## CLASSICAL AND QUANTUM SPREADING PROCESSES ON DISORDERED AND COMPLEX NETWORKS

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## ABSTRACT

Spreading processes on networks provide a valuable, abstract framework to study a vast array of problems using a unified formalism, from the spread of wildfires in forests to opinion formation in social groups. This thesis presents three specific problems that relate to different spreading processes on complex networks.

The first of these is a study of diffusive persistence on disordered lattices and complex networks to better understand the temporal characteristics and the lifetime of fluctuations in stochastic processes in networks. Diffusive persistence is defined as the probability that the diffusive field at a site (or node) has not changed sign up to a certain time (or in general, that the node remained active/inactive in discrete models). Applications of our research could help one better understand the lifetime and temporal dynamics of activity fluctuations and trends in social networks. We investigated disordered networks (characterized by the fraction of removed edges) and found that the behavior of the persistence depends on the topology of the network. In 2D networks we have found that above the percolation threshold diffusive persistence scales similarly as the original two-dimensional regular lattice, according to a power law with an exponent of  $0.186 \pm 1.4 * 10^{-4}$ . At the percolation threshold, the scaling exponent changes to one with  $0.141 \pm 5.3 * 10^{-5}$ , as the result of the interplay of diffusive persistence and the underlying structural transition in the disordered lattice at the percolation threshold. In contrast, we found that in random networks without a regular structure, such as Erdős-Rényi networks, no simple power-law scaling behavior exists above the percolation threshold. We also investigate finite-size effects for 2D lattices at the percolation threshold and find that the limiting value obeys a power-law with exponent  $z\theta$ , where  $z \approx 2.56 \pm 2.3 * 10^{-2}$  instead of the value of z = 2 normally associated with finite-size effects on 2D lattices.

Next, we discuss percolation on quantum networks. Quantum networks describe communication networks that are based on quantum entanglement. A concurrence percolation theory has been recently developed to determine the required entanglement to enable communication between two distant stations in an arbitrary quantum network. Unfortunately, concurrence percolation has been calculated only for very small networks or large networks without loops. Here, we develop a set of mathematical tools for approximating the concurrence percolation threshold for unprecedented large-scale quantum networks by estimating the path-length distribution, under the assumption that all paths between a given pair of nodes have no overlap. We show that our approximate method agrees closely with analytical results from concurrence percolation theory. The numerical results we present include 2D square lattices of  $200^2$  nodes and complex networks of up to  $10^4$  nodes. The entanglement percolation threshold of a quantum network is a crucial parameter for constructing a real-world communication network based on entanglement, and our method offers a significant speed-up for the intensive computations involved.

Finally, we study how public transportation data can be employed in the modeling of the spread of infectious diseases based on SIR dynamics. We present a model where public transportation data is used as an indicator of broader mobility patterns within a city, including the use of private transportation, walking etc. The mobility parameter derived from this data is used to model the infection rate. As a test case, we study the impact of the usage of the New York City subway on the spread of COVID-19 within the city during 2020. We show that utilizing subway transport data as an indicator of the general mobility trends within the city, and therefore as an indicator of the effective infection rate, improves the quality of forecasting COVID-19 spread in New York City. Our model predicts the two peaks in the spread of COVID-19 cases in NYC in 2020, unlike a standard SIR model that misses the second peak entirely.

## CHAPTER 1 INTRODUCTION

In this chapter we will give an overview of the key areas that serve as relevant background knowledge for the work presented in chapters 2-4. We start by giving a general overview of networks, including some mathematical properties of networks, and examples of regular and random networks. Next, we give an overview of percolation theory. Finally, we introduce the notion of quantum networks and discuss how they differ from classical networks.

### 1.1 Networks

A network, or graph, is a set  $\mathcal{G} = \{\mathcal{N}, \mathcal{E}\}$ , where  $\mathcal{N}$  is a set of nodes (or vertices) and  $\mathcal{E}$  is a set of edges (or links), where each edge is a pair of elements of  $\mathcal{N}$  and represents a connection between them [1]. Many real-world systems can be represented as networks, such as the internet, citation networks, and cellular networks [1], [2]. The adjacency matrix of a graph **A** has components  $A_{ij}$  which are 1 if there is an edge between nodes i and j, and is 0 otherwise [2]. In some networks  $A_{ij}$  may have some other value that represents the strength of the edge between these nodes. We say that a network is directed if  $A_{ij} \neq A_{ji}$ , with the direction of the edge  $A_{ij}$  being from j to i. In this work we will only be concerned with undirected graphs.

The degree of a node i refers to the number of edges connected to it

$$k_i = \sum_j A_{ij} \tag{1.1}$$

. The total number of edges in an undirected network is

$$E = \frac{1}{2} \sum_{i} k_i = \frac{1}{2} \sum_{ij} A_{ij}.$$
 (1.2)

The factor of  $\frac{1}{2}$  compensates for the fact that every edge in the sum on the right is counted twice. A graph in which every node is connected to every other node is known as a complete

graph. The number of edges in a complete graph with N nodes are

$$E = \frac{N(N-1)}{2}.$$
 (1.3)

We define the density of a graph with N nodes and E edges as

$$\rho = \frac{2E}{N(N-1)}.\tag{1.4}$$

A graph where  $\rho \to 0$  as  $N \to \infty$  is known as a sparse graph, while a graph where  $\rho \to \mathcal{O}(1)$  as  $N \to \infty$  is known as a dense graph [2]. So far we have not defined a notion of how graphs might grow, but in the next sections we will see how graphs might be constructed algorithmically and these notions of density will become helpful.

A path between two nodes s and t is said to exist if we start at node s and follow a series of edges that eventually bring us to node t. The longest shortest path connecting any two nodes in a network is called the diameter of the network. If, having left s, the only path to return to s is by following exactly the same edges as those already traversed, the network has no cycles [1]. Networks without cycles are called trees.

Networks where every node has the same degree is known as a regular network. Examples of regular networks are lattice graphs such as 1*d* chains  $(k_i = 2)$ , 2*d* square lattices  $(k_i = 4)$  and the Bethe lattice or Cayley tree.

#### 1.1.1 Complex Networks

#### Erdős-Rényi Networks

Networks where the edges are distributed randomly are known as random networks. The earliest systematic study of random networks was done by Paul Erdős and Alfréd Rényi [3]. In an Erdős-Rényi (ER) network E edges are distributed with equal probability among N nodes [1], [2], [3]. An alternative way of constructing an ER network is to define a probability, p, with which an edge exists between any pair of nodes. A graph constructed in this way is referred to as  $\mathcal{G}(N, p)$ . For a given p the expected number of edges is given by

$$\langle E \rangle = p \frac{N(N-1)}{2}.$$
 (1.5)

Ζ	Subgraph
$-\infty$	Disconnected Nodes
$-\frac{3}{2}$	Trees of order 3
$-\frac{4}{3}$	Trees of order 4
-1	Graphs with cycles
$-\frac{2}{3}$	Complete graphs of order 4
0	Complete graph of order $N$

Table 1.1: The appearance of subgraphs in  $\mathcal{G}(N,p)$  as  $p \sim N^z$  increases. All values taken from [1].

The average degree of a node in an ER network may then be written as

$$\langle k \rangle = \frac{2 \langle E \rangle}{N} = p(N-1).$$
 (1.6)

Given a graph consisting of N disconnected nodes we can increase p and, consequently, add more and more edges to the graph. We can visualize, for example, 3 of the original Nnodes forming a triangle at some probability p. In general, the average number of subgraphs with n nodes and e edges is given by [1], [4]

$$\langle X \rangle \approx \frac{p^e N^n}{a},$$
 (1.7)

where X is the number of subgraphs and a is the number of isomorphic subgraphs with the same number of nodes and edges. If we express the probability of the existence of an edge as  $p \sim N^z$  we can express what subgraphs will appear in  $\mathcal{G}(N, p)$  as a function of z [1]. Some examples are presented in Tab. 1.1.

The degree distribution of  $\mathcal{G}(N, p)$  is approximately a Poisson distribution in the limit of large N

$$P(k) \approx e^{-\langle k \rangle} \frac{\langle k \rangle^k}{k!} \tag{1.8}$$

#### Barabási-Albert (Scale-Free) Networks

Many real-world networks do not follow the degree distribution of ER networks. Instead, a wide variety of empirical networks follow a power-law degree distribution of the form [1], [5], [6]

$$P(k) \sim k^{-\gamma}.\tag{1.9}$$

Networks with power-law distribution have a long tail in the degree distribution such that there are a few nodes with a very large number of edges connected to them. In order to generate networks with such a degree distribution Barabási and Albert proposed a model of network growth based on preferential attachment, so that every node that is added to the network has a probability of being connected to an existing node based on that node's degree.

