since $t \mapsto x(t)$ is a continuous map, there exist $t^* \geq 0$, a set of indices $\mathcal{I} \subseteq \{1, \dots, n\}$, and a

positive number $\epsilon > 0$ such that, for every $i \in \mathcal{I}$,

$$x_i(t^*) = \max_{j \in \mathcal{N}_i} \{\beta(x_i(0), t^*), \psi_{ij} \|x_j\|_{[0, t^*]}, \|u_i\|_\infty\}, \quad (5.29)$$

and for every $i \in \mathcal{I}$ and every $t \in (t^*, t^* + \epsilon)$,

$$x_i(t) > \max_{j \in \mathcal{N}_i} \{\beta(x_i(0), t), \psi_{ij} \|x_j\|_{[0, t]}, \|u_i\|_\infty\}. \quad (5.30)$$

Let i be any index such that $i \in \mathcal{I}$. Since $\mathbb{R}_{\geq 0}^n$ is convex, by the Mean Value Theorem [123, Proposition 2.4.7],

$$f(x) - f(\mathbb{0}_n) = \left(\int_0^1 J(\tau x) d\tau \right) (x - \mathbb{0}_n). \quad (5.31)$$

By (5.29) and (5.30), we have $\|x_j\|_{[0, t]} \leq \psi_{ij}^{-1} x_i(t)$ for any $j \in \mathcal{N}_i$ and every $t \in [t^*, t^* + \epsilon)$. This inequality implies that for any $j \in \mathcal{N}_i$ and every $t \in [t^*, t^* + \epsilon)$,

$$x_j(t) \leq \psi_{ij}^{-1} x_i(t) \leq \kappa x_i(t). \quad (5.32)$$

Since $J(x)$ is Metzler for every $x \in \mathbb{R}_{\geq 0}^n$, by (5.31) and inequality (5.32), we have

$$\dot{x}_i(t) = f_i(x) \leq \left(\int_0^1 (J_{ii}(\tau x) + \sum_{j \in \mathcal{N}_i} J_{ij}(\tau x) \psi_{ij}^{-1}) d\tau \right) x_i(t). \quad (5.33)$$

We consider two cases in the following.

1. $x_i(t^*) = \beta(x_i(0), t^*)$: In this case, for every $t \in [t^*, t^* + \epsilon)$ and every $\tau \in [0, 1]$, we have $\tau x(t) \in B_i(x_i(t))$ and

$$B_i(x_i(t)) \subseteq B_i(x_i(t^*)) \subseteq B_i(x_i(0)).$$

Thus, by (5.33), we have

$$\dot{x}_i(t) \leq -\delta(x_i(0))x_i(t),$$

which implies that $x_i(t) \leq e^{-\delta(x_i(0))(t-t^*)}x_i(t^*)$. Thus, along with (5.29), we have, for every $t \in [t^*, t^* + \epsilon)$,

$$\begin{aligned} x_i(t) &\leq e^{-\delta(x_i(0))(t-t^*)}x_i(t^*) = e^{-\delta(x_i(0))t}x_i(0) \\ &\leq \max_j \{\beta(x_i(0), t), \psi_{ij}\|x_j\|_{[0,t]}, \|u_i\|_\infty\}, \end{aligned}$$

which is contradictory to (5.30).

2. $x_i(t^*) > \beta(x_i(0), t^*)$: In this case, we have

$$x_i(t^*) = \max_j \{\psi_{ij}\|x_j\|_{[0,t^*]}, \|u_i\|_\infty\}.$$

By (5.33), we have $\dot{x}_i(t) \leq 0$ for every $t \in [t^*, t^* + \epsilon)$. Since $\|x_j\|_{[0,t]}$ is nondecreasing with respect to t , for every $t \in [t^*, t^* + \epsilon)$,

$$x_i(t) \leq \max_j \{\psi_{ij}\|x_j\|_{[0,t]}, \|u_i\|_\infty\} \leq \max_j \{\beta(x_i(0), t), \psi_{ij}\|x_j\|_{[0,t]}, \|u_i\|_\infty\},$$

which is contradictory to (5.30).

