# First Passage and Machine Learning perspectives of RPS/RPSSL systems

Thesis submitted in partial fulfillment of the requirements for the degree of

Master of Science in Computational Natural Sciences by Research

by

Karthik Viswanathan 2019113015

karthik.viswanathan@research.iiit.ac.in



International Institute of Information Technology Hyderabad - 500 032, INDIA May 2024

Copyright © Karthik Viswanathan, 2024

All Rights Reserved

# International Institute of Information Technology Hyderabad Hyderabad, India

# CERTIFICATE

This is to certify that work presented in this thesis proposal titled *First Passage and Machine Learning perspectives of RPS/RPSSL systems* by *Karthik Viswanathan* has been carried out under my supervision and is not submitted elsewhere for a degree.

Date

Advisor: Dr. Chittaranjan Hens

#### Acknowledgements

The journey towards my Master's thesis has not only made me more knowledgable, but it has also made me a better and a stronger human. This journey wouldn't have reached this point without some; for it takes a village. From the bottom of my heart, I thank my advisor Dr. Chittaranjan Hens, who has been a teacher, guide, and a brother to me. He guided me diligently and provided me moral and emotional support whenever I seeked for it. He has been instrumental in responding, supervision, brainstorming, appreciating, and critiquing my work when necessary. I would like to thank my mom Malliga and dad Viswanathan who provided me moral, emotional, and financial support in my educational endeavours. They instilled in me great values, and helped me navigate this world through creativity, compassion, and courage. Finally, I would like to thank my brother Vignesh and my sister-in-law Sowmya for the support and company they provided me throughout this journey.

#### Abstract

The evolution of RPS/RPSSL can be studied from multiple perspectives. Once the rate reactions pertaining to birth, death, predation, and other activities including migration and mutation are drawn for the system, the simulation of the system can be done through multiple stochastic techniques like the stochastic lattice simulation or the Gillespie simulation. In this thesis, we study system evolution using two techniques. In a small-scale system with mutation, we study the extinction of a system under the lens of First-Passage formulation. We formulate a First-Passage Problem to derive the exact analytical solutions for extinction state and extinction time. We then verify the agreement between our First-passage solutions, Gillespie solutions, and mean-field theory. The first-passage solutions provide us a deeper look towards species extinction compared to stochastic simulations. Our findings suggest first-extinction time and state distribution in a system with mutation follows intriguing behaviour which promotes coexistence. There also exists a depression in the state space post which mutation extends the first-extinction time. Moreover, a system devoid of mutation exhibits a discernible inclination towards probabilities that lean in the direction of an endangered state space. However, the formulation of a first-passage problem is computationally very expensive and stochastic simulations become redundant for multiple initial conditions with same system parameters. Hence, we move towards a more complex problem of understanding and forecasting a system's evolution through Machine Learning. To provide the system with tractable information, we move to lattice-based simulation where we draw actions during each timestep using the Gillespie method. We also tackle a more intricate problem of migration, through which the spatio-temporal visualizations create spiral patterns in a system. Using Machine Learning we expedite the tasks of extinction prediction and system evolution by generating lattices using machine learning - which were computationally expensive using simulations and first-passage problems.

# Contents

Ch	apter		Page
1	Intro	duction	1
	1.1	Preliminary Works	. 1
	1.2	Thesis Scope	. 5
		1.2.1 Mutation through the eves of First Passage Formulation	. 6
		1.2.2 Migration through the eyes of Machine Learning	. 7
	1.3	Thesis Overview	. 8
2	Muta	ation and species co-existence	11
	2.1	Gillespie Simulations	. 11
	2.2	First Passage Problem	. 13
	2.3	Results	. 16
	2.4	Gillespie Simulations	. 17
	2.5	ODE model of the interacting five species ecosystem	. 18
	2.6	First Passage Probability and Time	. 22
	2.7	Initial Conditions in First-Passage problems	. 23
	2.8	Discussion	. 24
	2.9	Limitations	. 25
3	Mac	hine Learning for System Behaviour Prediction	33
	3.1	Lattice-based Simulation	. 33
	3.2	Convolutional Neural Networks	. 35
		3.2.1 U-Nets	. 38
		3.2.2 CNN Classifier	. 38
		3.2.3 Dropout	. 38
	3.3	Tasks	. 38
		3.3.1 Lattice Pattern Generation	. 39
		3.3.2 Species Extinction Prediction and Extrapolation	. 39
	3.4	Lattice Pattern Generation	. 40
	3.5	Extinction Prediction: Multiple Migration Rates	. 41
	3.6	Discussion	. 42
	3.7	Summary	. 43

#### CONTENTS

4	Conclusion	47
Bił	liography	48

# **List of Figures**

# Figure

1.1	A simple RPS model with various phenomenon. We define three species A,B, and C, and define some select phenomenon (migration, predation, reproduction). For each of these phenomenon, we show their effects on a lattice	2
1.2	(a). Initially, we define our rate equations, determine the rate constants and simulate the system using the Monte Carlo Method. Post this, we capture the data for spatio-temporal evolution for each Monte Carlo step. (b) and (c). Once we define and simulate the system, we capture the long-term nature of the system using lattices for varying rates and initial conditions. In (b), given lattices during earlier time steps of the simulation, we ask the CNN if the system goes to extinction in long-term. In (c), given a lattice of a system at a timestep $t$ , we ask the CNN to generate the system at timestep $t + dt$ after few steps of evolution.	9
1.3	Lattice-based for various migration rates $(M_r)$ and Monte Carlo time stamps $(T)$ . It can be observed that the spiral formation time increases and post a larger migration rate, spirals stop forming. Spirals are clearly visible for $M_r = 1$ and 8 post which they become less visible and more spread out	10
2.1	Schematic summary of the rate equations. Colors in the circle represent the species they belong to. (a) All possible species networks and interaction networks among them. (b) Examples of birth, mutation, and competition. (c) Evolution of a small scale system with various events occurring in discrete timesteps. (A1, A2,, A6) represent unique indexing for each of the actions / atomic processes in the system	13
2.2	Simulations obtained from long-term Gillespie simulations with Initial condi- tion $S_0 = (2, 2, 2, 2, 2)$ . <b>a.</b> Long-term Gillespie simulation for $\omega = 9$ without mutation. <b>b.</b> Long-term Gillespie simulation for $\omega = 30$ without mutation. <b>c.</b> Long-term Gillespie simulation for $\omega = 9$ with mutation. <b>d.</b> Long-term Gillespie simulation for $\omega = 30$ with mutation. We can observe that in the case without mutation, one species of the population survives, whereas in the case of mutation, we find various species of the population co-existing with each	15
	other	17

#### LIST OF FIGURES

- 2.3 Simulations obtained from short-term Gillespie simulations with  $\omega = 9$ . **a.** Short-term Gillespie simulation for initial state (2, 2, 2, 2, 2) without mutation. **b.** Short-term Gillespie simulation for initial state (7, 7, 7, 7, 7) without mutation. **c.** Short-term Gillespie simulation for initial state (2, 2, 2, 2, 2, 2) with mutation. **d.** Short-term Gillespie simulation for initial state (7, 7, 7, 7, 7, 7) with mutation. We observe a higher initial condition leading to a slower overall extinction in the case without mutation. With mutation, we observe multiple surges and plunges of population corresponding to various species.
- 2.4 First passage extinction probabilities: 2-Dimensional. Probabilities of the initial state (2, 2, 2, 2, 2) to be found at the following states during the first extinction event.  $P_abs$  represents the first-passage extinction probability. It can be noticed that the probability diminishes as the difference in the initial state and the possible extinction state increases indicating that it is less probable to find a state with rapid evolutionary dynamics during a first extinction event. . .
- 2.5 Stability diagram and time signals as a function of ω and β.(a-b) The light red color demarcates the unstable regime of Fp<sub>2</sub> ( α = 2.3 and α = 2.6 respectively). The blue area represents the stable parameter space of the same. (c) Time series of the system for a point (marked by X in (a)) from the stable region of the parameter space for α = 2.3. (d) the time series of the system for a point (marked by O in (a)) from the unstable region. Similarly, for α = 2.6 (e) and (f) correspond to the time series of the system for a point in the stable region and unstable region of the parameter space, respectively. Clearly, if we increase the predation term (α), the stable region decreases (light blue).

19

20

2.10	First passage extinction times: Number of states where an ecosystem with mutation leads to a slower first extinction than an ecosystem without mutation. Three variables $N_1, N_3, N_5$ are variables across the x and y axis under various line plots. The sum of states under these settings are taken where the difference in extinction times without and with mutation is positive	30
2.11	Correlation between the extinction probabilities of $1e6$ Gillespie simulations $(P_G)$ and first passage problem $(P_F)$ without (a) with R2 score 0.97 and with mutation (b) with R2 score 0.99.	30
2.12	<b>First passage extinction probabilities: 3-Dimensional</b> . Probabilities of the initial state (2, 6, 2, 2, 2) to be found at the following states during the first extinction event. It can be noticed that the probability diminishes as the difference in the initial state and the possible extinction state increases indicating that it is less probable to find a state with rapid evolutionary dynamics during a first extinction event.	31
2.13	<b>First passage extinction probabilities: 3-Dimensional</b> . Probabilities of the initial state (2, 6, 2, 2, 2) to be found at the following states during the first extinction event. It can be noticed that the probability diminishes as the difference in the initial state and the possible extinction state increases indicating that it is less probable to find a state with rapid evolutionary dynamics during a first extinction event	32
3.1	Schematic diagram for actions on lattice. Predation removes a species accord- ing to the cyclic predation order. Birthing results in a neighboring species giving birth to its offspring in a vacant site. Migration results in a species exchanging its lattice site with a neighboring species	34
3.2	A summary of CNN operations. Given an input image and a feature map, a visual representation of convolutions, pooling, flattening, and feed-forward network.	36
3.3	(a). U-Net Architecture. (i) Each block consists of a Conv Layer, followed by a Batch Norm, Max Pooling layer, and a ReLU non-linear activation. For each Conv block, we have downsampling kernels of shape 64, 128, 256, 512, post which upsampling occurs in the reverse order. (b). CNN architecture. With $N = 5$ , we have kernels 32, 64, 128, 256, 512. Our flattening layers downsamples each feature vectors into 256, 128, 64, and 2 post flattening followed by a softmax activation for binary class probabilities.	37

#### LIST OF FIGURES

- Results for pattern generation for model trained with single migration 3.4 rate. (a) Spiral formation from early-stage lattice predictions. Only t=5 lattice is provided as input to our model. Then the model outputs are used as successive inputs. (b) Spiral formation for data corresponding to lattice timesteps outside of training data temporally. In this task, the model extrapolates and generates spiral patterns for timesteps outside the training range. Only t=380 is provided as an input to our model. Then the model outputs are used as successive inputs. (c) Unseen Initial condition. (i) ML based predictions. Given t=5, use U-Net outputs for further simulation. (ii) Outputs from Monte Carlo algorithm (Simulation). (iii) Deviation in predictions. . . . . . . . . . . . . . 44 Results from model trained to generate patterns for multiple migration 3.5 rates. Lattices from random initial timesteps with input and output in difference of 40 Monte Carlo Timesteps. (i) Input Lattice. (ii) Expected output 45

# **List of Related Publications**

- [P1] K. Viswanathan, A. Wilson, S. Bhattacharyya, C. Hens, Ecological resilience in a circular world: Mutation and extinction in five-species ecosystems, Chaos, Solitons & Fractals, Volume 180, 2024.
- [P2] K. Viswanathan, U. Shekhar, A. Roy, C. Hens, Convolutional Nets for Lattice State Forecasting (under preparation)

# Chapter 1

## Introduction

#### **1.1 Preliminary Works**

The fundamental importance of coexistence within ecosystems cannot be overstated when it comes to bolstering the equilibrium of populations. In the intricate web of life, an ecosystem that experiences the extinction of species poses a substantial threat to its constituent organisms, creating disruptions that imperil biodiversity and the overarching stability of the entire ecological framework. In the tangible reality of our world, it becomes imperative to construct models of ecosystems to unravel the potential external influencers that can be introduced to fortify the system's equilibrium. Modeling an ecosystem is an exceedingly intricate endeavor, given the vast diversity of species and their interactions with one another. Within the tapestry of ecological dynamics, a multitude of intra- and inter-species relationships manifest, each playing a unique role in sustaining the ecosystem's vitality. Consequently, it is of paramount significance to meticulously investigate and seek to replicate these multifaceted interactions within an ecosystem, with the ultimate goal of comprehending their collective contributions to the overall stability and robustness of the ecosystem.

In the field of physics, theoretical investigations, primarily adopting an evolutionary game perspective, have ventured in various directions to comprehend the natural phenomenon of studying existence across multiple competing species with limited resources [1,2]. The rock-paper-scissors (RPS) model (as shown in Figure 1.1), particularly from the perspective of evolutionary game theory, has been widely studied to understand this natural process of biodiversity maintenance through interspecific cyclic competition. This model can be represented using multiple formalisms like Lotka-Volterra and May-Leonard systems [3–5]. The Lotka-Volterra formalism introduces a two-species model with the following rules: (1) There exists a prey and predator. (2) the prey dies through inherent death or predation by prey. (3) the predator die through inherent death, and their birth is positively affected by the rate at which they predate.