Starting with  $z_0$  nodes at every step a node is added to the network and connected to z existing nodes, where z is referred to as the coordination number. The probability of this new node connecting to an existing node with degree  $k_i$  is given by [1], [5]

$$\Pi(k_i) = \frac{k_i}{\sum_j k_j}.$$
(1.10)

As the number of steps in this process becomes very large the degree distribution of the network approaches

$$P(k) \approx 2z^2 k^{-\gamma},\tag{1.11}$$

where  $\gamma \approx 3$  [1]. We refer to networks constructed in this way as scale-free or Barabási-Albert (BA) networks.

#### 1.1.2 Processes on Networks

#### Percolation

Percolation refers to the process of removing nodes (site percolation) or edges (bond percolation) with probability  $1 - \phi$ , where  $\phi$  is called the occupation probability [7], [8]. Percolation can be used to describe a wide variety of systems, from phase transitions in the Ising spin model [9] to the emergence of flocking behavior in large groups of living organisms [10]. We define a cluster as a set of nodes in a network that are all connected through nearest-neighbor edges. As an example we consider a 2*d* lattice. We begin to remove edges from this lattice with probability  $1 - \phi$  and we are interested in whether there is a path connecting any node on the top boundary of the network to any node on the bottom. This process is illustrated in Fig. 1.1. We can see that as  $\phi$  decreases the network becomes more disordered but for  $\phi \geq 0.5$  we still see a cluster that spans the length of the lattice connecting its top and bottom boundaries. However, for  $\phi < 0.5$  we only have small disconnected clusters. The lattice undergoes a phase transition at a critical value of  $\phi$ , denoted  $\phi_c$ , at which an infinite cluster first appears. This value is known as the percolation threshold. For 2*d* lattices the bond-percolation threshold is  $\phi_c = 0.5$ .

More generally we can define the percolation threshold as the value of the occupation probability at which a giant, connected component first appears. If the size of the largest connected component of a network with N nodes is G then

$$\lim_{N \to \infty} \frac{G}{N} \to \mathcal{O}(1) \text{ for } \phi \ge \phi_c, \qquad (1.12)$$

$$\lim_{N \to \infty} \frac{G}{N} \to 0 \text{ for } \phi < \phi_c.$$
(1.13)

The fraction  $\frac{G}{N}$  for a 2*d* lattice, an ER network, and a BA network is plotted in Fig. 1.2. We can see that the 2*d* lattice shows the sharpest transition around  $\phi_c = 0.5$  while the percolation threshold for the ER network is roughly  $\phi_c \approx \frac{1}{\langle k \rangle}$ . The BA network, on the other hand, has a percolation threshold very close to 0.

The average correlation length,  $\xi$ , is a quantity proportional to the average cluster diameter near the percolation threshold and has associated with it a critical exponent  $\nu$  [11].

$$\xi \propto |\phi - \phi_c|^{-\nu},\tag{1.14}$$

where  $\nu \approx \frac{4}{3}$  [11], [12]. Many other quantities of interest in percolating systems follow a similiar power-law behavior near the critical threshold. For example, the average cluster size,  $S(\phi)$  is the average size of all connected components in the network when  $1 - \phi$  edges have been removed. This quantity is associated with a critical exponent  $\gamma$  [11]

$$S(\phi) \propto |\phi - \phi_c|^{-\gamma} = \xi^{\frac{\gamma}{\nu}}.$$
(1.15)

The above results hold only for the limit  $L \gg \xi$  (where L is the length of a d-dimensional lattice, such that  $L^d = N$ ). When  $L \ll \xi$  the behavior of these quantities is determined by L. If we introduce a scaling function

$$f(x) = \begin{cases} x^{\frac{\gamma}{\nu}} & x \ll 1\\ \text{constant} & x \gg 1 \end{cases},$$
(1.16)

we can write the behavior of the average cluster size as

$$S = \xi^{\frac{\gamma}{\nu}} f(\frac{L}{\xi}). \tag{1.17}$$

In general, the finite-size behavior of any quantity that is associated with a power-law of the form  $|\phi - \phi_c|^{-\theta}$  in the infinite limit can be expressed in terms of a scaling function [11].

#### Random Walks on Ordered and Disordered Lattices

A random walk is a process where we start at a given node and at every time step take a random step to one of the neighbors of that node [2], [13]. Consider a random walk on a 2d square lattice. If we define R as the distance from the starting node then at step t [8]



Figure 1.1: A 2d lattice where each edge is occupied with probability  $\phi$ . The largest connected component is shown in red.



Figure 1.2: (a) The giant component as a fraction of the network size for a 2d lattice, an ER network with  $\langle k \rangle = 4$  and a BA network with coordination number z = 4. All three networks have  $10^4$  nodes. (b) The giant component as a fraction of the network size for 2d lattices of different sizes.

$$R \propto t^{\frac{1}{2}}.\tag{1.18}$$

As the network becomes disordered, however, this relationship changes. At the percolation threshold the average distance travelled by a random walker on the network is given by

$$R \propto t^{\frac{1}{D'}},\tag{1.19}$$

where  $D' \approx 2.85 \pm 0.05$  [12].

#### Epidemics and Spreading of Infectious Diseases

A widely-used mathematical model for infectious diseases is the SIR (Susceptible-Infected-Recovered) model [14]. The model uses differential equations to relate the susceptible (s), infected (i), and recovered or dead (r) population densities as [2], [15]

$$\frac{ds}{dt} = -\beta si,\tag{1.20}$$

$$\frac{di}{dt} = \beta si - \gamma i, \tag{1.21}$$

$$\frac{dr}{dt} = \gamma i, \tag{1.22}$$

where  $\beta$  is the rate at which individuals transmit the disease to each other,  $\gamma$  is the rate at which individuals recover from the disease, and s(t)+i(t)+r(t) = 1. In general, these equations cannot be solved exactly. However, the steady state value of the final population of infected individuals goes to 0 ( $i(\infty) = 0$ ) while the susceptible and recovered populations satisfy [2]

$$s(\infty) = s(0)e^{-\frac{\beta}{\gamma}r(\infty)},\tag{1.23}$$

$$r(\infty) = 1 - s(0)e^{-\frac{\beta}{\gamma}r(\infty)}.$$
 (1.24)

We can also define a quantity known as the basic reproduction number, denoted by  $R_0$ , which is the average number of people infected by an infected individual over the course of the time period during which they remain infected. For the SIR model the reproduction number has the simple form [2]

$$R_0 = \frac{\beta}{\gamma}.\tag{1.25}$$

We can rewrite the differential equation for the infected population as

$$\frac{di}{dt} = \left(\frac{\beta}{\gamma}s - 1\right)\gamma i(t). \tag{1.26}$$

We see that when  $R_0 < 1$  the infection will quickly die out while when it  $R_0 > 1$  it will persist through the population until not enough of the susceptible population remains for the disease to maintain itself.

We can numerically solve these equations by discretizing them as follows

$$s(t + \Delta t) = s(t) - \Delta t \beta s(t)i(t), \qquad (1.27)$$

$$i(t + \Delta t) = i(t) + \Delta t\beta s(t)i(t) - \Delta t\gamma i(t), \qquad (1.28)$$

$$r(t + \Delta t) = r(t) + \Delta t \gamma i(t). \tag{1.29}$$

Fig. 1.3 plots SIR dynamics for two different reproduction numbers. The model is simple and more powerful models with additional compartments representing different phases of the disease, such as the SEIR (Susceptible-Exposed-Infected-Recovered) model, are built on it [15]. The model can also be modified to account for spatial patterns of disease spread due to the movements of population. For example, if we introduce a spatial variable and assume that our infected population travels and spreads the disease we may write a modified version of the model that incorporates a diffusive term tracking the movement of the population [16]. In chapter 4 we will use an alternative method to model the spatial spread of the disease by treating different locations, such as the neighborhoods of a city, as additional compartments in the SIR model.



(b)  $R_0 = 0.9$ 

Figure 1.3: Numerical evaluation of the SIR model with i(0) = 0.01. (a) When  $R_0 = \frac{\beta}{\gamma} > 1$  the disease infects a significant portion of the susceptible population before it dies out. (b) When  $R_0 = \frac{\beta}{\gamma} < 1$  the disease quickly dies out.

One can map the steady-state of an SIR process to bond percolation on networks [2], [17]. If we define  $\frac{1}{\gamma}$  as the amount of time that every every node remains infected then the probability that a node will become infected by its neighbor before the neighbor moves to the recovered state is given by  $\phi = 1 - e^{-\frac{\beta}{\gamma}}$ . We can then represent this process as bond percolation where the presence of an edge between two nodes indicates the possibility of transmission. When any node in a connected cluster is infected, the disease spreads to every node in that cluster.

## 1.2 Quantum Networks

Entangled pairs of particles shared between two parties can be used to transmit information, with entanglement acting as a physical resource [18]. Communication networks based on shared entangled particles have been proposed [19] and they exhibit several interesting properties. Before we describe quantum networks in detail we provide a brief overview of some key concepts from quantum information theory that determine many of the properties of quantum networks.