In both cases, we have a contradiction. Therefore, for every $t \geq 0$ and every $i \in \{1, \dots, n\}$, $x_i(t)$ satisfies (5.28). Moreover, Theorem 5.5.0.12 ensures that $\{\psi_{ij}\}_{(i,j) \in \mathcal{E}}$ satisfies $\psi_c < 1$, for every $c \in \Phi$. Therefore, by cyclic small-gain theorem 5.3.2.4, the control system (5.27) is ISS, which implies that $\mathbb{0}_n$ is globally asymptotically stable for nonlinear dynamical system (5.25).



Theorem 5.5.0.2 (Sum-interconnection stability) *Consider an interconnected non-linear system (5.25) evolving on the positive orthant $\mathbb{R}_{\geq 0}^n$ with the interconnection graph $\mathcal{G} = (V, \mathcal{E})$. Assume that $f(\mathbb{0}_n) = \mathbb{0}_n$, and for every $x \in \mathbb{R}_{\geq 0}^n$, the matrix $J(x)$ is Metzler with negative diagonal entries. Moreover, assume there exists a family of positive numbers $\{\gamma_{ij}\}$ for $i \in V$ and $j \in \mathcal{N}_i$ such that:*

1. *for every $i \in \{1, \dots, n\}$,*

$$\frac{J_{ij}(x)}{-J_{ii}(x)} \leq \gamma_{ij}, \quad \text{for all } x \in \mathbb{R}_{\geq 0}^n,$$

2. *for every $i \in \{1, \dots, n\}$ and $I = \{1, \dots, i\}$,*

$$\gamma_{M_I} < 1,$$

where the Metzler matrix M is defined as, for $i', j' \in V$

$$m_{i'j'} = \begin{cases} \gamma_{j'j'}, & \text{if } (j', i') \in \mathcal{E}, \\ -1, & \text{if } i' = j', \\ 0, & \text{otherwise.} \end{cases}$$

Then $\mathbb{0}_n$ is globally asymptotically stable for system (5.25).

Proof: By 2 and Theorem 5.4.4.51, M is Hurwitz. Thus, by Theorem 5.4.3.1, there exists a family of positive numbers $\{\psi_{ij}\}_{(i,j) \in \mathcal{E}}$ such that, for every $i \in \{1, 2, \dots, n\}$,

$$\sum_{j \in \mathcal{N}_i} \frac{m_{ij}}{-m_{ii}} \psi_{ij}^{-1} \leq 1,$$

and $\psi_c < 1$ for every $c \in \Phi$. This implies that, for every $x \in \mathbb{R}_{\geq 0}^n$, we have

$$\sum_{j \neq i} \frac{J_{ij}(x)}{-J_{ii}(x)} \psi_{ij}^{-1} \leq \sum_{j \neq i} \gamma_{ij} \psi_{ij}^{-1} = \sum_{i \neq j} \frac{m_{ij}}{-m_{ii}} \psi_{ij}^{-1} \leq 1.$$

Therefore, for the family of positive numbers $\{\psi_{ij}\}_{(i,j) \in \mathcal{E}}$,

$$\sum_{j \neq i} \frac{J_{ij}(x)}{-J_{ii}(x)} \psi_{ij}^{-1} \leq 1, \quad \text{for all } i \in \{1, \dots, n\},$$

and $\psi_c < 1$ for every $c \in \Phi$. Therefore, by Theorem 5.5.0.1, $\mathbb{0}_n$ is globally asymptotically stable for the dynamical system (5.25). ■

5.6 Additional Concepts and proofs

5.6.1 Cycle graphs, complementary cycle graphs and disjoint cycle sets

Let $M \in \mathbb{R}^{n \times n}$ be an irreducible Metzler matrix with negative diagonal elements and $\Phi = \{c_1, \dots, c_r\}$ be the set of simple cycles in $\mathcal{G}(M)$. Then the associated *cycle graph* of $\mathcal{G}(M)$ is the graph $\mathcal{G}_\Phi(M) = (V_\Phi, \mathcal{E}_\Phi)$ with the node set $V_\Phi = \{1, \dots, r\}$ and the edge set \mathcal{E}_Φ given by

$$\mathcal{E}_\Phi = \{(i, j) \mid c_i \in \Phi, c_j \in \Phi, c_i \cap c_j \neq \emptyset\}.$$