In the May-Lennard formalism, three-species models were introduced (A,B, and C), where phenomenons like predation could be cyclic (A predates B, B predates C, and C predates A); as shown in Figure 1.1. Such cyclic models demonstrate that all species have a fair chance to survive due to the cyclic dominance of predator-prey interactions. The RPS model has been applied to various biological examples, including the morph prevalence of three-morph mating systems in side-blotched lizards, the cyclic dominance of Pacific salmon, and microbial domains. [6–8].



**Figure 1.1** A simple RPS model with various phenomenon. We define three species A,B, and C, and define some select phenomenon (migration, predation, reproduction). For each of these phenomenon, we show their effects on a lattice.

Figure 1.1 provides insight into the various phenomenon that occur in a classic RPS system, where we denote the species by identifiers A, B, C. Each species undergoes a birth even (where the species multiplies), and a death event (where the species ceases to exist). More complex interactions like cyclic mutations, migrations, and predations can also take place in a system. Various works have analyzed such complex phenomenon through the help of a lattice. The analysis has been done both through the passage of time (temporal) in a defined lattice (space), termed as spatio-temporal evolution [9-14]. We explain a selection of such processes and phenomenon which have helped improve the realism of such system to that of real-world phenomenon in line with Figure 1.1 and Equation 1.1. **1 - Birth** All the works referenced in the context of evolution specify birth as a phenomenon for species proliferation. 2- Death Many formalisms including [3, 15, 16] introduce death as a part of their formalism. The site at which species was present earlier, becomes vacant. 3 - Predation Competitive interactions exist in ecological systems where predators prey on species for nutrition and survival [17, 18]. Various works have introduced competitive interactions in species through the eyes of cyclic predations [19, 20]. In cyclic predation, the species A can predate B, B can predate C can predate A as referenced in Equation 1.1. 4 - Mutation is an extremely important natural phenomenon which can cause crucial changes to a species on the genomic level [21]. These events have been extensively studied in cyclic RPS models [10, 22]. Through small mutation rates, species have been allowed to transform into another species, as a form of mutation, and their population dynamics have been extensively studied and concluded to promote co-existence [10, 12, 22]. **5** - Migration/Mobility. Just like species are allowed to move-across their assigned site, emulating this phenomenon in simulations can provide improved realism [13, 23–25]. In such systems, a species is allowed to exchange its position with a neighbor as shown in Figure 1.1. Migration (also termed as mobility), has been found to impact the chances of long-term survival of the species [26–28] and can even in some cases lead to the vanishing of all biodiversity and leading to the extinction of other species. These studies have also shown the formation of Turing spirals on lattices caused due to species migration [9, 29–31]. 6 - Misc. Further attempts were introduced apart from the above phenomenon to bridge the gap between realworld systems and simulated systems. For example, to emulate the elevated uncertainty of real-world systems, Reichenbach et al. propose addition of noise to RPS systems [32]. To address crucial problem of population shrink due to major evironmental phenomenon, epidemics, etc., Bhattacharya et al. spike the death rate across species for a brief period, providing further scope of agreement to real-world phenomenon [33]. Often techniques like the Monte Carlo Simulations [16, 34, 35], or Gillespie Simulations [36] are used to introduce stochasticity into ecological modeling. These simulations can be generalized roughly through a common algorithm: introducing a rate of occurence to each of the above phenomenon, and sampling an

action at a given timestep taking into account the rates, we can effectively model the evolution of a system. An insight of these phenomenon in the form of rate equations has been provided in Equation 1.1 and Figure 1.1.

$$AV \longrightarrow AA \ BV \longrightarrow BB \ CV \longrightarrow CC \text{ (Birth)}$$

$$AB \longrightarrow AV \ BC \longrightarrow BV \ CA \longrightarrow CV \text{ (Predation)}$$

$$A \longrightarrow V \ B \longrightarrow V \ C \longrightarrow V \text{ (Death)}$$

$$A \longrightarrow B \ B \longrightarrow C \ C \longrightarrow A \text{ (Mutation)} \tag{1.1}$$

$$AB \longrightarrow BA \ AC \longrightarrow CA \ AV \longrightarrow VA \text{ (Migration)}$$

$$BA \longrightarrow AB \ BC \longrightarrow CB \ BV \longrightarrow VB \text{ (Migration)}$$

$$CA \longrightarrow AC \ CB \longrightarrow BC \ CV \longrightarrow VC \text{ (Migration)}$$

In our thesis we will study on the role of mutation and migration in cyclically dominant eco-systems. At first we start with mutation. Mutation is a gradual process of incremental variation encompassing random changes in phenotypes. Researchers have abstracted this in a broader sense to encompass target mutations and birth of mutant species [10, 37]. Extinction and Survival analysis in ecological networks have been performed through the lens of multilayer networks and dispersal topologies to provide robust understanding of species persistence in complex networks [38, 39]. In a different context, exact solutions using first-passage extinction have been first attempted recently for an ecosystem extinction model by Barendgert et al. [40], inspired by Taylor and Karlin [41], Anderson and Kurtz [42] and Wilkinson [43]. In our thesis, we perform two formulations of the first-passage problem to obtain the first-passage probability and first-passage time for systems with and without mutation. In order to formulate these problems, we first define our state space. A single state in our state space is of the form  $(N_1, N_2, ..., N_k)$  where k is the number of species and  $N_i \in [0, \omega]$  where the carrying capacity,  $\omega$ is the maximum number of species our defined ecosystem can survive attributing to the limited resources crucial to survival in the system. First-passage probability for a state of interest Srepresents the probability at which systems with initial states  $S' \neq S$  first encounters state S during evolution. The first-passage time problem is the time taken for a system to reach this state S. These problems are formulated through using the adjoint of the Kolmogorov forward operator. We define the our state space, the rates at which transformations from one state  $S_i$ to the other state  $S_j$  can occur. Finally, we define the terminal state S for which we want to obtain first-passage probability and time from other states  $S' \neq S$ . We obtain exact solutions of species extinction using first-passage problems and show their correlation with Gillespie simulations for minimal modeling where single species persists. This scheme of studying extinction is certainly a potential host of investigating the effect of mutation. Our primary objective is to

understand the various mechanisms and conditions under which mutations foster co-existence. These effects of mutation have been extensively studied in Chapter 2.

In our thesis (apart from the investigation of mutation), we have also investigated the role of migration/mobility in three species model. In last two decades, researchers have studied the formation of several patterns in presence of migration (see the rate equation 1.1, Figure 1.3). It has been established that, a dying species can survive in presence of suitable migration [9]. On the other hand, high strength of diffusion may also jeopardize the entire state [9, 44]. Trying to capture the essence of physical systems through machine learning is an emerging endeavour with many related works. While stochastic simulations capture the patterns created through various phenomenon effectively, for larger lattices (> 100 \* 100), they are time-consuming as verifying conclusive results from long-term behaviour for multiple initial conditions occurs only after 4000-5000 iterations. Moreover, two different simulations with same parameters can have drastically different results, and hence, it is important to abstract an overall distribution for each rate interval. In this context, we search for ML tools capable of learning forecasting and event distribution across various system configurations.

CNNs and their variants have been extremely instrumental for applications including image and video recognition, image classification, image segmentation, etc [45-47]; inspired by cortical neurons which respond to stimuli only from their receptive field. Pooling multiple such receptive fields can be crucial to understanding the global impact caused by the stimuli and understand the overlap of various receptive fields. This is emulated in Convolutional Neural Networks through convolution operation, pooling, normalization, etc. From innovations like LeNet, ResNet, U-Nets, and Transformers, CNNs can now not only classify images but also produce high quality maps which can aid in various tasks including edge detection, depth estimation, etc [48–50]. This paper introduces a novel deep learning architecture, namely PeRCNN [51], for modeling and discovery of nonlinear spatio-temporal dynamical systems based on sparse and noisy data. In another paper, the authors propose a novel architechture, SciNet [52], that can be used to recover physical variables from experimental data in various physical toy settings. This paper [53], presented a data-driven method for discovering inter-pretable, low-dimensional dynamical models and their associated coordinates from highdimensional data. We take the inspiration of all the above works to emulate and abstract a distribution which can effectively predict long-term behaviour of RPS systems with migration.

#### 1.2 Thesis Scope

Our thesis aims at understanding RPS systems through the lens of First Passage Formulation, ODE, and, Machine Learning.

#### **1.2.1** Mutation through the eyes of First Passage Formulation

Mutation is an extremely important phenomenon which promotes diversity and co-existence in ecosystems [22, 54]. It is important to understand in-depth, the exact nuances of mutation, and more importantly, how mutation promotes co-existence. It is impossible to do an in-depth analysis through simulations as they do not provide us the effect of mutation on our state space. It is important to understand under which state spaces is the first extinction event imminent, and for each state space when does the first extinction even occur. This helps us from the multiple perspectives including development of conservation strategies, maintaining co-existence, etc. Hence, upon studying a system without mutations, and comparing it with a system in which mutation is present can help us understand the underlying effects of mutation and how it promotes co-existence. It is evident from Barendgert et al. that first-passage problems can be used to study the first extinction events of a system accurately [40]. First passage formulation of systems, as explained earlier provide more insights into the state space by deriving exact extinction probabilities and times for each state S to reach another state S'. Hence, it is only imperative to construct a first passage formulation of our system to derive exact analytical solutions to extinction states in the system to understand the mechanisms through which mutations prevents/delays our system from reaching extinction states. In the first part of our thesis Chapter 2, we aim to visualize a five-species system, with and without mutations and understand extinction with the exact solutions from the first passage probability and extinction models. By constructing first-passage formulations, we are able to show that an ecosystem with mutation promotes coexistence compared to an ecosystem without mutation. We also study through these first passage formulations how mutation prevents species extinction when extinction is imminent in a system. We construct infinitesimal matrix generators and obtain probabilities for absorption states. We explore symmetric probabilities among similar absorbing states when cyclic interactions exist. Gillespie simulations have been executed over long and short time scales. Mutation is shown to promote coexistence and diversity of the population even after a first extinction event. We also find symmetry in extinction events across different species. The extinction probability and times we obtain are symmetric across any permutation of  $(N_1, N_2, N_3, N_4, N_5)$  which verifies the correctness of our first-passage problems as each phenomenon we define is cyclic in nature. The extinction times obtained were using first passage formulation and we notice that it is not in all cases that mutation moves a population away from an extinction event when compared to the formulation where mutation is absent. There is a spike in population in minimal models when mutation is present. Finally, we show that our Gillespie simulations and First-passage formulation are in good agreement with each other with highly positive correlation scores. We also construct ODEs and simulate

them and show that our simulations and in extension, our first-passage problems follow similar patterns to that of ODEs.

#### **1.2.2** Migration through the eyes of Machine Learning

A species undergoing Migration / Mobility in a system shifts to a neighboring point in the lattice. When we study the spatio-temporal evolution of a system with migration, we find that such a system evolves with spiral patterns as described in Figure 2. These intricate spiral patterns are only visible in large-scale lattices for select rates of migration and such stable spirals act as a guard to the species residing inside them. Upon increasing the rates of migration, these spirals become more distorted and unstable. In the longer term, spirals vanish and extinction occurs. Migration rates which result in stable spirals foster co-existence of a system. To better understand the distribution of extinction events in such lattices, first-passage problems are not a viable option. While the solutions to the first-passage problems provides us insights into the system's absorbing states, it provides us little information about a systems evolution into its transient state. Moreover, formulation of LU decomposition for the first-passage problem is computationally inefficient. A sparse  $10^5 * 10^5$  can only model rates for a total of 50 species at maximum if we consider a five-species system. Hence, it is almost impossible to decompose such matrices with increasing complexities (and reducing sparseness) for larger systems where the intricate patterns created by migration is visible. Hence, we try to reduce the redundancy of simulations, but also provide a similar formulation to first-passage problems using Machine Learning. We prefer a stochastic lattice simulation for this task to provide rich input to our models. We aim to study the established patterns occurring in such a lattice when density preserving mutation (migration) is used in a system. Migration in lattice-based system causes spirals to occur. With increasing migration, in later stages of a stochastic simulation, extinction occurs. It is evident from Mobila et al. that forecasting of events can occur with the existing prior by implicitly estimating system parameters and translating them into spatio-temporal feedback [23]. Hence, using spatio-temporal dynamics at an earlier timestep as a prior and understanding its effect on long-term behaviour, can result in long-term system behaviour prediction for posterior data, hence optimizing the prediction timeline by reducing simulation time steps. Machine Learning can be crucial to optimizing this rate-limiting step, and providing us a rich higher-dimensional latent space for multitudes of system parameters from which observations can be drawn from. However, employing Machine Learning for RPS systems is extremely challenging as we must deal with the stochastic nature of our simulation data, simulating the spatio-temporal dynamics of the system, and bringing two elements: prediction of a system parameter, along with time-based forecasting fast-forwarded into the future

for the specific system parameter under a single roof. The first task to emulate the stochastic nature of our data can be solved by employing Dropouts during training and testing for better generalization and variability. The second complexity of spatio-temporal dynamics simulation can be solved by employing CNN-based image generation techniques. Finally, bringing multiple elements under a single prediction loop can be solved by employing ensemble based inputs to provide prior knowledge to our model about earlier system evolution which can be crucial to predict long-term behaviour. A schematic diagram of our tasks have been summarized in Figure 1.2.