#### 1.2.1 Entanglement

A quantum state describing multiple particles is said to be entangled if it cannot be decomposed as a product of the states of the individual particles. Using the Schmidt decomposition any pure bipartite entangled state may be written as

$$\left|\Psi\right\rangle = \sum_{i}^{n} \sqrt{\alpha_{i}} \left|\psi_{i}^{A}\right\rangle \left|\psi_{i}^{B}\right\rangle, \qquad (1.30)$$

where  $\{\alpha_i\}$  are the Schmidt coefficients of this state [18], [20]. By tracing out the degrees of freedom of one observer, we can define the partial density operator

$$\rho_A = \operatorname{Tr}_B |\Psi\rangle \langle \Psi| = \sum_i^n \alpha_i |\psi_i^A\rangle \langle \psi_i^A|.$$
(1.31)

A common measure of entanglement is the von Neumann entropy given by [18]

$$E = -\mathrm{Tr}\rho_A \log \rho_A = -\mathrm{Tr}\rho_B \log \rho_B = -\sum_i^n \alpha_i \log \alpha_i.$$
(1.32)

We can see from the above expression that the entropy ranges from 0 to 1. For a two qubit system the maximally entangled states are the singlet states known as the Bell states [20]

$$|\Psi^{+}\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle),$$
 (1.33)

$$|\Psi^{-}\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle),$$
 (1.34)

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle\right),\tag{1.35}$$

$$|\Phi^{-}\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle - |11\rangle\right). \tag{1.36}$$

We can transform a given entangled state into some other entangled state. Consider the following example taken from [18]: suppose that Alice and Bob each have a particle of the entangled state  $|\Phi^+\rangle$ . Alice then measures her particle by applying the measurement operators

$$M_1 = \begin{pmatrix} \cos \theta & 0\\ 0 & \sin \theta \end{pmatrix}, \tag{1.37}$$

$$M_2 = \begin{pmatrix} \sin \theta & 0\\ 0 & \cos \theta \end{pmatrix}.$$
 (1.38)

If Alice measures  $\sin \theta |00\rangle + \cos \theta |11\rangle$  she applies a NOT gate, and if she measures  $\cos\theta |00\rangle + \sin\theta |11\rangle$  she does nothing. She reports her result to Bob, who applies his own NOT gate for the first measurement, or does nothing in the case of the second measurement. At the end of this process of local operations and classical communications (LOCC) Alice and Bob have transformed  $|\Phi^+\rangle$  into  $\cos\theta |00\rangle + \sin\theta |11\rangle$ .

The above is an example of the general process of entanglement transformation where one pure bipartite state can be transformed into another using only LOCC [21]. In general, a state  $|\Psi\rangle$  may be converted to a state  $|\Phi\rangle$  with probability [22]

$$P(\Psi \to \Phi) = \min_{l \in [1,n]} \left( \left\{ \frac{\sum_{i=l}^{n} \alpha_i}{\sum_{i=l}^{n} \beta_i} \right\} \right), \tag{1.39}$$

where  $\{\alpha_i\}$  and  $\{\beta_i\}$  are the Schmidt coefficients of  $|\Psi\rangle$  and  $|\Phi\rangle$  respectively. A special

form of entanglement transformation is entanglement distillation, where some arbitrary pure state  $|\psi\rangle$  is converted to one of the Bell states [18], [23].

#### Concurrence

We now introduce the quantity known as concurrence, defined for two qubit systems as [24]

$$C = |\langle \Psi | \tilde{\Psi} \rangle|, \tag{1.40}$$

where  $|\tilde{\Psi}\rangle = \sigma_x \otimes \sigma_y |\Psi^*\rangle$ , and  $|\Psi^*\rangle$  is the complex conjugate of  $|\Psi\rangle$ . Concurrence can equivalently be expressed as [25]

$$C = 4\sqrt{1 - \operatorname{Tr}\rho^2}.\tag{1.41}$$

Concurrence is related to the von Neumann entropy as [24]

$$E = \mathcal{E}(C), \tag{1.42}$$

where

$$\mathcal{E}(C) = H\left(\frac{1+\sqrt{1-C^2}}{2}\right),\tag{1.43}$$

and

$$H(x) = -x \log_2 x - (1-x) \log_2(1-x).$$
(1.44)

Concurrence can be used to write an explicit formula for the entropy of formation for a two-qubit system [24]. In chapter 3 we still discuss concurrence percolation theory, which is a theory analogous to percolation used in the analysis of quantum networks.

#### 1.2.2 Quantum Random Networks

A quantum network is a model of a communication network where bipartite entangled qubits are shared between nodes [26]. For example, a 1d quantum network can be constructed using quantum repeaters [27], [28], [29].

A quantum random network consisting of N nodes can be constructed by assuming that any pair of nodes share one pair of particles that are in the non-maximally entangled state

$$|\Psi\rangle = \sqrt{\lambda_1} |00\rangle + \sqrt{\lambda_2} |11\rangle, \qquad (1.45)$$

where  $\lambda_1 + \lambda_2 = 1$ . By using local operations and classical communication (LOCC) we may transform this state into the maximally entangled Bell state  $\Phi = |00\rangle + |11\rangle$  with probability  $p = \min(1, \lambda_2)$ , which is the singlet conversion probability (SCP) [22], [26]. This is a percolation-like process which is reminiscent of the construction of classical random networks.

A remarkable property of quantum random networks is that for every possible subgraph there is a quantum random network with  $p \sim N^{-2}$  containing that subgraph, which can be obtained through local operations between the nodes [26]. This is in sharp contrast to classical random networks where there are critical values of  $p \sim N^{-z}$  below which certain subgraphs do not exist (see for example Tab. 1.1).

# CHAPTER 2 DIFFUSIVE PERSISTENCE ON DISORDERED LATTICES AND RANDOM NETWORKS

## 2.1 Introduction

#### 2.1.1 Persistence

The persistence probability is defined as the probability that some observable in a random process has not crossed some threshold value by time t (e.g., after initializing the system at t = 0) [30], [31]. The observable being studied may be global, such as a bulk order parameter, or local, such as the value of a field at a node.

Past research have investigated the persistence properties of stochastic systems on regular lattices. Examples include diffusion [32], [33], interface fluctuations [34], [35], magnetic and reaction-diffusion systems [36], [37], [38], and the contact process [30], [39]. The persistence probability is also of particular interest in non-equilibrium or disordered systems such as spin-relaxation in the Ising model [40], [41] and the Blume-Capel model [42], as well as the persistence of the bulk order parameter in inhomogenous magnetic systems with defects [43].

The fundamental question that researchers addressed (after initializing the system at time t = 0) is the probability  $P_i(t)$  that the state of the system at location *i* has not changed by time *t* (in homogeneous systems, e.g., in ones with translational invariance, this quantity is independent of the location *i*). For example, for simple diffusion, the persistence probability is the probability that the diffusion field  $\psi_i(t)$  has not changed its sign by time *t*. For an Ising or Voter model [36], [37], [38], it is the probability that the local state variable has never switched by time *t*.

In a wide variety of systems the persistence probability follows a power-law decay,  $P(t) \propto t^{-\theta}$  [31], [44]. For example, in one- and two-dimensional homogeneous diffusion, the local persistence probability follows a power law decay with exponents  $\theta \approx 0.12$  [32], [33] and  $\theta = 3/16$  respectively [45].

Beyond the fundamental diffusion processes, persistence characteristics of stochastic dynamics on network can clearly have important applications to complex systems. For example, in critical infrastructure networks, persistence can be defined as the probability that a local region remains operational up to time t. In influencing and opinion dynamics in social networks, persistence can be defined as the probability that certain nodes or network "regions" in a have not changed opinion since the beginning of a "campaign".

#### 2.1.2 Percolation

The percolation process on a lattice may be understood as removing either the connections between sites (bond-percolation) or the sites themselves (site percolation). The process is characterized by  $\phi$ , where  $1 - \phi$  is the probability of removal. Percolation on a 2D lattice creates a fractal structure, with the percolation threshold,  $\phi_c$ , marking the point at which an infinite cluster first appears [46]. The fractal dimension of the lattice for  $\phi \ge \phi_c$  is 2, while below the percolation threshold it is 1.896 [8]. Thus the topology of the lattice undergoes a phase transition as it becomes disordered.

The effect of this change in topology naturally affects any process on the lattice. Diffusion on lattices, for example, is associated with power-law behavior. When the 2D lattice is above the percolation threshold the distance traversed in a random walk behaves as  $R \propto t^{\frac{1}{2}}$ . However, when the network is at its site percolation threshold of  $\phi_c = 0.59$  the behavior changes to  $R \propto t^{\frac{1}{D'}}$ , where  $D' \approx 2.85 \pm 0.05$  [12].

In this paper, in order to study the effects of disorder on the temporal dynamics in lattices and networks, we investigate the local diffusive persistence behavior of various random graph topologies. In particular, we study the diffusive persistence probability of a diffusive process on disordered spatially-embedded and random networks, created by removing a fraction of edges, defined as  $1 - \phi$ .