We define the *complementary cycle graph* of $\mathcal{G}(M)$ by $\mathcal{G}_\Phi^c(M) = (V_\Phi, \mathcal{E}_\Phi^c)$. Note that while the graph $\mathcal{G}(M)$ is a weighted digraph, the graphs $\mathcal{G}_\Phi(M)$ and $\mathcal{G}_\Phi^c(M)$ are unweighted undirected graphs. Moreover, since M is irreducible, the cycle graph $\mathcal{G}_\Phi(M)$ is always connected. The *disjoint cycle set* K_ℓ^M is a set in which each element is a nonempty set

of $\ell \geq 1$ cycles in Φ that form a complete graph in $\mathcal{G}_\Phi^c(M)$.

Example 5.6.1.1 (Cycle graphs, complementary cycle graphs and K_ℓ^M) We illustrate the a few definitions using the Metzler matrix in Example 5.4.4.3, whose associated weighted digraph $\mathcal{G}(M)$ is shown in Fig. 5.1.

The cycle graph $\mathcal{G}_\Phi(M)$ is given in Fig. 5.4a and the complementary cycle graph $\mathcal{G}_\Phi^c(M)$ is given in Fig. 5.4b. From Fig. 5.4b, one can check that the disjoint cycle sets are clearly given by (5.18).

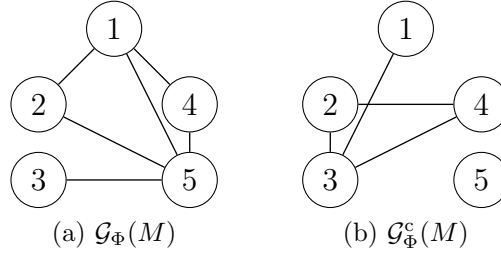


Figure 5.4: Cycle graph and complementary cycle graph

5.6.2 Graph expansion and proof of Theorem 5.4.4.53

In this subsection, we reverse the Schur complement process and propose a graph expansion algorithm for the associated graph of a Metzler matrix. The purpose of the expansion is to separate cycles so that no cycle is strictly contained in any other cycle. Once we complete this construction, a simple proof of Theorem 5.4.4.53 follows.

For a Metzler matrix $M \in \mathbb{R}^{n \times n}$ associated with $\mathcal{G}(M) = (V, \mathcal{E}, M)$, we construct the expansion digraph $\mathcal{G}_{\text{exp}}(M) = (V_{\text{exp}}, \mathcal{E}_{\text{exp}}, M_{\text{exp}})$ and the expanded Metzler matrix M_{exp} using Algorithm 1.

In words, for a Metzler matrix $M \in \mathbb{R}^{n \times n}$, Algorithm 1 inserts a node on each directed edge in $\mathcal{G}(M)$ and assigns proper weights to the added nodes and edges.

Algorithm 1 Graph expansion for Metzler matrices

```

1: Input: A Metzler matrix  $M \in \mathbb{R}^{n \times n}$  and  $\mathcal{G}(M) = (V, \mathcal{E}, M)$ 
2: Initialize:  $V_{\text{exp}} = V$ ,  $\mathcal{E}_{\text{exp}} = \emptyset$ ,  $M_{\text{exp}} = M$ ,  $k = 0$ 
3: for every edge  $(i, j) \in \mathcal{E}$  do
4:    $k = k + 1$ 
5:    $V_{\text{exp}} = V_{\text{exp}} \cup \{n + k\}$ 
6:    $\mathcal{E}_{\text{exp}} = \mathcal{E}_{\text{exp}} \cup \{(i, n + k), (n + k, j)\}$ 
7:    $M_{\text{exp}} = \begin{bmatrix} M_{\text{exp}} & \mathbb{0}_{(n+k-1) \times 1} \\ \mathbb{0}_{1 \times (n+k-1)} & -1 \end{bmatrix}$ 
8:    $M_{\text{exp}}(n + k, i) = M_{\text{exp}}(j, n + k) = \sqrt{m_{ji}}$ 
9: end for
10: return  $\mathcal{G}_{\text{exp}}(M) = (V_{\text{exp}}, \mathcal{E}_{\text{exp}}, M_{\text{exp}})$ 