#### **1.3 Thesis Overview**

The current chapter provides an introduction to RPS/RPSSL cyclic systems. We define the scope of our thesis, the challenges we will be facing, and the complexities involved in our work.

In Chapter 2, we present the theory and results of our Gillespie Simulations, First Passage Solutions, and ODE results, and compare the agreement between them. Concluding the chapter, we discuss the limitations of our work, and move towards Machine Learning.

In Chapter 3, we define the theory and tasks we perform through Machine Learning and present our results. We perform experiments to compare the stochastic lattice simulations to our Machine Learning results. We discuss how Machine Learning overcomes the limitations of both simulations and first-passage problems.

In Chapter 4, we conclude our thesis by summarizing our tasks and results. We provide further scope for our thesis.



Figure 1.2 (a). Initially, we define our rate equations, determine the rate constants and simulate the system using the Monte Carlo Method. Post this, we capture the data for spatio-temporal evolution for each Monte Carlo step. (b) and (c). Once we define and simulate the system, we capture the long-term nature of the system using lattices for varying rates and initial conditions. In (b), given lattices during earlier time steps of the simulation, we ask the CNN if the system goes to extinction in long-term. In (c), given a lattice of a system at a timestep t, we ask the CNN to generate the system at timestep t + dt after few steps of evolution.



**Figure 1.3** Lattice-based for various migration rates  $(M_r)$  and Monte Carlo time stamps (T). It can be observed that the spiral formation time increases and post a larger migration rate, spirals stop forming. Spirals are clearly visible for  $M_r = 1$  and 8 post which they become less visible and more spread out.

## Chapter 2

#### Mutation and species co-existence

#### 2.1 Gillespie Simulations

For the first section of our tasks, we model a five-species ecosystem as a stochastic process and evolve the system during each time step by updating the ecosystem's population in every time step following Gillespie algorithm. Since ecological systems are typically complex and composed of numerous interacting species; a five-species model is likely to provide a more realistic representation of the ecological dynamics within a particular ecosystem than a threespecies model. Moreover, we put our first-passage formulation into test by opening further stochastic systems and verifying its comparison to Gillespie simulations. Throughout the first section of our modelling, the minimal model has been used following Barendgert et al. [40] The species of the model have corresponding rates of heterocidal predation  $(\alpha_p, \beta_p, \gamma_p, \theta_p)$  as shown in Eq. 2.1. The homicidal competition may be thought of as death mechanism, where one member of a species competes with the another member of the same species. They also have birth rates for each species:  $r_a, r_b, r_c, r_d, r_e$ , and mutation rates denoted by  $\alpha_m, \beta_m, \gamma_m, \theta_m$ respectively (all shown in Eq. 2.1). The rates are normalized by the carrying capacity of our system barring the overflow of population given the limited resources in our ecosystem represented by  $\omega$ . Our predation strategy and the mutation strategy are cyclic, and the following rate equations cover our processes. The rate equations have been provided in Equation 1 and we have summarised the process in Figure 2.1.

$$A_{i} \longrightarrow 2A_{i} \text{ (with rate } r_{i} \text{ Birthing)}$$

$$A_{i} + A_{i+1} \longrightarrow A_{i+1} \text{ (with rate } \frac{\alpha_{p}}{\omega} \text{ :Heterocidal Predation)}$$

$$A_{i} + A_{i+2} \longrightarrow A_{i+2} \text{ (with rate } \frac{\beta_{p}}{\omega} \text{ :Heterocidal Predation)}$$

$$A_{i} + A_{i+3} \longrightarrow A_{i+3} \text{ (with rate } \frac{\gamma_{p}}{\omega} \text{ :Heterocidal Predation)}$$

$$A_{i} + A_{i+4} \longrightarrow A_{i+4} \text{ (with rate } \frac{\theta_{p}}{\omega} \text{ :Heterocidal Predation)}$$

$$2A_{i} \longrightarrow A_{i} \text{ with rate } \frac{2}{\omega} \text{ :Homocidal Predation)}$$

$$A_{i} \longrightarrow A_{i+1} \text{ (with rate } \frac{\alpha_{m}}{\omega} \text{ :Mutation)}$$

$$A_{i} \longrightarrow A_{i+2} \text{ (with rate } \frac{\beta_{m}}{\omega} \text{ :Mutation)}$$

$$A_{i} \longrightarrow A_{i+4} \text{ (with rate } \frac{\beta_{m}}{\omega} \text{ :Mutation)}$$

$$A_{i} \longrightarrow A_{i+4} \text{ (with rate } \frac{\theta_{m}}{\omega} \text{ :Mutation)}$$

The Gillespie algorithm at instant t updates the state as follows:

$$\boldsymbol{S_t} = \boldsymbol{S_0} + \sum_{0}^{k} a_k Y_K \int_0^t \lambda_k((\boldsymbol{S_n}) dn)$$
(2.2)

We first define states. A state **S** represents the population count  $(N_1, N_2, N_3, N_4, N_5)$  of the five-species ecosystem. The states are uniquely indexed for a time t in the Gillespie simulation. We represent  $a_k$  as a set of unitary actions for each rate equation mentioned in Eq. 2.1. For example, the vector associated with an increase in species 1 and a decrease in species 2 can be represented as (1, -1, 0, 0, 0). If these vectors correspond to the transition occurring in the above rate equation, they belong to our set of unitary actions. The propensity function  $(\lambda_k)$ , represents the intensity of the independent unit Poisson process  $Y_k$  for an action  $a_k$ . The propensity functions  $(\lambda_k)$  depend on the current state of the population. Birthing and Mutation events are first order; hence, the propensity function associated with them is represented by  $\nabla \times N_i$ , where  $\nabla$  represents the rate associated with the process. Similarly, predation is a second-order process; hence, the propensity function associated with it is represented by  $\nabla \times N_i \times N_j$ . Mutation is a first-order process, and the propensity is represented by  $\nabla \times N_i$ . We run the Gillespie algorithm as follows: we define a set of atomic actions, the rates associated with them, and the state changes corresponding to the atomic actions. For a given time t, we calculate the propensity functions and the next reaction time  $\delta t \sim exp(\sum_k \lambda_k)$  which depicts the minimum of the set of exponentially distributed random variables  $\lambda_k$ . We then determine the best course of action which occurs at  $t + \delta t$  by normalizing the propensities and obtaining the action corresponding to the maximum updated propensity. We then obtain the new state of the system by multiplying and adding the associated stoichiometric change for the action  $a_k$  to the original system to obtain the new state of the system. We run the Gillespie algorithm for the following system of rate equations long-term. We generalize the effects of mutation from the Gillespie Simulations and analyze first-time extinction events specifically.



**Figure 2.1** Schematic summary of the rate equations. Colors in the circle represent the species they belong to. (a) All possible species networks and interaction networks among them. (b) Examples of birth, mutation, and competition. (c) Evolution of a small scale system with various events occurring in discrete timesteps. (A1, A2, ..., A6) represent unique indexing for each of the actions / atomic processes in the system.

## 2.2 First Passage Problem

While our Gillespie simulation helps us understanding the long-term behavior, we aim to study the immediate dynamics of our extinction. The timing of extinctions helps us understand and prevent the collapse of an ecosystem. To model the extinction event, we construct an infinitesimal matrix generator  $\mathbf{L}$  where each entry  $L_{ij}$  in the generator matrix corresponds to the transition rate from state  $S_i$  to  $S_j$ . We follow the minimal model of Barendregt et al. [40], to obtain a distinct stationary distribution for which extinction events (as the state  $\mathbf{S} = (0, 0, 0, 0, 0)$ ) becomes inaccessible. An index in the matrix corresponding to the change of species count singularly in  $N_1$ , has a change in value of  $\pm 1$ . Similarly, a change of species count singularly in  $N_2$  corresponds to a change in the index by  $\pm \omega$ . A change in  $N_3, N_4, N_5$  are represented by a change in the index by  $\pm \omega^2$ ,  $\pm \omega^3$ , and  $\pm \omega^4$  respectively. For example, an increase of species of  $N_2$ , a decrease in a single species  $N_3$  at the same instant would be represented by  $L_{i,i+(1+\omega)-(1+\omega)^2}$ . The following set of elements in the transition matrix represents birthing in species.

$$L_{i,i+1} = r_1 N_1, \ L_{i,i+(1+\omega)} = r_2 N_2, \ L_{i,(1+\omega)^2} = r_3 N_3, L_{i,i+(1+\omega)^3} = r_4 N_4, \ L_{i,i+(1+\omega)^4} = r_5 N_5.$$
(2.3)

On the other hand, death in species is represented by

$$L_{i,i-1} = \frac{(N_1 \times (N_1 - 1))}{\omega} + \frac{\alpha_p}{\omega} N_1 N_2 + \frac{\beta_p}{\omega} N_1 N_3 + \frac{\gamma_p}{\omega} N_1 N_4 + \frac{\theta_p}{\omega} N_1 N_5.$$

$$L_{i,i-(1+\omega)} = \frac{\theta_p}{\omega} N_2 N_1 + \frac{(N_2 \times (N_2 - 1))}{\omega} + \frac{\alpha_p}{\omega} N_2 N_3 + \frac{\beta_p}{\omega} N_2 N_4 + \frac{\gamma_p}{\omega} N_2 N_5.$$

$$L_{i,i-(1+\omega)^2} = \frac{\gamma_p}{\omega} N_3 N_1 + \frac{\theta_p}{\omega} N_3 N_2 + \frac{(N_3 \times (N_3 - 1))}{\omega} + \frac{\alpha_p}{\omega} N_3 N_4 + \frac{\beta_p}{\omega} N_3 N_5.$$

$$L_{i,i-(1+\omega)^3} = \frac{\beta_p}{\omega} N_4 N_1 + \frac{\gamma_p}{\omega} N_4 N_2 + \frac{\theta_p}{\omega} N_4 N_3 + \frac{(N_4 \times (N_4 - 1))}{\omega} + \frac{\alpha_p}{\omega} N_4 N_5.$$

$$L_{i,i-(1+\omega)^4} = \frac{\alpha_p}{\omega} N_5 N_1 + \frac{\beta_p}{\omega} N_5 N_2 + \frac{\gamma_p}{\omega} N_5 N_3 + \frac{\theta_p}{\omega} N_5 N_4 + \frac{(N_5 \times (N_5 - 1))}{\omega}.$$
(2.4)

Each of the above elements representing death has twofold mechanism: homocidal death (represented by  $\frac{N_i \times (N_i-1)}{\omega}$  and heterocidal death through predation. The following set of elements

represents the occurrences of mutation in species:

$$L_{i,i-1+(1+\omega)} = \frac{\alpha_m}{\omega} N_1, \ L_{i,i-1+(1+\omega)^2} = \frac{\beta_m}{\omega} N_1, \\ L_{i,i-1+(1+\omega)^3} = \frac{\gamma_m}{\omega} N_1, \ L_{i,i-1+(1+\omega)^4} = \frac{\theta_m}{\omega} N_1 \\ L_{i,i-(1+\omega)+1} = \frac{\theta_m}{\omega} N_2, \ L_{i,i-(1+\omega)+(1+\omega)^2} = \frac{\alpha_m}{\omega} N_2, \\ L_{i,i-(1+\omega)+(1+\omega)^3} = \frac{\beta_m}{\omega} N_2, \ L_{i,i-(1+\omega)+(1+\omega)^4} = \frac{\theta_m}{\omega} N_2 \\ L_{i,i-(1+\omega)^2+1} = \frac{\gamma_m}{\omega} N_3, \ L_{i,i-(1+\omega)^2+(1+\omega)} = \frac{\theta_m}{\omega} N_3, \\ L_{i,i-(1+\omega)^2+(1+\omega)^3} = \frac{\alpha_m}{\omega} N_3, \ L_{i,i-(1+\omega)^3+(1+\omega)} = \frac{\gamma_m}{\omega} N_4, \\ L_{i,i-(1+\omega)^3+1} = \frac{\beta_m}{\omega} N_4, \ L_{i,i-(1+\omega)^3+(1+\omega)^4} = \frac{\alpha_m}{\omega} N_4, \\ L_{i,i-(1+\omega)^3+(1+\omega)^2} = \frac{\theta_m}{\omega} N_5, \ L_{i,i-(1+\omega)^4+(1+\omega)} = \frac{\beta_m}{\omega} N_5, \\ L_{i,i-(1+\omega)^4+(1+\omega)^3} = \frac{\gamma_m}{\omega} N_5, \ L_{i,i-(1+\omega)^4+(1+\omega)^4} = \frac{\theta_m}{\omega} N_5. \end{cases}$$

Since we are studying the first passage extinction events, the elements corresponding to a state  $S_i$  where at least one species is extinct (absorbing state) are

$$L_{i,j} = 0 \tag{2.6}$$

The identity positions in the matrix generator with non-absorbing states are given as follows:

$$L_{i,i} = -\sum_{j} L_{i,j} \text{ (non-absorbing state)}$$
(2.7)

For an absorbing state, the identity positions are given by

$$L_{i,i} = 1$$
 (absorbing state) (2.8)

The first passage problem is formulated as [40]

$$L\tau = \mathbf{e}_{\mathbf{S}} \tag{2.9}$$

S is a fixed absorbing state, and  $\tau$  is the probability of hitting state S. es is a matrix of zeros except the state s, where the value is 1. We define an initial condition  $\mathbf{S}(\mathbf{0}) = (2, 2, 2, 2, 2, 2)$ , solve the first passage problem for a small carrying capacity ( $\omega = 10$ ) to understand the immediate effects of mutation in the first extinction event, and obtain the probabilities corresponding to the initial condition hitting an absorbing state. For the first passage time problem, we obtain the exact time of extinction for a non-absorbing state by setting  $e_{S_i} = -1$  where  $S_i$  is a set of all absorbing states (in our case, states that represent extinction). Given the computational complexity of the first passage problem, with the infinitesimal matrix operator containing elements of the order ( $10^5 \times 10^5$ , depending on our choice of  $\omega$ ), we perform a LU Decomposition [55] of the following type:

$$L = P^{-1}L'U'Q^{-1}$$

$$P^{-1}L'U'Q^{-1}\tau = e_{S}$$

$$L'U'Q^{-1}X = Pe_{S}$$

$$\tau = QU'^{-1}L'^{-1}Pe_{S}$$
(2.10)

This method of LU decomposition factorizes sparse matrix into a unit lower triangular matrix L, an upper triangular matrix U, a row permutation matrix P, and a column permutation matrix Q. We solve the first passage problem for two cases, with and without mutation, and plot the difference in probabilities to understand the effect of mutation during extinction events.