### 2.2 Methods

We define a diffusive field variable  $\psi_i$  for the  $i^{\text{th}}$  node of the network. The value of this variable for each node in the network is initialized by sampling from a normal distribution with 0 mean and a standard deviation of 1. Following previous work [32], [33], the discretized diffusion equation that we will study is

$$\psi_i(t + \Delta t) - \psi_i(t) = -\alpha \Delta t \sum_j A_{ij}(\psi_i(t) - \psi_j(t)), \qquad (2.1)$$



Figure 2.1: Persistence on a 2D lattice with  $10^4$  nodes. The diffusive persistence exhibits a power-law behavior. However, as edges are removed from the network, the power-law exponent changes. At the percolation threshold, the power-law exponent is  $\theta \approx 0.14 \pm 5.3 * 10^{-5}$ . The flattening out of the curves is due to the finite size of the network.

where  $A_{ij}$  is the adjacency matrix associated with the network and the RHS of the equation represents the graph Laplacian operator. We choose  $\alpha = 1$  and  $\Delta t = \frac{1}{8}$ . In order to track the progress of diffusion we define persistence, P(t), as the fraction of nodes for which  $\psi_i(t)$ has not changed sign.

To create disordered networks we iterate through the edge list and randomly remove edges with probability  $1 - \phi$ . We then repeat the diffusive process on the giant component of the resulting disordered network. The bond-percolation threshold of 2D lattices is 0.5, and we vary  $\phi$  in the range [0.5, 1].

While our main focus is disordered 2D lattices we also investigate other network topologies, such as percolating Erdős-Rényi (ER) networks and percolating k-regular random networks.

For every network configuration we generate 100 samples and simulate the diffusion

Table 2.1: Values of the power-law exponent,  $\theta$ , associated with diffusive persistence on 2D lattices with  $300^2$  nodes as a function of  $\phi$ , where  $1 - \phi$  is the edge-removal probability.

$\phi$	$\theta$
1	$0.186 \pm 1.4 * 10^{-4}$
0.9	$0.189 \pm 1.6 * 10^{-4}$
0.8	$0.189 \pm 1.4 * 10^{-4}$
0.5	$0.141 \pm 5.3 * 10^{-5}$

equation with randomized initial conditions.

### 2.3 2D Lattices

Fig. 2.1 shows the local persistence probability as diffusion proceeds on a 2D network with a million nodes. P(t) exhibits power-law behavior. For the fully-intact network (i.e  $\phi = 1$ ) we obtain,  $\theta = 0.186 \pm 1.4 * 10^{-4}$ . For different values of  $\phi$  the persistence maintains this power-law behavior, although we observe a different slope at the percolation threshold.

In order to characterize the change in the power-law exponent as a function of  $\phi$  we fit the different persistence curves. The results are shown in Tab. 2.1. The exponent undergoes a dramatic shift at the percolation threshold. The persistence at the percolation threshold follows a power-law with novel exponent  $\theta = 0.141 \pm 5.3 * 10^{-5}$ .

Away from the percolation threshold the power-law exponent maintains its value of approximately  $0.186 \pm 1.4 * 10^{-4}$  for  $\phi > 0.8$ . We were not able to clearly discern the behavior of the power-law exponent for intermediate values of  $\phi$ .

#### 2.3.1 Finite-size Behavior at and Above the Percolation Threshold

We can see from Fig. 2.2a that there is a finite-size effect in the persistence curves where they flatten at some non-zero value. We refer to this limiting value as  $P(\infty)$  and the time at which this limiting value is reached as  $t_x$ . On lattices of length L, where  $L^2$  is the number of nodes in a 2D lattice, the crossover time behaves as  $t_x \sim L^z$  and the limiting value of persistence has a power-law behavior  $P(\infty) \propto L^{-z\theta}$  [47], where  $\theta$  is the exponent associated with the power-law decay of P(t). Following previous work [12], [47], [48] we take the scaling behavior of the persistence to be of the form



Figure 2.2: (a) Finite-size effects on 2d lattices with  $\phi = 1$ . (b) Scaling behavior of 2d lattices for  $\phi = 1$  with  $\theta = 0.186$  and z = 1.99.



Figure 2.3: (a) Finite-size effects on 2d lattices with  $\phi = 0.9$ . (b) Scaling behavior of 2d lattices for  $\phi = 0.9$  with  $\theta = 0.189$  and z = 1.99.



Figure 2.4: (a) Finite-size effects on 2d lattices with  $\phi = 0.5$ . (b) scaling behavior of 2d lattices for  $\phi = 0.5$  with  $\theta = 0.141$  and z = 2.62.



Figure 2.5: The limiting value,  $P(\infty)$ , of the 2D lattice with  $\phi = 0.5$  obeys a power-law relation as a function of the system length, L. The error bars show the standard error over 100 runs. The dotted black line is the best-fit power-law for  $P(\infty) \propto L^{-z\theta}$ .

$$P(t,L) = L^{-z\theta} f(t/L^z), \qquad (2.2)$$

where

$$f(x) = \begin{cases} x^{-\theta} & \text{if } x \ll 1, \\ \text{constant} & \text{if } x \gg 1. \end{cases}$$
(2.3)

For  $\phi = 1$  we calculate  $z = 1.99 \pm 2.8 * 10^{-3}$ , in good agreement with the literature value of the scaling exponent [47]. The scaling behavior of 2D lattices with  $\phi = 1$  is shown in Fig. 2.2b and we see good collapse of all the curves.



Figure 2.6: (a) Local persistence for ER networks with  $n = 10^4$ . The dotted lines show the segment that has been fit with a power-law. (b) The power-law exponent of the persistence curves as a function of the average degree.

We also observe finite-size effects for disordered lattices, as shown in Fig. 2.3a. In comparison to the fully-intact network this effect is observed at longer time-scales. Using the same value of z that we determined for  $\phi = 1$  we plot the scaling behavior in Fig. 2.3b. We see that as the network size increases the collapse of the persistence curves onto a single curve improves.

When the 2D lattice is at the percolation threshold with  $\phi = 0.5$  we observe that the flattening of the persistence curves appears at a much longer time scale as can be seen in Fig. 2.4a. We obtain z for this case by plotting  $P(\infty, L)$  against L and fitting a power-law with exponent  $-z\theta$ , as shown in Fig. 2.5. We obtain  $z = 2.56 \pm 2.3 * 10^{-3}$ . Fig. 2.4b plots  $L^{z\theta}P(t)$  against  $t/L^{z}$  for our calculated values of  $\theta$  and z. We can see from the figure that there is reasonably good collapse of the different curves onto a single curve.

The finite-size behavior that we have studied in this section stems from the underlying diffusive process. The distance traveled in a random walk behaves as  $R \propto t^{\frac{1}{2}}$  for  $\phi = 1$ , but is  $R \propto t^{\frac{1}{D'}}$  on 2D lattices at the site percolation threshold, where  $D' \approx 2.85 \pm 0.05$  [7, 12]. This implies that  $t_x \sim L^{D'}$ . The difference between our value of z and the literature value of D' may stem from the greater sensitivity of the persistence process to finite-size effects. We expect to see closer agreement by looking at longer time-scales and larger network sizes.



Figure 2.7: (a) Diffusive persistence on Erdős-Rényi networks  $(n = 10^4)$  for different average degrees,  $\langle k \rangle$ , and different edge removal probabilities,  $1 - \phi$ . (b) Diffusive persistence for ER networks of different sizes with  $\langle k \rangle = 4$ .



Figure 2.8: (a) Local persistence for k-regular networks with n = 10<sup>4</sup>. The dotted lines show the segment that has been fit with a power-law.
(b) The power-law exponent of the persistence curves as a function of the network degree.

## 2.4 Complex Networks

For complex networks we use  $\Delta t = \frac{1}{100}$  since we study networks with higher average degrees than the case of 2D lattices.

### 2.4.1 Erdős-Rényi (ER) Networks

The behavior of persistence is shown in Fig. 2.6a. In contrast to the clear power-law scaling of 2D networks no such behavior is observed for ER networks.

Fig. 2.7b also shows that the particular shape of the curves is not defined by the



Figure 2.9: (a) Diffusive persistence on k-regular networks  $(n = 10^4)$  for different k, and different edge removal probabilities,  $1 - \phi$ . (b) Diffusive persistence for k-regular networks of different sizes with k = 4.

network size but is a function of the particular network topology.

Fig. 2.6a shows persistence curves for different average degrees and different values of  $\phi$ . As more edges are removed from a network of a given average degree we see that its persistence behavior changes to that of a network with a smaller average-degree. This is not surprising, since removing a certain fraction of edges from an ER network does not cause its topology to change, rather only its degree distribution is changed.

While we do not see any clear power-law scaling, we do notice that as the average degree of the network increases the persistence curves cluster increasingly close to each other. By fitting a power-law to a segment of the persistence curves (marked by the dotted lines in Fig. 2.6a) we are able to characterize this effect, as shown in Fig. 2.6b.