```

Lemma 5.6.2.1 *For a Metzler matrix $M \in \mathbb{R}^{n \times n}$ and its expansion M_{exp} , M is Hurwitz if and only if M_{exp} is Hurwitz.*

Proof: The Metzler matrix M can be recovered from M_{exp} by removing all the added nodes using the Schur complement, and the diagonal elements of the remaining nodes do not change during the elimination. Therefore, by Lemma 5.2.2.3, M is Hurwitz if and only if M_{exp} is Hurwitz. ■

Now we are ready to give a proof to Theorem 5.4.4.53. *Proof:* [Proof of Theorem 5.4.4.53] By construction, any cycle in $\mathcal{G}_{\text{exp}}(M)$ can show up as a leading principal submatrix after a permutation on M_{exp} . Since M is Hurwitz, M_{exp} is also Hurwitz and by Lemma 5.2.2.1(iii), the determinant of the negative leading principal submatrix must be positive, i.e., the cycle gain must be less than 1. ■

5.7 Conclusion

In this chapter, we obtained and characterized the graph-theoretic necessary and sufficient conditions for the Hurwitzness of Metzler matrices. By establishing connections with the well-known input-to-state stability theory and small-gain theorems, we were able

to derive stability conditions for linear Metzler systems based on two different forms of ISS gains. Our conditions are also related to the classic Hicksian stability condition. These conditions give insights on how the cycles and cycle structures in the associated digraph of the Metzler matrices play a role in determining system stability. We also extended our results to the case of nonlinear monotone systems and obtained sufficient conditions for stability.

5.8 Appendix

5.8.1 Proof of Lemma 5.4.4.4

In order to prove Lemma 5.4.4.4, we need a few results regarding the graph-theoretic interpretations of determinants. For a weighted digraph $\mathcal{G} = (V, \mathcal{E}, W)$, a *factor* $F = \{c_1, \dots, c_r\}$ of \mathcal{G} satisfies

1. each $c_i \in F$ is either a self loop or a simple cycle;
2. $c_i \cap c_j = \emptyset$, for all $i \neq j$;
3. $\cup_{i=1}^r c_i = V$.

Note that the set of factors may be empty and in this case the determinant of the matrix corresponding to the digraph is 0.

For a matrix $A \in \mathbb{R}^{n \times n}$, the determinant of A can be computed based on the factors of $\mathcal{G}(A)$. For a simple cycle or a self loop c in $\mathcal{G}(A)$, we define $A(c)$ to be the product of the edge weights along the cycle or the self loop. Then, we have the following lemma.

Lemma 5.8.1.1 (Graph-theoretic interpretation of determinants [124, Theorem 1]) *Let $A \in \mathbb{R}^{n \times n}$ be a matrix with digraph $\mathcal{G}(A) = (V, \mathcal{E}, A)$. Suppose $\mathcal{G}(A)$ has*

factors $F_k = \{c_{k_1}, c_{k_2}, \dots, c_{k_{r_k}}\}$, $k = 1, \dots, q$, then

$$\det(A) = (-1)^n \sum_{k=1}^q (-1)^{r_k} A(c_{k_1}) A(c_{k_2}) \cdots A(c_{k_{r_k}}). \quad (5.34)$$

In the case of irreducible Metzler matrices with negative diagonal elements, we can rewrite (5.34) in terms of the cycle gains. Let $M \in \mathbb{R}^{n \times n}$ be an irreducible Metzler matrix with negative diagonal elements and $\Phi = \{c_1, \dots, c_r\}$ be the set of simple cycles of $\mathcal{G}(M)$, then a *cycle factor* $F^c = \{c_1, \dots, c_t\}$ of $\mathcal{G}(M)$ satisfies

1. $F^c \subset \Phi$ and $F^c \neq \emptyset$;
2. $c_i \cap c_j = \emptyset$, for all $c_i, c_j \in F^c$ and $i \neq j$.