#### 2.3 Results

All the results visualized in this section involve the five species starting their journey from a coexisting state. In Subsection 2.4, we visualize the outputs of our Gillespie algorithm under varying circumstances. We then draw observations from them and compare the Gillespie simulations with cyclic mutation and without cyclic mutation. In Subsection 2.5, we analyze the mean-field behaviour of our model and show their agreement to our Gillespie Simulations. In Subsection 2.6, we visualize the probabilities under the first passage extinction problem for the ecosystem with a carrying capacity of 50 members. We again start from a coexisting state and derive the exact probabilities of the first extinction. We then compare the first passage problems for cases with and without mutation and draw our observations from the same. Finally, we check the agreement between the first passage problem and the Gillespie algorithm using correlation plots.

Throughout all our simulations and first-passage formulations, we have used the following rates across all species: ( $r_i = r = 1$ ,  $\alpha_p = 0.11$ ,  $\beta_p = 0.14$ ,  $\gamma_p = 0.08$ ,  $\theta_p = 0.11$ ,  $\alpha_m = 0.1$ ,

 $\beta_m = 0.3$ ,  $\gamma_m = 0.2$ ,  $\theta_m = 0.4$ ). All of the values corresponding to the predation and mutation have been normalized by the single-species carrying capacity of our population.



**Figure 2.2** Simulations obtained from long-term Gillespie simulations with Initial condition  $S_0 = (2, 2, 2, 2, 2)$ . **a.** Long-term Gillespie simulation for  $\omega = 9$  without mutation. **b.** Long-term Gillespie simulation for  $\omega = 30$  without mutation. **c.** Long-term Gillespie simulation for  $\omega = 9$  with mutation. **d.** Long-term Gillespie simulation for  $\omega = 30$  with mutation. We can observe that in the case without mutation, one species of the population survives, whereas in the case of mutation, we find various species of the population co-existing with each other.

## 2.4 Gillespie Simulations

Figure 2.2 represents the Gillespie simulations for five-species models. Figure 2.2(a) and Figure 2.2(b) represent the long-range dynamics for the ecosystem with  $\omega = 30$  and  $\omega = 9$  for the case without mutation, respectively. Figure 2.2(c) and Figure 2.2(d) represent the long-range dynamics for the ecosystem with  $\omega = 30$  and  $\omega = 9$  for the case with mutation, respectively. We observe that cyclic mutation promotes co-existence in a system. Even if a

species count drops to zero, cyclic mutation ensures that the same species can resurface and thrive among the population. Extinction is imminent in the case without mutation, with a single species surviving long term. In the case where cyclic mutation exists, extinction is imminent, yet the chance of long-term survival is possible for multiple species. With our cyclic mutation, it is equally likely for Species A to go extinct at time  $t_i$ , Species B to mutate to Species A at time  $t_j$  where  $t_j > t_i$ , and the population for A to spike up. It is also equally likely (unlike an ecosystem where cyclic mutation is absent) for species already facing a an abundance in population to plunge into extinction. Our Gillespie simulations suggest that the five-species model without mutation follows a transient behavior. In the case of mutation, it is evident that we do not reach a transient behavior and the population dynamics keep evolving. It is also intriguing that the long-term simulations of a system with cyclic mutation include burst phases, where the population from a species undergoes a burst with a steep population increase in a short time and plunges towards extinction later due to the effect of mutation.

Figure 2.3 represents the short-term Gillespie Algorithm for  $\omega = 9$  for two different initial conditions:  $S_1 = (2, 2, 2, 2, 2)$  and  $S_2 = (7, 7, 7, 7, 7)$  for both ecosystems with and without mutations for a shorter period to make the unit changes more evident. The change in initial conditions makes an evident difference in the condition where the mutation is absent, pushing the species extinction at t < 10. When the mutation is present, the initial condition plays little role as mutation introduces more stochasticity into the system causing random species burst, extinction events, etc. While it is evident from Figure 2.4 that mutation promotes co-diversity, it is intriguing to understand under what conditions does extinction events take place when mutation is present, and how does this differ from a case where mutation is absent. Understanding the difference between the states of the population during the first extinction event with and without mutation can help us determine if mutation effectively helps avoid the extinction of other species. We analyze this in the first passage problems in Section 2.6.

## **2.5 ODE model of the interacting five species ecosystem**

We aim to to understand the mean-field dynamics of the system in this section as ODEs provide us a mathematical model for predicting system behaviour over time. While the ODE cannot provide us state-wise extinction parameters, it is crucial to check the agreement of our ODE with our simulations to ensure similarity in system behaviour. Solving ODEs can help us understand system behaviour and help us choose appropriate rates to conduct our simulations and first-passage problems. The ordinary differential equations corresponding to rate equations of the five species RPS model (see Eqn. (1) in the main text) are shown below. The parameters  $\alpha_p$ ,  $\beta_p$ ,  $\gamma_p$ ,  $\theta_p$  correspond to heterocidal predation while the terms  $\alpha_m$ ,  $\beta_m$ ,  $\gamma_m$ ,  $\theta_m$  correspond



**Figure 2.3** Simulations obtained from short-term Gillespie simulations with  $\omega = 9$ . **a.** Short-term Gillespie simulation for initial state (2, 2, 2, 2, 2, 2) without mutation. **b.** Short-term Gillespie simulation for initial state (7, 7, 7, 7, 7) without mutation. **c.** Short-term Gillespie simulation for initial state (2, 2, 2, 2, 2) with mutation. **d.** Short-term Gillespie simulation for initial state (7, 7, 7, 7, 7) with mutation. We observe a higher initial condition leading to a slower overall extinction in the case without mutation. With mutation, we observe multiple surges and plunges of population corresponding to various species.

to mutation. The coefficient of birth rate is denoted as r. The rate of change of size of each sub-population is reduced by 2nd-degree (in sub-population size) heterocidal and homocidal predation terms. The rate also increases from birthing and cross-mutation terms and decreases from self-mutation terms all of which are of degree one in sub-population size.



**Figure 2.4** First passage extinction probabilities: 2-Dimensional. Probabilities of the initial state (2, 2, 2, 2, 2, 2) to be found at the following states during the first extinction event.  $P_abs$  represents the first-passage extinction probability. It can be noticed that the probability diminishes as the difference in the initial state and the possible extinction state increases indicating that it is less probable to find a state with rapid evolutionary dynamics during a first extinction event.

$$\begin{aligned} \frac{da}{dt} &= a(r - \frac{2}{\omega}a - \frac{\alpha_p}{\omega}b - \frac{\beta_p}{\omega}c - \frac{\gamma_p}{\omega}d - \frac{\theta_p}{\omega}e) + \frac{\theta_m}{\omega}b + \frac{\gamma_m}{\omega}c + \frac{\beta_m}{\omega}d + \frac{\alpha_m}{\omega}e - (\frac{\alpha_m + \beta_m + \gamma_m + \theta_m}{\omega})a \\ \frac{db}{dt} &= b(r - \frac{2}{\omega}b - \frac{\theta_p}{\omega}a - \frac{\alpha_p}{\omega}c - \frac{\beta_p}{\omega}d - \frac{\gamma_p}{\omega}e) + \frac{\alpha_m}{\omega}a + \frac{\theta_m}{\omega}c + \frac{\gamma_m}{\omega}d + \frac{\beta_m}{\omega}e - (\frac{\alpha_m + \beta_m + \gamma_m + \theta_m}{\omega})b \\ \frac{dc}{dt} &= c(r - \frac{2}{\omega}c - \frac{\gamma_p}{\omega}a - \frac{\theta_p}{\omega}b - \frac{\alpha_p}{\omega}d - \frac{\beta_p}{\omega}e) + \frac{\beta_m}{\omega}a + \frac{\alpha_m}{\omega}b + \frac{\theta_m}{\omega}d + \frac{\gamma_m}{\omega}e - (\frac{\alpha_m + \beta_m + \gamma_m + \theta_m}{\omega})c \\ \frac{dd}{dt} &= d(r - \frac{2}{\omega}d - \frac{\beta_p}{\omega}a - \frac{\gamma_p}{\omega}b - \frac{\theta_p}{\omega}c - \frac{\alpha_p}{\omega}e) + \frac{\gamma_m}{\omega}a + \frac{\beta_m}{\omega}b + \frac{\alpha_m}{\omega}c + \frac{\theta_m}{\omega}c - (\frac{\alpha_m + \beta_m + \gamma_m + \theta_m}{\omega})d \\ \frac{de}{dt} &= e(r - \frac{2}{\omega}e - \frac{\alpha_p}{\omega}a - \frac{\beta_p}{\omega}b - \frac{\gamma_p}{\omega}c - \frac{\theta_p}{\omega}d) + \frac{\theta_m}{\omega}a + \frac{\gamma_m}{\omega}b + \frac{\beta_m}{\omega}c + \frac{\alpha_m}{\omega}d - (\frac{\alpha_m + \beta_m + \gamma_m + \theta_m}{\omega})e \end{aligned}$$

The set of equations has one trivial fixed points:  $FP_1 = (0, 0, 0, 0, 0)$  and the non-trivial fixed point:  $FP_2 = (\frac{r\omega}{\alpha_p + \beta_p + \gamma_p + \theta_p + 2})(1, 1, 1, 1, 1)$  where the 5 species coexist with the same population density. For the sake of brevity, r is taken as 1, and the conditions  $\alpha_p = \beta_p = \gamma_p = \theta_p = \alpha$  and  $\alpha_m = \beta_m = \gamma_m = \theta_m = \beta$  are applied. Under these conditions, the fixed point (0,0,0,0,0) is globally unstable (the stability is not shown here). Now we will check the stability of the non-trivial fixed point, the coexistence steady-state whose *Jacobian* is shown below.

$$\begin{bmatrix} -\frac{4\beta}{\omega} - \frac{2}{4\alpha+2} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{4\beta}{\omega} - \frac{2}{4\alpha+2} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{4\beta}{\omega} - \frac{2}{4\alpha+2} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{4\beta}{2\alpha+2} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} \\ -\frac{\alpha}{4\alpha+2} + \frac{\beta}{\omega} & -\frac{\alpha}{4\alpha$$

The eigen values of the matrix above are -1,  $\frac{-20\alpha\beta+\alpha\omega-10\beta-2\omega}{4a\omega+2\omega}$ . Therefore, for  $-10\beta(2\alpha + 1) + \omega(\alpha - 2) < 0$ , the coexisting steady-state is a stable node .i.e, for  $\alpha <= 2$ , this fixed point is stable for all values of  $\beta >= 0$ . However, if  $\alpha > 2$  the system is unstable around the aforementioned equilibrium point for certain non-negative values of  $\beta$ . This bifurcation around  $\beta$  is discussed in Figure 2.5. With increasing predation parameter, the bifurcation line faces an upward shift owing to species domination. The bifurcation line across the mutation-predation space represented in 2.6 is piecewise and with reducing carrying capacity, moves downward attributing to the fact that with lesser resources, every other species except for one is bound to go extinct. For parameter tuples from the stable region of parameter space, numerically, the system was observed to eventually converge to the fixed point calculated above irrespective of the starting point. However, for parameter values from the unstable region of the parameter space, the system appeared to converge to different steady states which are represented through phasic bursts in Figure 2.7. We will explore this behavior in the near future.

For varying carrying capacities, we also vary the  $\alpha - \beta$  parameters to obtain the bifurcation points in the cyclic mutation-predation plane. Figure 2.6 represents the stability diagram as a function of  $\alpha$  and  $\beta$  for three different carrying capacities. We observe a downward shift of the unstable region for non-negative values of  $\alpha$  and  $\beta$  with a reduction in the carrying capacity.