#### 2.4.2 k-Regular Random Networks

The behavior of diffusive persistence for k-regular random networks is shown in Fig. 2.8a. We see a distinct segment of the curve that shows power-law scaling. Similar to ER networks, we notice that as k increases the persistence curves become closer, and by plotting the power-law exponent  $\theta$  as a function of k in Fig. 2.8b we see that this exponent reaches an asymptotic value of approximately 0.22 as k becomes larger.

As we delete edges from the network we can see from Fig. 2.9a that the persistence maintains its power-law behavior for some segment of the curve.

### 2.5 Conclusion

Our investigations shows that regular networks, such as the 2D network, show persistence behavior with clear power-law scaling. As the network becomes more disordered through the percolation process, the power-law exponent remains constant at  $\theta \approx 0.186$  for  $\phi > \phi_c$  but with some strong corrections to the scaling behavior. However, at  $\phi_c$  we observe the novel power-law exponent  $\theta \approx 0.141 \pm 5.3 * 10^{-5}$ . This change may likely be associated with the phase-transition that the network topology undergoes at the percolation threshold.

We also study finite-size effects for 2D lattices at the percolation threshold and discovered that the limiting value of the persistence is associated with a different exponent of  $z \approx 2.56 \pm 2.3 * 10^{-3}$  instead of the known value of z = 2 for ordered lattices.

We also observe interesting behavior for k-regular random networks where the persistence curves show clear power-law behavior. However, we observe no such behavior for ER networks.

Portions of this chapter are available as a preprint: O. Malik, Melinda Varga, Alaa Moussawi, David Hunt, Boleslaw Szymanski, Zoltan Toroczkai, Gyorgy Korniss, "Diffusive Persistence on Disordered Lattices and Random Networks," preprint arXiv:2207.05878 July 12, 2022.

# CHAPTER 3 CONCURRENCE PERCOLATION THRESHOLD OF LARGE-SCALE QUANTUM NETWORKS

## 3.1 Introduction

The application of network science to problems in quantum physics is a relatively new and rapidly developing field [50]. Quantum networks, where the links between nodes represent entangled qubits [19], [26], [29], [51], [52] are expected to form the basis of the quantum internet. Recent advances in quantum repeater technology have made long-distance, noiseresilient quantum communication possible [53], [54], [55], [56], [57]. These networks have quantum correlations that can be exploited by performing specific local measurements on any node.

Protocols for quantum communication rely on the conservation of correlations in entangled states, and the generation and distribution of entanglement are necessary for quantum networks [58]. For a given network topology, we want to determine the minimum amount of entanglement necessary between qubits to maintain a giant component in the network, which is a problem analogous to percolation on classical networks [2], [8], [59], [60]. However, there are crucial differences between classical and quantum networks, limiting the extent to which we can map a classical percolation theory to quantum networks. For example, in a classical random network with N nodes, if an edge between nodes exists with probability p, a subgraph with n nodes and l edges exists above a critical threshold of p given by  $p_c \propto N^{-n/l}$  [61]. For a quantum network, however,  $p_c \sim N^{-2}$  for all subgraphs for large N [62]. We can also use measurement strategies to alter the topology of a quantum network, meaning that the optimal entanglement percolation threshold needs to be minimized over all possible measurement strategies [51].

Recently, Meng et al. [49] proposed a concurrence percolation theory (ConPT), predicting a considerably lower entanglement percolation threshold for quantum networks than previously known thresholds. Despite the compelling result, the computational complexity of ConPT, given that it can only be calculated for networks consisting of  $\sim 60$  nodes at

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Table 3.1: Comparison of results for  $\theta_{th}$ , the threshold of long-distance entanglement transmission for various quantum network topologies, given that each link is a bipartite state of qubits,  $|\Psi\rangle = \cos \theta |00\rangle + \sin \theta |11\rangle, \ \theta \in [0, \pi/4].$ 

Network topology	$(\pi/4)^{-1} heta_{ m th}$ (Fast ConPT)	$(\pi/4)^{-1} heta_{ m th}~({ m Ref.}~[49])$
Bethe Lattice (Cayley Tree) $(L = 100, k = 3)$	0.5	0.5
Be the Lattice (Cayley Tree) $(L = 100, k = 4)$	0.39	0.3918
2D square $(n = 8^2, S_9)$	0.40	0.416
2D square $(n = 20^2, S_3)$	0.44	n/a
2D square $(n = 200^2, S_2)$	0.5	n/a
ER ( $n = 10^3, \langle k \rangle = 3, S_5$ )	$0.6 \pm 0.002$	n/a
ER ( $n = 10^3, \langle k \rangle = 4, S_5$ )	$0.53 \pm 0.0019$	n/a
ER ( $n = 10^4, \langle k \rangle = 2, S_1$ )	$0.85 \pm 0.0021$	n/a
BA ( $n = 10^3, z = 5, S_1$ )	$0.3 \pm 0.0018$	n/a
BA ( $n = 10^4, z = 1, S_5$ )	$0.86 \pm 0.0057$	n/a

maximum, puts great limitation on its utility.

Here, we present a fast and tangible solution for the calculation of the ConPT threshold. Our method relies on two approximations. The first is the parallel approximation, which treats all paths in the network as non-overlapping. The second is what we call the  $S_m$ approximation, where we calculate the total concurrence between nodes using a subset of paths consisting of the *m*-th shortest paths on the network, with m = 1 referring to the shortest paths. We find that our approximate method agrees closely with the analytical results provided by Meng et al. [49]. Depending on the choice of  $S_m$ , the computation based on this method can be several orders of magnitude faster than the analytical approach, as shown in Fig. 3.7. By combining our method with combinatorial expressions for shortest and second-shortest paths we can calculate, for the first time, an approximation for the concurrence for much larger networks than would be analytically possible. Here, we calculate the sponge-crossing concurrence for 2D lattices with up to  $200^2$  nodes. We also extend the notion of concurrence to networks without boundaries and present results for Erdős–Rényi and Barabási–Albert networks of up to  $10^4$  nodes. Our results are summarized in Table 3.1.

# **3.2** Quantum Networks and Entanglement Percolation

Quantum networks [26] are used to model a scalable communication network based on quantum teleportation. It consists of nodes that denote a local set of qubits and edges, which represent a bipartite and entangled state of qubits shared between the two connected nodes (Fig. 3.1a). The simplest practical quantum network can be built from quantum re-



Figure 3.1: Schematic representation of a quantum network. (a) Each link in the network represents a pair of entangled qubits shared between the two connected nodes. (b) The entanglement swapping protocol. Node B performs a Bell state measurement (BSM) on its qubits, causing the qubits in A and C to become entangled. Entanglement swapping can modify the topology of a quantum network, changing its percolation threshold.

peaters [27], [28] which share only one entangled pair between nodes [29]. Quantum communication networks are expected to have several advantages over classical communication networks, including the ability to use quantum cryptography and send "quantum software" [19], [26].

The bipartite state of any entangled qubits in the network can be defined as

$$|\Psi\rangle = \cos\theta \,|00\rangle + \sin\theta \,|11\rangle \tag{3.1}$$

up to a unitary transformation, where  $\theta$  can change from 0 to  $\pi/4$ . Each entangled pair can be converted to a maximally entangled pair with a certain probability p, known as the singletconversion probability (SCP), given by  $p = 2 \sin^2 \theta$  [22]. This represents the probability of establishing a perfect communications channel [62]. Converting every entangled pair in the network to a singlet is equivalent to a bond-percolation process and this measurement strategy is called classical entanglement percolation (CEP) [8], [51].

Having established the mapping to percolation, it is natural to ask what is the minimum level of entanglement necessary for the formation of a perfect communication channel between Unfortunately, CEP does not give us the lowest possible percolation threshold value for a quantum network because it is possible to lower the entanglement threshold necessary for creating an infinite cluster by changing the network's topology. This is done through a process known as entanglement swapping, shown in Fig. 3.1b, where two previously unentangled qubits are entangled using local operations and classical communication (LOCC) [63].

The network topology may be altered to lower the percolation threshold before converting every link to a singlet by performing a series of entanglement swapping operations. This strategy is known as quantum entanglement percolation (QEP) [51], [64]. The limitation of QEP is that it is not generally adaptable to arbitrary network topology as CEP is. For most network topologies, QEP cannot improve the percolation threshold in general. Note also that neither CEP nor QEP are optimal, meaning that it is impossible to determine if any given measurement strategy results in the lowest potential value of the percolation threshold [50].

# 3.3 Concurrence Percolation Theory

In order to address the above limitations, a new local statistical theory has recently been proposed to explain the observed quantum advantage in quantum networks over the prediction of classical percolation theory [49]. This theory is analogous to classical percolation theory but fundamentally different, as it is not built on probability measure p but a new variable c for each link, which stands for *concurrence*—a key measure of bipartite entanglement [65]. For pure bipartite states, the concurrence is defined as [25]

$$c = \sqrt{2(1 - \operatorname{Tr}\rho_r^2)},\tag{3.2}$$

where  $\rho_r$  is the reduced density matrix of one party (subsystem) of the bipartite state. For qubits, Eq. (3.1), the concurrence is simply

$$c = 2\cos\theta\sin\theta. \tag{3.3}$$

Meng et al. then use this quantity in place of probability to construct a concurrence percolation theory (ConPT) on arbitrary network topologies [49].