Suppose $\mathcal{G}(M)$ has cycle factors $F_k^c = \{c_{k_1}, c_{k_2}, \dots, c_{k_{t_k}}\}$, $k = 1, \dots, q$, then each cycle factor F_k^c can be expanded to a factor of $\mathcal{G}(M)$ by adding the self loops at the nodes that are not on any simple cycles in F_k^c and by doing this, all the factors except the one that consists of purely self loops can be recovered. Since the diagonal elements of M are negative, we can factor out $\prod_{i=1}^n (-m_{ii})$ in the general formula (5.34) and rewrite the equation for M as follows,

$$\det(M) = \prod_{i=1}^n m_{ii} + \prod_{i=1}^n m_{ii} \sum_{k=1}^q (-1)^{t_k} \gamma_{c_{k_1}} \gamma_{c_{k_2}} \cdots \gamma_{c_{k_{t_k}}}. \quad (5.35)$$

By definition, the disjoint cycle sets are related to the cycle factors as $K_\ell^M = \{F_k^c \mid t_k = \ell\}$, thus we can group the cycle factors with the same cardinality in (5.35) and obtain (5.20) for $I = \{1, \dots, n\}$. For $i = \{1, \dots, n-1\}$ and $I = \{1, \dots, i\}$, the same procedure works for the leading principal submatrices M_I and (5.20) follows except for the case when Φ_{M_I} is empty. If Φ_{M_I} is empty, i.e., $\mathcal{G}(M_I)$ is acyclic, then the determinant $\det(M_I)$ is equal to the product of the diagonal elements. By (5.17), we have $\gamma_{M_I} = 0$ in this case

and thus (5.20) holds.

5.8.2 Proof of Corollary 5.4.3.2

(i) \implies (ii): Since M is Hurwitz, by Theorem 5.4.3.1, for every $(j, i) \in \mathcal{E}$, there exists $\psi_{ij} > 0$ such that

$$\sum_{j \in \mathcal{N}_i} \left(\frac{m_{ij}}{-m_{ii}} \right) \psi_{ij}^{-1} < 1, \quad \forall i \in \{1, \dots, n\}, \quad (5.36)$$

$$\psi_c < 1, \quad \forall c \in \Phi. \quad (5.37)$$

Let $c \in \Phi$ and assume that $c = (1, \dots, k, 1)$. Then, for every $k' \in \{1, \dots, k\}$, we define

$$\widehat{\theta}_{k'}^c = \begin{cases} \left(\frac{m_{k'+1, k'}}{-m_{k'+1, k'+1}} \right) \psi_{k'+1, k'}^{-1}, & k' \leq k-1, \\ \left(\frac{m_{1, k}}{-m_{11}} \right) \psi_{1, k}^{-1}, & k' = k. \end{cases}$$

First note that (5.37) can be written as

$$\prod_{i \in c} \widehat{\theta}_i^c > \gamma_c, \quad \forall c \in \Phi.$$

Since $\mathcal{G}(M)$ is connected and cactus, no two simple cycles share an edge. Therefore, one can write (5.36) as follows:

$$\sum_{c \in \Phi} \widehat{\theta}_i^c < 1, \quad \forall i \in c.$$

By a straightforward continuity argument, one can show that, for every $c \in \Phi$ and $i \in c$, there exists $\theta_i^c > 0$ such that

$$\begin{aligned} \prod_{i \in c} \theta_i^c &> \gamma_c, & \forall c \in \Phi, \\ \sum_{c \in \Phi} \theta_i^c &= 1, & \forall i \in c. \end{aligned}$$

(ii) \implies (i): Now suppose that, for every $c \in \Phi$ and every $i \in c$, there exists $\theta_i^c > 0$ which satisfies (5.15). Let $c = (1, \dots, k, 1)$, and for every $k' \in \{1, \dots, k-1\}$

$$\psi_{k'+1, k'} = \left(\frac{m_{k'+1, k'}}{-m_{k'+1, k'+1}} \right) (\theta_{k'}^c)^{-1},$$

and

$$\psi_{1, k} = \left(\frac{m_{1, k}}{-m_{11}} \right) (\theta_k^c)^{-1}.$$

By a continuity argument, (5.15) can be written as (5.36) and (5.37). Thus, by Theorem 5.4.3.1, the matrix M is Hurwitz.

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