In our endeavor to replicate the outcomes derived from stability analysis, we turn to Gillespie simulations. As depicted in Figure 2.7, we present the outcomes of Gillespie simulations across a spectrum of mutation rates, focusing on a singular predation rate and carrying capacity. With increasing mutation rates, we find our system going to more stable conditions with phasic bursts of population ensuring the same density average over timesteps. As our mutation rate increases, the time period of the phasic bursts reduces. Hence, our system becomes more chaotic, yet, the overall species density remains the same. However, our findings point towards the emergence of instability in the ordinary differential equations (ODEs) owing to the dominance of a single species. Upon elevating the mutation rate, we observe an increase in the frequency of peaks across multiple species, giving rise to co-existing states. In these states, multiple species exhibit recurrent fluctuations in population, characterized by pronounced bursts and declines. These population dynamics can be interpreted as a collective oscillation of the overall species count around a shared sub-population size. This phenomenon signifies a convergence into a non-zero state, ultimately leading to the establishment of a stable converging fixed point in the stability analysis conducted for the ODEs.

### 2.6 First Passage Probability and Time

While mutations through the eyes of simulations have been extensively studied, it is crucial to understand at what states does the actions of mutation kick in, and in what states are species endangered beyond the purpose of mutation. Hence, it is useful to formulate the exact analytical solutions of extinction probability and time for various states to better understand the mechanism of mutation. We formulate a small-scale first passage problem with the carrying capacity of every species  $\omega = 9$ . With a coexisting state  $S_0$ , we obtain the probabilities of  $S_0$  reaching an absorbing first extinction state,  $S_e$ . Figure 2.4 represents the extinction probabilities for the following fixed conditions: one species goes extinct, two are fixed, and two are variable. The intensities of the probabilities are represented using the size of the circles. Figure 2.4 can be read as follows: the probability of the initial state  $S_0 = (2, 2, 2, 2, 2)$  reaching the state  $S_i = (x, 0, y, a, b)$ . We scale this up to three dimensions to get a better observation. Figure 2.8 represents the extinction probabilities in 3-D.

We now use this visualization method for the probabilities obtained from the first passage problem for cases with and without mutation. We compare both cases by subtracting the respective state probabilities for conditions with and without mutation and representing them in the same graph. We notice from Figure 2.8. that combining our constants and variables in any possible way gives us symmetric outputs. This indicates that our cyclic process of mutation and predation combined with our birth process results in symmetric first-passage probabilities. Similarly, it can be inferred from Figure 2.5. that the probabilities reduce from our initial state of coexistence symmetrically across all the remaining variations of  $N_1, N_3, N_4, N_5$ . This is precisely the results obtained from Barendregt et al. which indicated the 5-species model is an extension of the Rock-Paper-Scissors model [40]. Moreover, it can also be inferred from Figure 2.9. that it is more likely to find the first extinction state, closer to the initial state  $S_0$ , when mutation exists. An ecosystem without mutation will likely experience a first extinction event when other species in the environment are endangered or close to extinction. This is evident from the probability differences in Figure 2.9. near the regions  $N_1, N_2, N_5 = (0, 0, 0)$  where probabili-

ties in a case without mutation highly exceed that of a case with mutation indicating that it is likely to find  $N_1, N_2, N_5$  close to extinction when the first extinction event takes place. Furthermore, there is a high probability in the case of mutation to observe first extinction events when  $N_1, N_2, N_5 > (2, 2, 2)$  (initial state), indicating that mutation aims at diversifying the population among species, compared to that of an ecosystem without mutation and plays a major role in the coexistence of species. It can also be observed that it is as unlikely to find the first extinction event occurring at a state  $S'_e$  such that  $|S_0 - S'_e| > \epsilon$  derived from the fact that mutation, a gradual genetic change, is ill-suited for rapid transformation in real-time environments. In such dynamic settings, immediate adaptation is crucial, necessitating mechanisms other than slow mutation to cope with swift changes and maintain competitiveness. Hence, extinction probabilities in such circumstances are similar to those of an ecosystem where mutation is absent. We formulate the first-passage extinction probabilities for a non-uniform initial condition in Section 2.7. We observe that there is a general trend for systems without mutations to have a higher probability to exist in an endangered state compared to that of a system with mutations. Moreover, A system with mutation is likely to experience an increase in first extinction time as the overall species count in an ecosystem increases. This can be observed from Figure 2.10. While there is a spike in the number of states where mutation slows first extinction  $(S_m)$  near  $N_i = 1$ , there is a dip as we progress towards  $N_i > 2$ , attributing to the fact that stochastic pathways with mutation lead to extinction faster due to lack of diversity among species. But as the species count and diversity of the ecosystem increases, there is a huge surge in the number of states where the first extinction event is slower when mutation is present. This is evident with the surge we observe in regions  $N_i > 6$  of Figure 2.10. We find that even when mutation is present, there needs to be a minimum co-existing state of the population for mutation to increase first extinction time, and that, it is not in all cases that mutation moves a population away from an extinction event. We validate our inferences by comparing the correctness of our first-passage problem with Gillespie Simulations. Figure 2.11 shows the correlation plot between the first-passage problem probabilities and Gillespie simulation probabilities for the first extinction event represented Equation 2.10. Both cases show good agreement given that both have an R2 score  $\geq 0.97$ . Due to denser matrices and larger matrix sizes, the exact solutions of the first passage problem for  $\omega \gtrsim 10$  become intractable.

## 2.7 Initial Conditions in First-Passage problems

In our formulation of the first-passage problem, the solutions for the extinction distribution obtained for a uniform initial state. In this section, we vary the initial state to follow a non-uniform initial condition and extract the first-passage probabilities for the new initial states.

Our new non-uniform initial state, labelled by  $\mathbf{S}'$  follows the species distribution: (2, 6, 2, 2, 2). Figure 2.12 represents the conditional probability distribution given a first extinction event occurs for a species. Change of conditional probabilities across species still remain symmetrical with respect to the change of population of single species with the peak at the closest hyperplane with respect to the initial condition. An analog of Figure 2.9 for  $\mathbf{S}'$  has been shown in Figure 2.13. Within this comparative framework, we observe a general trend; a system devoid of mutation exhibits a higher probability to linger around an endangered state space (characterized by a species population less than 2) - more visible when a non-uniform initial condition is taken and near the vicinity of the initial condition. Furthermore, in comparison to our uniform formulation, we observe fewer red spots in states characterized by increased coexistence. This suggests that a higher species count facilitates the transition towards a more coexisting state when the first extinction event takes place.

#### 2.8 Discussion

This work introduces mutations in five-species models and performs first-passage formulation to obtain exact state-wise probabilities for the first extinction event. We demonstrate the use of cyclic mutations and employ them mathematically in an infinitesimal matrix generator to observe more nuanced differences during the first extinction event. It is to be noted that works including Kang *et al.* [56] and Vukov *et al.* [57] motivated us to construct mean field ODE equations (see the Appendix A) of five species model. While they have investigated the coexistence of species from the perspective of multiple invasion rates, our study focuses on the extinction for a single parameter through the lens of varying initial conditions.

Furthermore, our mean-field approach varies the  $\alpha - \beta$  (mutation - predation) parameter space as opposed to the cyclic predation parameters to observe the boundary between extinction and stable states where species ideally oscillate across a fixed point. We hope to study co-existence along with a joint perturbation across various cyclic domains of both mutation and predation in our further studies. When compared to the range of models dicussed in [58], our model assumes a cyclic mutation where each species mutates to the other. The study operates on spiral-generating lattices including migration to study the effects of mutations. In our study, we do not take into consideration the spatio-temporal dynamics of the system, but rather, understand the behaviour of the system from the perspective of extinction and co-existence. Unlike the stability analysis presented for generic RPS systems with mutations where stability in the predation-birth space was explored, we provide stability analysis in the predation-mutation space for uniform cyclic parameters. We find through the Gillespie simulations that cyclic mutation promotes co-existence among the population and promotes population diversity. We also observe that population bursts occur frequently, in a phased manner, when mutation exists. We also uncover that mutations offer more diverse and robust pathways to a first extinction event, preventing further species endangerment and providing room for coexistence compared to an ecosystem where mutation does not exist. We observe that it is not always the case that mutation extends our first-extinction time. There is a sudden increase of the number of states where mutation extends the first-extinction time near the endangered states, followed by a dip, and then a rise, as the population reaches co-existing states. We also uncover symmetric extinctions in first-passage problems of five-species models, indicating that they are extensions of three-species models with birth and cyclic predation.

In our simulations, we observe population size oscillations rather than full extinction, as mutation reactions make the underlying Markov chain irreducible. Our first-passage probabilities are symmetric across various combinations of our constants, reflecting the uniform cyclic parameters used in our rate equations. The trend of sudden increase, and dip, followed by a rise again in our first-passage extinction times can be attributed to more stochastic pathways leading to a reduction in population (with contributing actions being mutation and predation) are higher than proliferation pathways in the set of states where the dip is observed. Once the population reaches a non-endangered, and co-existing state the effects of mutations are observed more effectively, as it drives our population away from a first extinction event. In both our scenarios with and without mutations, our formulations show near-perfect agreement with our Gillespie simulations.

#### 2.9 Limitations

Although we obtained exact results using first-passage formulation, our studies were limited to small carrying capacities only. The fact is that increasing the single-species carrying capacity, even by a small factor, rapidly increased the size of our infinitesimal matrix generator (L), and reduced the sparsity of our matrix. Hence, after a small carrying capacity, it was impossible to carry out LU decompositions of our matrix. Moreover, in a real-world scenario, extinction only occurs in a given probability, and hence, the absorbing states are confined by a probability which is not taken into account in the first-passage formulation. For larger systems, thousands of simulations to estimate extinction probability for a given set of parameters can take hours. Hence, a Machine Learning formulation which can extrapolate to data points is more suitable for studying extinction events. Finally, through first-passage formulations and time-based sampling of the Gillespie simulation, it become impossible to study the evolution of the system. Hence, an ML approach based upon step wise lattice evolution is more suited for our purpose of studying spatio-temporal evolution of a system.



Figure 2.5 Stability diagram and time signals as a function of  $\omega$  and  $\beta$ .(a-b) The light red color demarcates the unstable regime of  $Fp_2$  ( $\alpha = 2.3$  and  $\alpha = 2.6$  respectively). The blue area represents the stable parameter space of the same. (c) Time series of the system for a point (marked by X in (a)) from the stable region of the parameter space for  $\alpha = 2.3$ . (d) the time series of the system for a point (marked by O in (a)) from the unstable region. Similarly, for  $\alpha = 2.6$  (e) and (f) correspond to the time series of the system for a point in the stable region and unstable region of the parameter space, respectively. Clearly, if we increase the predation term ( $\alpha$ ), the stable region decreases (light blue).



Figure 2.6 Stability diagram as a function of  $\alpha$  and  $\beta$ . For non-negative values of mutation and predation parameters, we observe a downward shift of unstable region indicating that for a lower carrying capacity, smaller values of mutation enforces the system towards a more stable behaviour where all species converge around a specific point.



Figure 2.7 Gillespie Simulations: For  $\omega = 50$  and  $\alpha = 2.6$  and  $\beta$  varying accross (a): 0, (b): 0.1, (c): 0.3, (d): 0.7, (e): 1.0, (f): 1.5. With increasing mutation rates, we find frequent population bursts accross multiple difference species which is in correspondence to our ODE results.



**Figure 2.8** First passage extinction probabilities ( $P_{abs}$ ): 3-Dimensional. Probabilities of the initial state (2, 2, 2, 2, 2) to be found at the following states during the first extinction event. It can also be noticed that extinction occurs symmetrically across all 3-D graphs.



Figure 2.9 First passage problem extinction probabilities ( $P_{abs}$ ), mutation comparison, Configuration 2 ( $N_5$  fixed,  $N_2 = 0$ , ( $N_1$ ,  $N_3$ ,  $N_4$ ): Variable; 3-Dimensional. Red Spheres represent that the difference in first passage probabilities between the cases of mutation and without mutation is negative. The blue spheres represent that this probability is positive.



Figure 2.10 First passage extinction times: Number of states where an ecosystem with mutation leads to a slower first extinction than an ecosystem without mutation. Three variables  $N_1, N_3, N_5$  are variables across the x and y axis under various line plots. The sum of states under these settings are taken where the difference in extinction times without and with mutation is positive.



**Figure 2.11** Correlation between the extinction probabilities of 1e6 Gillespie simulations ( $P_G$ ) and first passage problem ( $P_F$ ) without (a) with R2 score 0.97 and with mutation (b) with R2 score 0.99.



**Figure 2.12 First passage extinction probabilities: 3-Dimensional**. Probabilities of the initial state (2, 6, 2, 2, 2) to be found at the following states during the first extinction event. It can be noticed that the probability diminishes as the difference in the initial state and the possible extinction state increases indicating that it is less probable to find a state with rapid evolutionary dynamics during a first extinction event.



**Figure 2.13 First passage extinction probabilities: 3-Dimensional**. Probabilities of the initial state (2, 6, 2, 2, 2) to be found at the following states during the first extinction event. It can be noticed that the probability diminishes as the difference in the initial state and the possible extinction state increases indicating that it is less probable to find a state with rapid evolutionary dynamics during a first extinction event.