To be more specific, recall that for classical bond percolation on a lattice, any link in the lattice is active with probability p—a variable that should be considered as the link weight. We may then define a "sponge-crossing" (SC) quantity,  $P_{\rm SC}$ , as the probability that at least one path connecting the two distant boundaries is fully active.  $P_{\rm SC}$ , as a function of p, can be calculated by summing up all paths that connect the two boundaries of the lattice, following basic addition and multiplication rules of probability measures [8]. Essentially, we treat  $P_{\rm SC}$  as a "weighted sum of all paths".

Now, given an *n*-node quantum network,  $\mathbb{G}_{\theta}(n)$ , where all the link weights are  $\theta$ , by the CEP/QEP schemes we have the mapping  $p \equiv 2\sin^2\theta$  (i.e. the SCP). From classical percolation theory, it is known that a minimum value of p exists, below which the spongecrossing probability,  $P_{SC}$ , becomes zero in the thermodynamic limit  $n \to \infty$ :

$$p_{\rm th} = \inf \left\{ p \subset [0,1] | \lim_{n \to \infty} P_{\rm SC}[\mathbb{G}_{\theta}(n)] > 0 \right\}.$$

$$(3.4)$$

This minimum value,  $p_{\rm th}$ , is known as the percolation threshold.

The ConPT is constructed differently, using the mapping  $c \equiv \sin 2\theta$  instead [49]. Still, an analogous quantity,  $C_{SC}$ , referred to as the sponge-crossing concurrence can be defined as the weighted sum of all paths in terms of this new weight c [49]. It is believed that a nontrivial threshold on c also exists:

$$c_{\rm th} = \inf \left\{ c \subset [0, 1] | \lim_{n \to \infty} C_{\rm SC}[\mathbb{G}_{\theta}(n)] > 0 \right\}, \tag{3.5}$$

such that  $c_{\rm th}$  is the minimum value of the concurrence c per link, below which  $C_{\rm SC}$  becomes zero when  $n \to \infty$ .

It remains to show how the "weighted sum of paths" is calculated for ConPT. As a problem of path connectivity, the calculation turns out to closely resemble the analysis of an electrical resistor network, where a set of *series and parallel rules* are needed as the basic connectivity rules [49], [66]. Fundamental quantum communication theorems demand that, for k links connected in series, the total concurrence must be given by

$$c_{\text{seri}} \equiv \text{seri}(c_1, c_2, \dots c_k) = \prod_{i=1}^k c_i.$$
(3.6)

The rule for k links connected parallel to each other is more involved,

$$\frac{1+\sqrt{1-c_{\text{para}}^2}}{2} = \max\left\{\prod_{i=1}^k \frac{1+\sqrt{1-c_i^2}}{2}, \frac{1}{2}\right\},\tag{3.7}$$

which may be restated as

$$c_{\text{para}} \equiv \text{para}(c_1, c_2, \dots c_k) = \begin{cases} 2\sqrt{f(c_1, \dots c_k) - f(c_1 \dots c_k)^2} & f(c_1 \dots c_k) > 1/2, \\ 1 & f(c_1 \dots c_k) \le 1/2, \end{cases}$$
(3.8)

where  $f(c_1 \dots c_k) = \prod_{i=1}^k \frac{1+\sqrt{1-c_i^2}}{2}$ . A caveat lies in the fact that if the network topology is not *series-parallel* [67] but has nontrivial loops (e.g., a bridge-circuit topology), then  $C_{\rm SC}$ cannot be calculated using only series and parallel rules. Higher-order connectivity rules are needed, of which general forms are unknown. There is, however, a heuristic way to approximate these higher-order rules: by employing the so-called *star-mesh transform*, all possible higher-order rules can be approximated using only the series and parallel rules [49].

Equations (3.6) and (3.7), together with the star-mesh transform, allow us to calculate the "weighted sum of paths" between arbitrary two nodes in a quantum network of arbitrary topology. Formally, we denote the two nodes as the source node (s) and the target node (t), respectively, and we define the final concurrence between them as the s-t concurrence,  $C_{st}$ . Note that although s and t are named differently, they are symmetric and exchangeable. Hence, between any two nodes, a  $C_{st}$  can be calculated by the connectivity rules mentioned above (see Fig. 3.2 for example).

On regular lattices, the sponge-crossing concurrence  $C_{\rm SC}$  can be calculated by contracting two separate boundaries into two "mega" nodes [49] and calculate the *s*-*t* concurrence between them. As we increase the network size *n*, a threshold  $c_{\rm th}$  will emerge, accompanied with a sudden jump of  $C_{\rm SC}$  as soon as the concurrence *c* per link becomes larger than  $c_{\rm th}$ . This observation supports the existence of ConPT. Also, the observed  $c_{\rm th}$  is significantly smaller than all previously known classical-percolation-theory-based schemes [49], exhibiting



Figure 3.2: Example of calculating the *s*-*t* concurrence  $C_{st}$  between nodes 1 and 6 on a 2D rectangular lattice using ConPT connectivity rules [series and parallel rules, Eqs. (3.6) and (3.7), respecitively]. (Left to right: step i-v.) Step i: original lattice; Steps ii and iii: series rules; Step iv: star-mesh transform on the star-graph (edges  $4 \leftrightarrow 1$ ,  $4 \leftrightarrow 3$ ,  $4 \leftrightarrow 6$ ), then parallel rule for edges  $1 \leftrightarrow 3$  and  $3 \leftrightarrow 6$ ; Step v: series rule for edges  $1 \leftrightarrow 3$  and  $3 \leftrightarrow 6$ , then parallel rule for edge  $1 \leftrightarrow 6$ .

a quantum advantage in large-scale quantum networks that is purely structural.

Despite the fresh insights the ConPT has offered, it has two main limitations:

- 1. The heuristic approximation (star-mesh transform) used for higher-order connectivity rules is a double-recursive process that is computationally intensive, thus only feasible for networks of very small size.
- 2. Although an *s*-*t* concurrence can be calculated between any two nodes in any network topology, the sponge-crossing concurrence  $C_{\rm SC}$  is only defined for regular lattices that have apparent boundaries, and thus so is  $c_{\rm th}$ . It is unknown how to define  $c_{\rm th}$  on complex network topology where we cannot define a boundary, and, provided a proper definition, how (non)trivial the numerical result of  $c_{\rm th}$  would be.

Unlike cluster-based percolation theories, ConPT is based on path connectivity, which is arguably more general [49]. This is why  $c_{\rm th}$  simply cannot be defined by clusters like in classical percolation theory for complex network topology. A proper definition and feasible calculation of  $c_{\rm th}$  will be of great interest for the theory itself as well as for its applications. Below, we will show our suggested solution that can satisfactorily handle these two limitations of ConPT.

# 3.4 A Fast and Tangible Solution for Concurrence Percolation

We start by generalizing  $C_{\rm SC}$  from being defined between two apparent boundaries to two *arbitrary sets* of nodes, denoted S and T. It is reasonable that Eq. (3.5) will yield a nontrivial ConPT threshold  $c_{\rm th}$  for this generalized  $C_{\rm SC}$ , as long as the lengths of all paths connecting S and T increase with the network size n. We contract the two sets S and T into two "mega" nodes, which amounts to erasing the internal network topologies of S and T, and then calculate the s-t concurrence between them. This provides us a definitive way of calculating  $C_{\rm SC}$  for arbitrary network topology and inferring  $c_{\rm th}$  from Eq. (3.5).

Our numerical computation of  $c_{\rm th}$  ("Fast ConPT computation") on large-scale quantum networks is further made possible by introducing two key simplifying approximations: the parallel approximation and the  $S_m$  approximation.

#### Parallel Approximation

In this Section, we introduce the parallel approximation, where we treat all paths connecting nodes of interest to be parallel, i.e. we treat them as if they have no shared edges. For an arbitrary network with n nodes and uniform edge-weights c, the parallel approximation  $C'_{SC}$  of the true sponge-crossing concurrence between two sets of nodes, Sand T, is given by

$$\frac{1+\sqrt{1-C_{\rm SC}^{\prime 2}}}{2} = \max\left\{\prod_{l=1}^{n} \left(\frac{1+\sqrt{1-c^{2l}}}{2}\right)^{N_l}, \frac{1}{2}\right\},\tag{3.9}$$

where  $N_l$  is the total number of self-avoiding paths of length l that connect s and t for all  $s \in S$  and  $t \in T$ , respectively. Equation (3.9) is the mathematical statement of the parallel approximation, indicating that we are taking each of the  $N_l$  paths to be parallel (Fig. 3.3). We illustrate the approximation with a simple example, and then show that on series-parallel networks [67] the concurrence calculated under the parallel approximation forms an upper bound to the true concurrence. First, we consider the case where our network is *essentially parallel*, i.e., it can be expressed as the parallel combination of k subnetworks each with



Figure 3.3: The parallel approximation preserves the number of paths and their lengths, but ignores overlap between the paths. In this example, k branches of a network, each with concurrence  $c_{p_i}$ , all join to a segment with concurrence  $c_s$ . Under the parallel approximation the network is transformed so that the k branches have no overlap with each other.

concurrence  $c_i$ . In this case, the parallel approximation is exact:

$$C'_{\rm SC} = C_{\rm SC} = \text{para}(c_1, c_2, \dots c_k).$$
 (3.10)

The more interesting case is that of an essentially series network, i.e., a network that can be decomposed as a combination of subnetworks in series. We consider an exemplary network that splits into k branches, each with concurrence  $c_{p_i}$  (Fig. 3.3). The concurrence of the segment before branching is  $c_s$ . Following the series and parallel rules [Eqs. (3.6) and (3.7)], the sponge-crossing concurrence from the left of this network segment to the right is

$$C_{\rm SC} = \begin{cases} c_s \left( 2\sqrt{f(c_{p_0}, \dots c_{p_k}) - f(c_{p_0}, \dots c_{p_k})^2} \right) & f(c_{p_0}, \dots c_{p_k}) > 1/2, \\ c_s & f(c_{p_0}, \dots c_{p_k}) \le 1/2, \end{cases}$$
(3.11)

where  $f(c_{p_0}, \ldots c_{p_k}) = \prod_{i=1}^k g(c_{p_i}) = \prod_{i=1}^k \left(\frac{1+\sqrt{1-c_{p_i}^2}}{2}\right)$ . Under the parallel approximation, the network is transformed so that the concurrence of the segment is given by

$$C_{\rm SC}' = \begin{cases} 2\sqrt{f(c_s c_{p_0}, \dots c_s c_{p_k}) - f(c_s c_{p_0}, \dots c_s c_{p_k})^2} & f(c_s c_{p_0}, \dots c_s c_{p_k}) > 1/2, \\ 1 & f(c_s c_{p_0}, \dots c_s c_{p_k}) \le 1/2. \end{cases}$$
(3.12)

Since  $c_s c_{p_i} \leq c_{p_i}$ , it follows that  $g(c_s c_{p_i}) \geq g(c_{p_i})$  and  $f(c_s c_{p_0}, \dots, c_s c_{p_k}) \geq f(c_{p_0}, \dots, c_{p_k})$ . There are three cases:

- 1.  $1/2 \ge f(c_s c_{p_0}, \dots, c_s c_{p_k}) \ge f(c_{p_0}, \dots, c_{p_k})$ . In this case, it is obvious that  $C'_{SC} = 1 \ge C_{SC}$ .
- 2.  $f(c_s c_{p_0}, \ldots c_s c_{p_k}) \ge f(c_{p_0}, \ldots c_{p_k}) > 1/2$ . Now we consider the fraction

$$\left(\frac{C_{\rm SC}'}{C_{\rm SC}}\right)^2 = \frac{f(c_s c_{p_0}, \dots c_s c_{p_k})(1 - f(c_s c_{p_0}, \dots c_s c_{p_k}))}{c_s^2 f(c_{p_0}, \dots c_{p_k})(1 - f(c_{p_0}, \dots c_{p_k}))}.$$
(3.13)

The behavior of this expression can be inferred by considering some limiting cases. When  $c_{p_i} = 0$  for all *i* it results in  $C_{SC} = C'_{SC} = 0$ . If we increase the concurrence of a single branch *i* to be greater than 0 while holding the other branches to be zero, then the expression becomes

$$\frac{\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - c_s^2 c_{p_i}^2}\right)\left(1 - \left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - c_s^2 c_{p_i}^2}\right)\right)}{c_s^2 \left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - c_{p_i}^2}\right)\left(1 - \left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - c_{p_i}^2}\right)\right)} = 1,$$
(3.14)

which may be reexpressed as  $g(c_s c_{p_i})(1 - g(c_s c_{p_i})) = c_s^2 g(c_{p_i})(1 - g(c_{p_i}))$ . This result is simply a statement of the fact that, given only one branch, the parallel approximation is identical to the exact result (since there is one and only one path). We now add a second branch, j, while leaving the remaining k - 2 branches with zero concurrence. The ratio of the two values of concurrence now becomes

$$\left(\frac{C_{\rm SC}'}{C_{\rm SC}}\right)^2 = \frac{g(c_s c_{p_i})g(c_s c_{p_j})\left(1 - g(c_s c_{p_i})g(c_s c_{p_j})\right)}{c_s^2 g(c_{p_i})g(c_{p_j})\left(1 - g(c_{p_i})g(c_{p_j})\right)}.$$
(3.15)

For  $c_s \ll 1$  the fraction above reduces to

$$\frac{2c_{p_i}^2 + 2c_{p_j}^2}{c_{p_i}^2 + c_{p_j}^2 - \frac{1}{2}c_{p_i}^2 c_{p_j}^2 + c_{p_j}^2 \sqrt{1 - c_{p_i}^2} + c_{p_i}^2 \sqrt{1 - c_{p_j}^2}} \ge 1,$$
(3.16)

and approaches 1 as  $c_s$  goes to 1. The derivative with respect to  $c_s$ ,

$$\frac{\partial}{\partial c_s} \left(\frac{C_{\rm SC}'}{C_{\rm SC}}\right)^2 = -\frac{c_s c_{p_i}^2 c_{p_j}^2 \left(\sqrt{1 - c_s^2 c_{p_i}^2} + \sqrt{1 - c_s^2 c_{p_j}^2} + \sqrt{1 - c_s^2 c_{p_i}^2}\sqrt{1 - c_s^2 c_{p_j}^2}\right)}{2^3 g(c_{p_i}) g(c_{p_j}) \left(1 - g(c_{p_i}) g(c_{p_j})\right) \sqrt{1 - c_s^2 c_{p_i}^2} \sqrt{1 - c_s^2 c_{p_j}^2}},$$
(3.17)

is non-positive for  $0 \le c_s \le 1$ , indicating that the expression of the parallel approximation is never smaller than the true percolation. This tells us that the addition of another branch results in the expression of the parallel approximation becoming larger than the true concurrence calculated through series-parallel rules. As more branches are added to the expression the concurrence calculated through the parallel approximation remains larger than the true concurrence

$$\frac{C_{\rm SC}'}{C_{\rm SC}} = \sqrt{\frac{f(c_s c_{p_0}, \dots c_s c_{p_k})(1 - f(c_s c_{p_0}, \dots c_s c_{p_k}))}{c_s^2 f(c_{p_0}, \dots c_{p_k})(1 - f(c_{p_0}, \dots c_{p_k}))}} \ge 1.$$
(3.18)

Notice that while  $\{c_{p_i}\}$  need to be constrained such that  $f(c_{p_1} \dots c_{p_k}) > \frac{1}{2}$ , the above expression holds for all  $\{c_{p_i}\}$ .

3.  $f(c_s c_{p_0}, \ldots c_s c_{p_k}) > 1/2 \ge f(c_{p_0}, \ldots c_{p_k})$ . As before, we consider the fraction

$$\frac{C_{\rm SC}'}{C_{\rm SC}} = \sqrt{\frac{f(c_s c_{p_0}, \dots c_s c_{p_k})(1 - f(c_s c_{p_0}, \dots c_s c_{p_k}))}{c_s^2(1/4)}}$$
(3.19)

Since we require that  $f(c_{p_1} \ldots c_{p_k}) \leq 1/2$ , there is a lower bound to the smallest value of concurrence that any branch can have given by  $\min(\{c_{p_i}\}) \geq 4\left(\frac{1}{2}\right)^{1/k} \left(1 - \left(\frac{1}{2}\right)^{1/k}\right)$ . Additionally, as  $c_s \to 1$  the function  $f(c_s c_{p_1}, \ldots c_s c_{p_2})$  will becomes less than  $\frac{1}{2}$  and we will revert to case 1. Therefore there is also an upper bound on  $c_s$ . If we remain below this value and  $f(c_s c_{p_1} \ldots c_s c_{p_k}) > 1/2$  then for small  $c_s$  the expression reduces to

$$\frac{C_{\rm SC}'}{C_{\rm SC}} \approx \sqrt{\sum_{i=1}^{k} c_{p_i}^2},\tag{3.20}$$

$$\geq \sqrt{4k\left(\frac{1}{2}\right)^{1/k}\left(1-\left(\frac{1}{2}\right)^{1/k}\right)} \geq 1,\tag{3.21}$$

where the equality only holds for k = 1. As  $c_s$  approaches its allowed upper bound and  $f(c_s c_{p_1} \dots c_s c_{p_k}) \to 1/2$ 

$$\lim_{f(c_s c_{p_1} \dots c_s c_{p_k}) \to 1/2} \frac{C'_{\rm SC}}{C_{\rm SC}} = \sqrt{\frac{1}{c_s^2}} \ge 1.$$
(3.22)

Since this expression only differs from the previous case by terms in the denominator that do not depend on  $c_s$ , the derivative with respect to  $c_s$  for this case will also be non-positive for all values of  $c_s$ . Therefore

$$\frac{C'_{\rm SC}}{C_{\rm SC}} = \sqrt{4 \frac{f(c_s c_{p_0}, \dots c_s c_{p_k})(1 - f(c_s c_{p_0}, \dots c_s c_{p_k}))}{c_s^2}} \ge 1$$
(3.23)

We have shown that  $C'_{\rm SC}$  is an upper bound for  $C_{\rm SC}$  on series-parallel networks. Interestingly, as we will see, this upper bound seemingly becomes tighter as the network becomes larger. We hence expect that a new concurrence threshold on  $C'_{\rm SC}$  could even emerge, which should numerically approach the true  $c_{\rm th}$  from below and completely match  $c_{\rm th}$  in the thermodynamic limit  $n \to \infty$ .