#### Chapter 3

#### **Machine Learning for System Behaviour Prediction**

The subsequent sections of this chapter are arranged as follows: we describe our algorithm for lattice-based simulation in Section 3.1 and the theory behind our ML work in Section 3.2. We then describe the tasks performed in Section 3.3. The results of the tasks along with the data and model hyperparameters is presented in Section 3.4, and Section 3.5. Finally we conclude with discussion of the results and outlook in Section 3.6.

## 3.1 Lattice-based Simulation

For the third chapter of our thesis, we model the three-species ecosystem as a stochastic process with birth, predation, and migration as stated in Reichenbach et al. [23]. We perform a Lattice based Monte-Carlo Simulation which is restricted to the lattice using Periodic Boundary Conditions to emulate the spatio-temporal dynamics of the system. The rate equations have been provided in Equation 3.1. Migrations can be interpreted as mutations in a lattice which preserves density in a lattice and prevents species resurfacing. A schematic diagram on lattice for the respective actions have been provided in Figure 3.1. For various  $M_r$ , the patterns formed have been visualized in Figure 1.3.

$$A_{i} \longrightarrow 2A_{i} \text{ (with rate } r \text{ Birthing), i=(0,1,2)}$$

$$A_{i} + A_{(i+j)\%3} \longrightarrow A_{(i+j)\%3} \text{ (with rate } p : \text{Predation), i = (0,1,2) and j=(1,2,3)}$$

$$A_{i} + A_{(i+j)\%4} \longrightarrow A_{(i+j)\%4} + A_{j} \text{ (with rate } M_{r} : \text{Exchange), i = (0,1,2) and j=(1,2,3)}$$

$$A_{i} + \phi \longrightarrow \phi + A_{i} \text{ (with rate } M_{r} : \text{Exchange)} \text{ (3.1)}$$

Our lattice simulation algorithm is as follows. We initialize a lattice with a uniform distribution of all the three species and vacant sites. For each Monte Carlo (MC) time step, we obtain a random configuration of lattice sites. We iterate over this order, choose a sample a random



**Figure 3.1** Schematic diagram for actions on lattice. Predation removes a species according to the cyclic predation order. Birthing results in a neighboring species giving birth to its offspring in a vacant site. Migration results in a species exchanging its lattice site with a neighboring species.

action sampled through the Gillespie algorithm given the rates, and perform the action. This way, we evolve the lattice for T Monte Carlo timesteps. In one Monte Carlo timestep, every entry in a lattice is randomly updated by randomly sampling one action (with the probability of choosing being directly proportional to the rate of the action) for every non-vacant entry in the lattice. We set r = 1 and p = 1 and chose an arbitrary migration rate  $M_r$ . We then normalize these values  $r' = \frac{r}{r+p+M_r}$ ,  $p' = \frac{p}{r+p+M_r}$  and  $M'_r = \frac{M_r}{r+p+M_r}$  and simulate lattice using the above algorithm. For varying migration rates with multiple initial conditions, simulations become redundant as multiple initial conditions must be chosen to observe long-term behaviour and generalize. This is because, the long-term behaviour of the above system varies for different  $M_r$  and there is a probability distribution with which species survive, as explained in Chapter 1. Analytically, this probability curve can be predicted [23]. Here, we want to explore an alternative framework. Hence, to reduce the redundancy of time-taking simulations with varying initial conditions, and learning a survival probability distribution for varying migration rates, and hence, faster long-term prediction, we employ Machine Learning. We know in suitable diffusion, we will obtain spiral pattern in 2D space (see Fig 1.3, where migration rates are 1,8,15, and 22). The more we increase the migration the spiral becomes larger (see figure 1.3). For higher migration rates, after crossing the critical diffusion, the species will go to extinction [9, 33]. Here we raise a precise question: Can we predict/forecast the future evaluation of the spiral pattern? In particular, we are able to show that CNN based ML technique can predict the future evaluation of spatiotemporal pattern of RPS dynamics, In the next section we describe the basic principles around CNN. Multiple realizations with varying migration rates  $(M_r)$  are taken as datasets for the Machine Learning tasks to train the CNNs presented in this

paper. With respect to the rate equations and the system presented in Equation 3.1, Figure 1.3 represents the evolution for various migration rates,  $M_r$ .

## 3.2 Convolutional Neural Networks

Convolutional Neural Networks (CNNs) are variants of feed-forward neural networks which are designed to handle images, and information where spatial and temporal stream of data decide the outcome of the task. CNNs are typically used for image data including tasks like classification [59–61], segmentation [61–63], and image generation [64–66]. In feed-forward neural network of L layers, each layer has  $N_l$  neurons which are connected to the next layers of neurons  $N_{l+1}$  through weights  $W_l$ . Simply, multiplying the weights  $W_l$  and activations  $A_{il}(i = (0, ..., N_l))$  provides us  $A_{i(l+1)}(i = (0, ..., N_{l+1}))$ . Typically, learnable kernels replace weights in feed-forward networks. These learnable kernels are just 2-D versions of weights W present in feed-forward neural networks. An Image contains of N \* M pixels, which are treated as feature blocks. These feature blocks act as 2-D neurons which are then operated by the kernel to create feature block for the next layer. The kernels are convoluted (instead of multiplied) with existing feature blocks as follows. Given a multi-channel feature f as an input, the convolution operation for a given kernel h is defined as follows:

$$G[m,n] = (f*h)[m,n] = \sum_{j} \sum_{k} h[j,k] \times f[m-j,n-k]$$
(3.2)

where G is the resultant matrix and  $\times$  is multiplication. If we want to use multiple feature maps of varying sizes as inputs, we may pad the image to have uniform image sizes across all images. Convolutions are usually performed in a strided format with each convolution occuring over specific stride length given by s. Given a kernel, s decides how many units to shift the kernel after each step of the convolution. If p is the padding used, and  $n_c$  is the number of channels in an image and n is the size of the image, and if our kernel has  $n_f$  filters, the convolution operation results in the output of the following size:

$$[n, n, n_c] * [f, f, n_c] = [\lfloor \frac{n+2p-f}{s} + 1 \rfloor, \lfloor \frac{n+2p-f}{s} + 1 \rfloor, n_f]$$
(3.3)

The resultant matrix G as mentioned in Equation 3.2 is used as the new feature set on which new set of kernels are used to perform convolution. Kernel sizes may be choosen to downsample or upsample for the existing feature set. For tasks involving image generation, both upsampling and downsampling kernels are used. For tasks involving classification, kernels

are used to downsample images and feature maps. Post the convolution operation, typically, to generalize local features in a region accross a feature set, we use pooling by extracting particular values in a partition of a feature set through a selection operation as follows:

$$G[i, j] = S_{(k-0, k-1, \dots, M/q), (k-0, k-1, \dots, N/q)}(A_{(qi-k, qj-k)})$$
(3.4)

The operator S can perform max pooling, mean pooling, sum pooling, etc. We use batch normalization and activation functions to tackle exploding gradients. For example, if we have a feature set F of shape  $150 \times 150 \times 3$  and we use a downsampling operation to perform max pooling operation of size  $2 \times 2$ , for every  $2 \times 2$  block in our feature set F, the maximum value is selected, and the resulting feature set is  $75 \times 75 \times 3$ . This way, we obtain the global features from more scattered low-level features in a map. For tasks involving lattice pattern generation, we can select kernels such that the output feature map is of the same shape as input feature map. For tasks including classification, we may flatten 2-D feature maps into a 1-D feature set, and treat each of these features just like neurons in feed-forward networks and apply more layers to the feed-forward neural network for classification. For the purpose of Image generation we use a special class of CNNs called UNets which can output a 2-D image (feature map). For classification purposes, we use a simple CNN classifier, where after few convolution blocks, the 2-D feature maps are flattened as mentioned above. An overview of the CNN Architecture is presented in Figure 3.2.



**Figure 3.2** A summary of CNN operations. Given an input image and a feature map, a visual representation of convolutions, pooling, flattening, and feed-forward network.



**Figure 3.3 (a)**. U-Net Architecture. (i) Each block consists of a Conv Layer, followed by a Batch Norm, Max Pooling layer, and a ReLU non-linear activation. For each Conv block, we have downsampling kernels of shape 64, 128, 256, 512, post which upsampling occurs in the reverse order. (b). CNN architecture. With N = 5, we have kernels 32, 64, 128, 256, 512. Our flattening layers downsamples each feature vectors into 256, 128, 64, and 2 post flattening followed by a softmax activation for binary class probabilities.

#### 3.2.1 U-Nets

U-Nets are a special class of CNNs used for tasks like map generation and image segmentation. Pooling operations are performed followed by upsampling operators. [47] These upsampling operators are responsible for improving the resolution of the output by merging embeddings downsampling layers. This residual connection helps the model construct maps using the local features of an image which are learnt during earlier convolutional layers. The U-Net model used by us is represented in Figure 3.3(a).

#### 3.2.2 CNN Classifier

Given an image I, a binary classifier module consists of multiple downsampling modules followed by a flattening layer which converts feature maps into dense embeddings. These flattened layers are further downsampled to smaller feature vectors as shown in Figure 3.3(b). Followed by this, we apply a softmax operation to convert the output layer's values to probabilities. These probabilities represent the classification output for our downstream task [67].

#### 3.2.3 Dropout

Randomly switching off some neurons in CNNs and nullifying their contribution to the output can help prevent overfitting of data, and generalize posterior distribution by creating ensemble of networks by randomly switching across different neuron combinations [68, 69]. Moreover, for tasks in which data is stochastic, we can learn a variable predictive distribution that emulates the stochasticity in our real-world data. During evaluation, multiple predictions can be made across various ensembles and the mean across the predictions can be estimated as the model output, and its variance can be estimated as the model uncertainty corresponding to the data point.

#### 3.3 Tasks

Our tasks aim at introducing Machine Learning for spatio-temporal forecasting and longterm system behaviour prediction for RPS systems. We perform two important tasks: image generation by future forecasting and long-term survival prediction which has not been performed using Machine learning. Future behaviour of spirals have not been estimated from a distribution perspective through the eyes of Machine Learning, and we attempt to forecast spiral behaviour using our MC data for various downstream tasks using CNNs and U-Nets.

#### 3.3.1 Lattice Pattern Generation

Single Migration rate: For a single migration rate  $(M_r)$ , we vary the initial configuration for every simulation and provide our U-Net model a random configuration at timestep t. We then ask our U-Net to predict the configuration at timestep  $t + \delta t$ . We then input the output of our U-Net predictions as an input to itself to perform a to predict lattice for  $t + 2\delta t$ . We extrapolate the prediction timestep  $t_p > t_e$  where  $t_e$  represents the latest data MC time stamp provided to our model during training. We compare the time evolution of the lattice of U-Net and an original configuration.

Multiple Migration rate: For multiple migration rates  $(M_1, M_2, ..., M_k)$  we generate multiple MC simulations. Given a random configuration at timestep t, we ask our U-Net to predict the approximate lattice configuration at timestep  $t + \delta t$ . For this downstream task, the U-Net completely relies on two factors: the current MC step pertaining to the lattice configuration and the migration rate corresponding to the current MC step of the input lattice. We aim to obtain the spiral pattern of  $t + \delta t$  using our UNets.

#### **3.3.2** Species Extinction Prediction and Extrapolation

For multiple migration rates  $(M_1, M_2, ..., M_k)$ , given an ensemble of lattices at MC steps  $(t_{k_1}, t_{k_2}, ..., t_{k_n})$ , we ask our model to predict if the system in the long-term observes extinction: prevelance of a single species over the others. The results of this task can vary across various simulations for a single migration rate  $M_r$ . Hence, during training, we use Dropouts to ensure variability in outputs and calibrate our model to match the simulation distribution. In this task, the binary classification task has two aspects: the migration rate corresponding to the lattice ensembles, forecasting at an MC timestep far away from the input time steps. We train the model in intervals of migration rates and ask out model to extrapolate predictions to unseen regions and analyze model predictions.

In Section 3.4, we visualize the outputs of lattice generation for single migration rate a successive simulation  $\delta t = 20$ . Followed by this, we visualize the immediate lattice generation post  $\delta t = 40$  MC steps for multiple migration rates. In Section 3.5, we draw observations from our classification task. For tasks in 3.3.1, we use the Cross Entropy loss for loss backpropogation. For each pixel in the output image, we calculate the cross-entropy loss corresponding to the simulation ground truth as follows:

$$L_{i} = -\sum_{C} \sum_{i=(0,\dots,N), j=(0,\dots,M)} I(s_{(i,j)}) log(F(s_{(i,j)}))$$
(3.5)

where  $I(s_{(i,j)})$  represents the species present at the (i, j) point in the lattice at time  $t + \delta t$ ,  $s_{(i,j)}$  represents the input pixel, C represents the classes (four in our case including vacant species) and  $F(s_{(i,j)})$  represents the model outputs for the corresponding input pixel and N, M are the length and width of the lattices.

For task in 3.3.2, we use the Binary cross entropy loss which is a reduced form of Cross Entropy loss for 2 classes (0 or 1). Given an image matrix I, prediction  $Y_m$ , and ground truth value obtained from simulation  $Y_s$ , the Binary cross entropy loss is given as:

$$L_{i} = Y_{m} log(1 - Y_{s}) + (1 - Y_{s}) log(Y_{m})$$
(3.6)

The above loss function maximizes loss on increasing difference between  $Y_m$  and  $Y_s$ . Adam Optimizer with learning rate  $10^{-3}$  is used for all the training processes. A learning rate scheduler is also used to reduce learning rate at plateau regions.

#### 3.4 Lattice Pattern Generation

Single Migration rate: 400 MC steps are simulated using single migration with a given update order. The U-Net is trained by pairing any two timesteps with difference  $\delta = 20$ . Our validation set 400 MC steps from simulation with completely different initial conditions. We train the U-Net for 15 epochs and achieve a Cross Entropy loss of 0.07 on our validation set. Fig 3.4(a). visualizes an early stage simulation forming into a spiral pattern completely by our U-Net model in increments of  $\delta t = 20$ . We notice that given a initial condition, for a given migration rate, our model is able to develop the spatio-temporal evolution of the lattice effectively. Figure 3.4(b), shows the lattice at t and  $t + \delta t$  as predicted by our model and simulation respectively. During testing, we also input a terminal timestep to our model (t =360) and make 8 successive predictions till (t = 520). Noting that the model has been only trained on data till (t = 400), We compare the quality of extrapolation of our model with the results obtained from our simulation. We observe accurate results across the lattice generations. However, we observe an increasing distortion between the lattices generated via simulation and U-Net predictions. This is due to increased stochasticity with increasing  $\delta_t$  which results in compounding errors as only image at t is given as input and the model outputs for t + 20, t + 40, t + 60, t + 80 and t + 100 are used as inputs to generate successive time steps.

Multiple Migration rate: 8000 values from a uniformly distributed interval of migration rates  $M_r \in [0.2, 10]$  are extracted from a larger set of  $M_r \in [0.2, 30]$ . MC Simulations for each of these migration values are performed for 650 timesteps, and for each simulation, 5 pairs are

formed between input and output lattices whose difference is  $\delta t = 40$ . From each simulation, we sample 30,000 points are used for training and the rest 10,000 of the data points are used for testing. Figure 3.5 shows the input lattice, U-Net outputs, and the simulation result. The machine learning predictions are accurately able to model the patterns in the target lattice. Moreover, it can be observed that the patterns are generated accurately across various input lattice timesteps. We obtain a Cross Entropy loss of 0.76 when predictions are made through our validation set. However, unlike Task 1, our model is not able to accurately estimate vacant sites as the their density and distribution in the lattice varies across varying migration rates.

#### **3.5 Extinction Prediction: Multiple Migration Rates**

35,000 from a uniformly distributed interval of migration rates  $M_r \in [0.2, 30]$  are extracted. MC Simulations for each of these migration values are performed for 5000 timesteps, and four lattice states at timesteps 500, 800, 1500, 1750 are collected. We then calculate the system density at long-range 4000th timestep. Given these lattice states, we predict if the system goes to extinction in the long-term. We use a CNN with flattening layer and fully connect neural network along with dropouts as described in Figure 3.5. We use Binary Cross Entropy loss across our training batch to minimize our error. We conduct three experiments to analyze the generalization of our model:

Accuracy on validation: We obtain 96 % accuracy in extinction prediction. Furthermore, since class imbalance is prevalent in these tasks, we check the class accuracy for data in our validation set. We obtain 92 % for tasks where extinction occurs.

**Multiple realizations of Single data point:** We split our data into buckets, and for each migration rate, we obtain 250 simulations and long-term ground truths. We then make model predictions using the ensembles from simulations. For each migration rate, we calculate the extinction probability as follows:

$$R_e = \frac{N_e}{N_e + N_{ne}} \tag{3.7}$$

where  $R_e$  is the extinction probability and  $N_e$  is the number of realizations for a single migration rate where extinction occurs and  $N_{ne}$  is the number of realizations for a single migration rate where species survive long-term. Figure 3.6(a) shows the plot for  $R_e$  versus migration rates for results obtained simulations and model predictions. The results match to a great extent, but diverges towards larger migration rates due to class imbalance. **Model Extrapolation:** We modify our dataset to include migration rates only from certain intervals. The other intervals are then used for testing purposes. Figure 3.6(a) shows the plot for  $R_e$  versus migration rates for all intervals. For positive points where extinction occurs, we obtain an accuracy of 80 % by tuning dropouts and an overall accuracy of 93 %. We observe a slight dip in accuracy due to the large length of validation intervals used to test prediction extrapolation.

## 3.6 Discussion

The results presented in this paper demonstrate the efficacy and limitations of utilizing machine learning techniques, specifically U-Net and CNN models, for lattice generation and extinction prediction tasks in complex systems governed by migration rates. In Subsection 3.4, we focused on single migration rate scenarios, where our U-Net model showed remarkable performance in predicting lattice evolution over successive time steps. Despite being trained on data up to a certain time point, our model exhibited the ability to extrapolate beyond the training range, capturing the underlying dynamics of lattice formation accurately. However, as the prediction horizon extended, we observed increasing distortions between simulated and predicted lattices due to the accumulation of stochasticity and compounded errors across multiple predictions used as inputs. Expanding our pattern generation to encompass multiple migration rates (Subsection 3.4), we encountered additional challenges stemming from the variability in lattice patterns induced by different migration rates. While our model demonstrated competence in capturing general patterns across various migration rates, accurately estimating vacant sites proved to be a more formidable task due to their varying density and distribution. This highlights the importance of considering the intricacies of the system dynamics when designing and training predictive models. In Subsection 3.5, we tackled the task of extinction prediction, leveraging a CNN architecture and Binary Cross Entropy loss function. Our model achieved high accuracy in predicting the long-term fate of the system, demonstrating its proficiency in capturing complex relationships between migration rates and extinction probabilities. This task not only tackles classification among images, but also tackles classification post long-range forecasting. It is feasible because the model inherently grasps the delicate balance between spiral size and extinction. As the spiral size increases, it deviates further from the lattice's boundaries. Our model predicts the likelihood of spirals exceeding these boundaries, leading to one species eventually dominating the other within the lattice, by analyzing spiral evolution based on early-stage ensembles. Notably, our analysis revealed the impact of class imbalance on model performance, particularly evident at higher migration rates. Despite this, our model's ability to generalize across different migration rate intervals was demonstrated through rigorous experimentation and analysis.

#### 3.7 Summary

This research work introduces an innovative approach to modeling ecosystems using machine learning techniques, particularly focusing on lattice-based simulations. The ecosystem dynamics considered include birth, death, predation, and migration of three species. The key contributions of this work lie in the application of machine learning, specifically Convolutional Neural Networks (CNNs), for both image generation and binary classification tasks within the context of ecosystem simulation.

The study progresses through three main tasks, each increasing in complexity. Firstly, we simulate lattices for a single migration rate. Then, we extend this to generate lattices for multiple migration rates. Finally, we tackle the challenging task of long-term extinction prediction within the ecosystem. Throughout these tasks, the authors leverage advancements in computer vision to achieve accurate results.

Validation of the ML tasks is performed using unseen data points for each task. Notably, in the third task, we employ a method where certain intervals of data are masked, prompting the model to extrapolate predictions over large intervals where training data is lacking. Furthermore, we acknowledge the stochastic nature of the data, and recognize that short-term changes can accumulate and perturb long-term behavior. To address this, we incorporate Monte Carlo Dropouts into our models to accommodate variability. During testing, these dropouts are retained to ensure variability across test data, enhancing the robustness of the model.

The results demonstrate the effectiveness of the proposed approach in accurately predicting extinction events across various scenarios, including cases of premature extinction, the presence of large spirals, and instances where smaller spirals lead to extinction. Overall, the study showcases the potential of machine learning techniques, particularly CNNs, in advancing our understanding and prediction capabilities within complex ecological systems.



Figure 3.4 Results for pattern generation for model trained with single migration rate. (a) Spiral formation from early-stage lattice predictions. Only t=5 lattice is provided as input to our model. Then the model outputs are used as successive inputs. (b) Spiral formation for data corresponding to lattice timesteps outside of training data temporally. In this task, the model extrapolates and generates spiral patterns for timesteps outside the training range. Only t=380 is provided as an input to our model. Then the model outputs are used as successive inputs. (c) Unseen Initial condition. (i) ML based predictions. Given t=5, use U-Net outputs for further simulation. (ii) Outputs from Monte Carlo algorithm (Simulation). (iii) Deviation in predictions.



Figure 3.5 Results from model trained to generate patterns for multiple migration rates. Lattices from random initial timesteps with input and output in difference of 40 Monte Carlo Timesteps. (i) Input Lattice. (ii) Expected output lattice post t + 40. (iii) U-Net predictions.



**Figure 3.6 (a).** Extinction Probability  $R_e$  versus Migration rate  $M_r$  across 250 realizations of 9 different points in validation. For this task, the CNN had been trained across a uniformly sampled dataset across migration rates 0 to 30. (b). Extinction Probability  $R_e$  versus Migration rate  $M_r$  across 250 realizations of 11 different points in validation. For this task, the regions shaded in red were masked during training, but solely used for validation purposes.

# Chapter 4

## Conclusion

In this thesis, we study RPS/RPSSL system from two perspectives: first-passage problems and Machine learning. While first-passage problems provides us in-depth analysis on statebased probability conditioned on initial configuration and first-extinction time, it is only viable for small-scale systems. With multiple initial configurations, combined with increasing species and the need to study extinction from an evolutionary perspective, neither multiple large-scale systems or first-passage problems rise up to the occasion. Hence, we train Machine Learning based lattice generators capable of generating evolutionary snapshots of lattices. We also train a Machine learning predictor capable of learning extinction probabilities and extrapolating to unknown regions accurately. This thesis advances the domain by optimization, expedition, and intricate analytical formulation of complex rate reactions pertaining to a system.

Further scope of this thesis can be realized through efficient LU decomposition using distributed computing for sparse systems. Furthermore, the Machine Learning aspects can be diversified by conducting multiple simulations for multiple migration rates through a streamlined ML channel. For accurate vacant space prediction, recent developments like Transformers and ConvLSTMs can be used. Moreover, a uniform framework through transfer learning can be performed for both extinction prediction and lattice generation. Furthermore, the Machine Learning work can be extended to more complex systems involving fitness-based mutations, immigration, etc.

## **Bibliography**

- M. Frean and E. R. Abraham, "Rock-scissors-paper and the survival of the weakest," *Proceedings: Biological Sciences*, vol. 268, no. 1474, pp. 1323–1327, 2001. [Online]. Available: http://www.jstor.org/stable/3068026
- [2] M. Pekkonen, T. Ketola, and J. T. Laakso, "Resource availability and competition shape the evolution of survival and growth ability in a bacterial community," *PLOS ONE*, vol. 8, no. 9, p. null, 09 2013.
- [3] A. J. Lotka, "Analytical note on certain rhythmic relations in organic systems," *Proceed*ings of the National Academy of Sciences, vol. 6, no. 7, pp. 410–415, 1920.
- [4] V. Volterra, "Fluctuations in the abundance of a species considered mathematically," *Nature*, vol. 118, no. 2972, pp. 558–560, 1926.
- [5] R. M. May and W. J. Leonard, "Nonlinear aspects of competition between three species," *SIAM journal on applied mathematics*, vol. 29, no. 2, pp. 243–253, 1975.
- [6] B. Kerr, M. A. Riley, M. W. Feldman, and B. J. Bohannan, "Local dispersal promotes biodiversity in a real-life game of rock-paper-scissors," *Nature*, vol. 418, no. 6894, pp. 171–174, 2002.
- [7] B. Sinervo and C. M. Lively, "The rock–paper–scissors game and the evolution of alternative male strategies," *Nature*, vol. 380, no. 6571, pp. 240–243, 1996.
- [8] C. Guill, B. Drossel, W. Just, and E. Carmack, "A three-species model explaining cyclic dominance of pacific salmon," *Journal of Theoretical Biology*, vol. 276, no. 1, pp. 16–21, 2011.
- [9] M. M. Tobias Reichenbach and E. Frey, "Mobility promotes and jeopardizes biodiversity in rock-paper-scissors games," *Nature*, vol. 448, no. 7157, pp. 1046–1049, 2007.
   [Online]. Available: https://doi.org/10.1038/nature06095

- [10] D. F. P. Toupo and S. H. Strogatz, "Nonlinear dynamics of the rock-paper-scissors game with mutations," *Phys. Rev. E*, vol. 91, p. 052907, May 2015. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevE.91.052907
- [11] J. Park, "Fitness-based mutation in the spatial rock-paper-scissors game: Shifting of critical mobility for extinction," EPL (Europhysics Letters), vol. 126, no. 3, p. 38004, 2019.
- [12] W. Huang, B. Haubold, C. Hauert, and A. Traulsen, "Emergence of stable polymorphisms driven by evolutionary games between mutants," *Nature Communications*, vol. 3, no. 1, p. 919, 2012. [Online]. Available: https://doi.org/10.1038/ncomms1930
- [13] A. Szolnoki and M. c. v. Perc, "Zealots tame oscillations in the spatial rock-paperscissors game," *Phys. Rev. E*, vol. 93, p. 062307, Jun 2016. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevE.93.062307
- [14] J. Menezes, B. Moura, and T. Pereira, "Uneven rock-paper-scissors models: patterns and coexistence," *EPL (Europhysics Letters)*, vol. 126, no. 1, p. 18003, 2019.
- [15] R. M. May, "Will a large complex system be stable?" *Nature*, vol. 238, no. 5364, pp. 413–414, 1972.
- [16] S. Bhattacharyya, P. Sinha, R. De, and C. Hens, "Mortality makes coexistence vulnerable in evolutionary game of rock-paper-scissors," *Physical Review E*, vol. 102, no. 1, p. 012220, 2020.
- [17] S. Roxburgh, K. Shea, and J. Wilson, "The intermediate disturbance hypothesis: Patch dynamics and mechanisms of species coexistence," *Ecology*, vol. 85, no. 2, pp. 359–371, Feb. 2004.
- [18] A. M. Ellison, E. J. Farnsworth, and R. R. Twilley, "Facultative mutualism between red mangroves and root-fouling sponges in belizean mangal," *Ecology*, vol. 77, no. 8, pp. 2431–2444, 1996. [Online]. Available: http://www.jstor.org/stable/2265744
- [19] G. E. Hutchinson, "Homage to santa rosalia or why are there so many kinds of animals?" *The American Naturalist*, vol. 93, no. 870, pp. 145–159, 1959.
- [20] R. MacArthur and R. Levins, "The limiting similarity, convergence, and divergence of coexisting species," *The american naturalist*, vol. 101, no. 921, pp. 377–385, 1967.
- [21] L. Loewe and W. Hill, "The population genetics of mutations: Good, bad and indifferent," *Philosophical transactions of the Royal Society of London. Series B, Biological sciences*, vol. 365, pp. 1153–67, 04 2010.

- [22] J. Park, "Fitness-based mutation in the spatial rock-paper-scissors game: Shifting of critical mobility for extinction," *Europhysics Letters*, vol. 126, no. 3, p. 38004, jun 2019.
   [Online]. Available: https://dx.doi.org/10.1209/0295-5075/126/38004
- [23] T. Reichenbach, M. Mobilia, and E. Frey, "Mobility promotes and jeopardizes biodiversity in rock-paper-scissors games," *Nature*, vol. 448, no. 7157, pp. 1046–1049, 2007.
- [24] L. Frachebourg, P. L. Krapivsky, and E. Ben-Naim, "Spatial organization in cyclic lotka-volterra systems," *Phys. Rev. E*, vol. 54, pp. 6186–6200, Dec 1996. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevE.54.6186
- [25] S. Islam, A. Mondal, M. Mobilia, S. Bhattacharyya, and C. Hens, "Effect of mobility in the rock-paper-scissor dynamics with high mortality," *Phys. Rev. E*, vol. 105, p. 014215, Jan 2022. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevE.105.014215
- [26] J. Menezes and E. Rangel, "Trade-off between reproduction and mobility prolongs organisms' survival in rock-paper-scissors models," *Europhysics Letters*, vol. 142, no. 4, p. 47002, may 2023. [Online]. Available: https://dx.doi.org/10.1209/0295-5075/acd418
- [27] J. Park, "Fitness-based mutation in the spatial rock-paper-scissors game: Shifting of critical mobility for extinction," *Europhysics Letters*, vol. 126, no. 3, p. 38004, jun 2019.
   [Online]. Available: https://dx.doi.org/10.1209/0295-5075/126/38004
- [28] M. Mobilia, A. M. Rucklidge, and B. Szczesny, "The influence of mobility rate on spiral waves in spatial rock-paper-scissors games," *Games*, vol. 7, no. 3, 2016. [Online]. Available: https://www.mdpi.com/2073-4336/7/3/24
- [29] L.-L. Jiang, T. Zhou, M. c. v. Perc, and B.-H. Wang, "Effects of competition on pattern formation in the rock-paper-scissors game," *Phys. Rev. E*, vol. 84, p. 021912, Aug 2011.
   [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevE.84.021912
- [30] P. P. Avelino, D. Bazeia, L. Losano, J. Menezes, and B. F. Oliveira, "Junctions and spiral patterns in generalized rock-paper-scissors models," *Phys. Rev. E*, vol. 86, p. 036112, Sep 2012. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevE.86.036112
- [31] C. R. Hasan, H. M. Osinga, C. M. Postlethwaite, and A. M. Rucklidge, "Spatiotemporal stability of periodic travelling waves in a heteroclinic-cycle model," *Nonlinearity*, vol. 34, no. 8, p. 5576, jul 2021. [Online]. Available: https: //dx.doi.org/10.1088/1361-6544/ac0126

- [32] T. Reichenbach, M. Mobilia, and E. Frey, "Noise and correlations in a spatial population model with cyclic competition," *Phys. Rev. Lett.*, vol. 99, p. 238105, Dec 2007. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevLett.99.238105
- [33] S. Chatterjee, R. De, C. Hens, S. K. Dana, T. Kapitaniak, and S. Bhattacharyya, "Response of a three-species cyclic ecosystem to a short-lived elevation of death rate," *Scientific Reports*, vol. 13, no. 1, p. 20740, 2023.
- [34] S. Raychaudhuri, "Introduction to monte carlo simulation," in 2008 Winter Simulation Conference, 2008, pp. 91–100.
- [35] Q. He, M. Mobilia, and U. C. Täuber, "Spatial rock-paper-scissors models with inhomogeneous reaction rates," *Physical Review E*, vol. 82, no. 5, p. 051909, 2010.
- [36] D. T. Gillespie, "Exact stochastic simulation of coupled chemical reactions," *The Journal of Physical Chemistry*, vol. 81, no. 25, pp. 2340–2361, 1977. [Online]. Available: https://doi.org/10.1021/j100540a008
- [37] J. Park, Y. Do, B. Jang, and Y.-C. Lai, "Emergence of unusual coexistence states in cyclic game systems," *Scientific reports*, vol. 7, no. 1, p. 7465, 2017.
- [38] S. Kundu, S. Majhi, S. K. Sasmal, D. Ghosh, and B. Rakshit, "Survivability of a metapopulation under local extinctions," *Phys. Rev. E*, vol. 96, p. 062212, Dec 2017.
   [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevE.96.062212
- [39] S. Kundu, S. Majhi, and D. Ghosh, "Persistence in multilayer ecological network consisting of harvested patches," *Chaos: An Interdisciplinary Journal of Nonlinear Science*, vol. 31, p. 033154, 03 2021.
- [40] N. W. Barendregt and P. J. Thomas, "Heteroclinic cycling and extinction in may–leonard models with demographic stochasticity," *Journal of Mathematical Biology*, vol. 86, no. 2, p. 30, 2023. [Online]. Available: https://doi.org/10.1007/s00285-022-01859-4
- [41] H. M. Taylor and S. Karlin, An introduction to stochastic modeling., 3rd ed. Boston, MA: Academic Press, 1998.
- [42] D. F. Anderson and T. G. Kurtz, *Stochastic analysis of biochemical systems*, ser. Math. Biosci. Inst. Lect. Ser., Stoch. Biol. Syst. Cham: Springer, 2015, vol. 2.
- [43] D. J. Wilkinson, *Stochastic modelling for systems biology*. Boca Raton, FL: Chapman & Hall/CRC, 2006.

- [44] M. Mobilia, A. M. Rucklidge, and B. Szczesny, "The influence of mobility rate on spiral waves in spatial rock-paper-scissors games," *Games*, vol. 7, no. 3, p. 24, 2016.
- [45] M. D. Zeiler and R. Fergus, "Visualizing and understanding convolutional networks," 2013.
- [46] F. Sultana, A. Sufian, and P. Dutta, "Evolution of image segmentation using deep convolutional neural network: A survey," *Knowledge-Based Systems*, vol. 201–202, p. 106062, Aug. 2020. [Online]. Available: http://dx.doi.org/10.1016/j.knosys.2020.106062
- [47] O. Ronneberger, P. Fischer, and T. Brox, "U-net: Convolutional networks for biomedical image segmentation," 05 2015.
- [48] Y. Lecun, L. Bottou, Y. Bengio, and P. Haffner, "Gradient-based learning applied to document recognition," *Proceedings of the IEEE*, vol. 86, no. 11, pp. 2278–2324, 1998.
- [49] K. He, X. Zhang, S. Ren, and J. Sun, "Deep residual learning for image recognition," 2015.
- [50] A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, and I. Polosukhin, "Attention is all you need," 2023.
- [51] C. Rao, P. Ren, Q. Wang, O. Buyukozturk, H. Sun, and Y. Liu, "Encoding physics to learn reaction–diffusion processes," *Nature Machine Intelligence*, vol. 5, no. 7, pp. 765–779, 2023. [Online]. Available: https://doi.org/10.1038/s42256-023-00685-7
- [52] R. Iten, T. Metger, H. Wilming, L. del Rio, and R. Renner, "Discovering physical concepts with neural networks," *Phys. Rev. Lett.*, vol. 124, p. 010508, Jan 2020. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevLett.124.010508
- [53] K. Champion, B. Lusch, J. N. Kutz, and S. L. Brunton, "Data-driven discovery of coordinates and governing equations," *Proceedings of the National Academy* of Sciences, vol. 116, no. 45, pp. 22445–22451, 2019. [Online]. Available: https://www.pnas.org/doi/abs/10.1073/pnas.1906995116
- [54] T. Nagatani, G. Ichinose, and K.-i. Tainaka, "Heterogeneous network promotes species coexistence: metapopulation model for rock-paper-scissors game," *Scientific Reports*, vol. 8, no. 1, p. 7094, 2018.
- [55] R. Mittal and A. Al-Kurdi, "Lu-decomposition and numerical structure for solving large sparse nonsymmetric linear systems," *Computers & Mathematics with Applications*,

vol. 43, no. 1, pp. 131–155, 2002. [Online]. Available: https://www.sciencedirect.com/ science/article/pii/S0898122101002796

- [56] J. Vukov, A. Szolnoki, and G. Szabó, "Diverging fluctuations in a spatial five-species cyclic dominance game," *Phys. Rev. E*, vol. 88, p. 022123, Aug 2013. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevE.88.022123
- [57] Y. Kang, Q. Pan, X. Wang, and M. He, "A golden point rule in rock-paper-scissorslizard-spock game," *Physica A: Statistical Mechanics and its Applications*, vol. 392, no. 11, pp. 2652–2659, 2013.
- [58] A. Szolnoki, M. Mobilia, L.-L. Jiang, B. Szczesny, A. M. Rucklidge, and M. Perc, "Cyclic dominance in evolutionary games: A review," *Journal of The Royal Society Interface*, vol. 11, no. 100, p. 20140735, 2014.
- [59] A. Krizhevsky, I. Sutskever, and G. E. Hinton, "Imagenet classification with deep convolutional neural networks," *Commun. ACM*, vol. 60, no. 6, p. 84–90, may 2017.
   [Online]. Available: https://doi.org/10.1145/3065386
- [60] K. Simonyan and A. Zisserman, "Very deep convolutional networks for large-scale image recognition," arXiv preprint arXiv:1409.1556, 2014.
- [61] C. Szegedy, W. Liu, Y. Jia, P. Sermanet, S. Reed, D. Anguelov, D. Erhan, V. Vanhoucke, and A. Rabinovich, "Going deeper with convolutions," in 2015 IEEE Conference on Computer Vision and Pattern Recognition (CVPR), 2015, pp. 1–9.
- [62] J. Long, E. Shelhamer, and T. Darrell, "Fully convolutional networks for semantic segmentation," in 2015 IEEE Conference on Computer Vision and Pattern Recognition (CVPR), 2015, pp. 3431–3440.
- [63] L.-C. Chen, G. Papandreou, I. Kokkinos, K. Murphy, and A. L. Yuille, "Deeplab: Semantic image segmentation with deep convolutional nets, atrous convolution, and fully connected crfs," *IEEE Transactions on Pattern Analysis and Machine Intelligence*, vol. 40, no. 4, pp. 834–848, 2018.
- [64] I. J. Goodfellow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley, S. Ozair, A. Courville, and Y. Bengio, "Generative adversarial nets," in *Proceedings of the 27th International Conference on Neural Information Processing Systems - Volume 2*, ser. NIPS'14. Cambridge, MA, USA: MIT Press, 2014, p. 2672–2680.

- [65] T. Karras, T. Aila, S. Laine, and J. Lehtinen, "Progressive growing of gans for improved quality, stability, and variation," *ArXiv*, vol. abs/1710.10196, 2017. [Online]. Available: https://api.semanticscholar.org/CorpusID:3568073
- [66] T. Karras, S. Laine, and T. Aila, "A style-based generator architecture for generative adversarial networks," in 2019 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR), 2019, pp. 4396–4405.
- [67] Y. Lecun and Y. Bengio, "Convolutional networks for images, speech, and time-series," 01 1995.
- [68] N. Srivastava, G. E. Hinton, A. Krizhevsky, I. Sutskever, and R. Salakhutdinov, "Dropout: A simple way to prevent neural networks from overfitting," *Journal of Machine Learning Research*, vol. 15, no. 1, pp. 1929–1958, 2014.
- [69] Y. Gal and Z. Ghahramani, "Dropout as a bayesian approximation: representing model uncertainty in deep learning," in *Proceedings of the 33rd International Conference on International Conference on Machine Learning - Volume 48*, ser. ICML'16. JMLR.org, 2016, p. 1050–1059.