## $S_m$ Approximation

For most regular lattices and complex networks, however, the distribution of  $N_l$  [Eq. (3.9)] is not so trivial. When we look at arbitrary networks, the calculation for the sponge-crossing concurrence is essentially a path-counting problem which may require approximation as well.

Although the literature of path counting on graphs is rich and well studied, unfortunately, there is almost no closed-form solution for enumeration of self-avoiding walks of arbitrary length for even the simplest network (like 2D lattices) [68]. While approximate path enumerations exist for both 2D lattices [69] and random networks [70], we find them impractical, since the concurrence calculation is very sensitive to  $N_l$  for small l. Indeed, observation of Eq. (3.9) implies that a single path's contribution to the total concurrence decreases with increasing l and increases with increasing  $N_l$ . Even though longer paths  $(l \simeq n)$  will outnumber shorter paths by several orders of magnitude, shorter paths will still contribute significantly more to the concurrence.

Based on this, if we define  $S_m$  as the set which contains up to the *m*th shortest paths (i.e., the shortest paths, the 2nd shortest paths, and so on up to the *m*th shortest paths) between s and t for all  $s \in S$  and  $t \in T$ , then it is possible to approximate the sponge-crossing concurrence between S and T using only these paths. When  $m = m_{\text{max}}$ ,  $S_m$  becomes the set of all sponge-crossing paths.

## 3.5 Results

In this Section, using our Fast ConPT computation, we present numerical results for different networks of large size n. We numerically estimate the finite-size ConPT threshold in terms of  $\theta_{\rm th} \equiv \frac{1}{2} \sin^{-1} c_{\rm th}$ , determining its position on the critical curve by matching the corresponding sponge-crossing concurrence at the half point,  $C_{\rm SC} = 1/2$ .

### 3.5.1 Bethe Lattice (Cayley Tree)

Given a finite Bethe lattice (i.e., a Cayley tree) with L layers and coordination number k [71], [72] all paths from the root node to any one of the boundary nodes have the same length, L. Since only one path exists from the root node to any node on the boundary, the number of paths of length L is

$$N_L = k(k-1)^{L-1}. (3.24)$$

There is no need to employ the  $S_m$  approximation since all paths are exactly known. Only the parallel approximation  $C'_{SC}$  of the sponge-crossing concurrence  $C_{SC}$  is to be calculated, which is given by [following Eq. (3.9)]

$$\frac{1+\sqrt{1-C_{\rm SC}'^2}}{2} = \max\left\{\left(\frac{1+\sqrt{1-c^{2L}}}{2}\right)^{N_L}, \frac{1}{2}\right\}.$$
(3.25)

To solve for  $c_{\rm th}$ , near  $C'_{\rm SC} = 0$  we let

$$\left(\frac{1+\sqrt{1-c_{\rm th}^{2L}}}{2}\right)^{N_L} = 1-\epsilon \tag{3.26}$$

given an arbitrarily small positive  $\epsilon$ . This gives rise to

$$c_{\rm th}^{2L} = 1 - \left[2\left(1-\epsilon\right)^{1/N_L} - 1\right]^2 \simeq -4N_L^{-1}\ln\left(1-\epsilon\right) + O(N_L^{-2}),\tag{3.27}$$

and thus

$$c_{\rm th} \simeq \left(\frac{4\epsilon}{k}\right)^{\frac{1}{2L}} \left(\frac{1}{k-1}\right)^{\frac{L-1}{2L}} \simeq \frac{1}{\sqrt{k-1}} \tag{3.28}$$

in the limit of large L. This is identical to the exact ConPT threshold calculated in Ref. [49] using a recursive renormalization trick on the series and parallel rules [Eqs. (3.6) and (3.7)].

Interestingly, it is known that a saturation point  $c_{\text{sat}} < 1$  also exists in ConPT [49], namely, before c reaches unity,  $C_{\text{SC}}$  will already reach unity at  $c = c_{\text{sat}}$ . This is because of the maximum function appearing in the parallel rule [Eq. (3.7)]. It is also obvious that  $c_{\text{sat}} \ge c_{\text{th}}$ , given the monotonicity of the series and parallel rules. To see if we can solve for  $c_{\text{sat}}$  using the parallel approximation too, let

$$\left(\frac{1+\sqrt{1-c_{\rm sat}^{2L}}}{2}\right)^{N_L} = \frac{1}{2},\tag{3.29}$$

set by  $C'_{\rm SC} = 1$ . This yields

$$c_{\text{sat}}^{2L} = 1 - \left[2\left(1/2\right)^{1/N_L} - 1\right]^2 \simeq 4N_L^{-1}\ln 2 + O(N_L^{-2}),\tag{3.30}$$



Figure 3.4: Sponge-crossing concurrence  $C_{SC}$  for the Bethe lattice with the parallel approximation for (a) k = 3 and (b) k = 4. As the network becomes larger the numerical values of  $\theta_{th}$  approaches the analytical value.

and thus

$$c_{\text{sat}} \simeq \left(\frac{4\ln 2}{k}\right)^{\frac{1}{2L}} \left(\frac{1}{k-1}\right)^{\frac{L-1}{2L}} \simeq \frac{1}{\sqrt{k-1}}.$$
 (3.31)

We see that the saturation point calculated using the parallel approximation is equal to  $c_{\rm th}$ , which is underestimated, since the true saturation point is given by [49]

$$c_{\rm sat} = \sqrt{\frac{(1/2)^{1/k} - (1/4)^{1/k}}{(1/2)^{(k-1)/k} - (1/4)^{(k-1)/k}}},$$
(3.32)

which can calculated similarly using a recursive renormalization trick on the series and parallel rules [Eqs. (3.6) and (3.7)].

For validation purposes, numerical results of the sponge-crossing concurrence on the Bethe lattice using the parallel approximation versus the true ConPT results are shown in Fig. 3.4. We see that as L increases, both  $c_{\rm th}$  and  $c_{\rm sat}$  (where  $c = 2\cos\theta\sin\theta$ ) approach  $1/\sqrt{k-1}$  from below and above, respectively, consistent with our theoretical result. Hence, it is highly suggested that the parallel approximation can correctly estimate the true ConPT threshold  $c_{\rm th}$  in the thermodynamic limit.

## 3.5.2 2D Square Lattices

In a 2D square lattice of n nodes  $(\sqrt{n} \in \mathbb{Z})$ , the length of the mth shortest selfavoiding path, between source and target nodes of coordinates  $s = (x_s, y_s)$  and  $t = (x_t, y_t)$  $(1 \le x_s, x_t \le \sqrt{n} \text{ and } 1 \le y_s, y_t \le \sqrt{n})$ , is simply

$$l_m = |x_s - x_t| + |y_s - y_t| + 2(m-1).$$
(3.33)

Now, let S and T denote the left  $(x_s = 1)$  and right  $(x_t = \sqrt{n})$  boundaries. Let  $s = (1, y_s) \in S$  and  $t = (\sqrt{n}, y_t) \in T$ . Under the  $S_m$  approximation, the total number of self-avoiding paths of length l between S and T is given by

$$N_{l} \approx \sum_{y_{s}=1}^{\sqrt{n}} \sum_{y_{t}=1}^{\sqrt{n}} \delta_{l_{1}l} N_{l_{1}}(s \to t) + \delta_{l_{2}l} N_{l_{2}}(s \to t) + \dots + \delta_{l_{m}l} N_{l_{m}}(s \to t), \qquad (3.34)$$

where  $\delta_{ij}$  is the Kronecker delta. This approximation of  $N_l$  is then substituted into the parallel approximation [Eq. (3.9)] to calculate  $C_{\rm SC}$  between S and T.

For  $m \leq 2$ , it is possible to directly enumerate the 1st and 2nd shortest self-avoiding paths between every pair of s and t. The general expressions are given by

$$N_{l_1}(s \to t) = \begin{pmatrix} |x_s - x_t| + |y_s - y_t| \\ |x_s - x_t| \end{pmatrix},$$
(3.35)

and

$$N_{l_{2}}(s \to t) = \sum_{x'=\max\{x_{s},2\}}^{\min\{x_{t}+1,\sqrt{n}\}} \sum_{y'=y_{s}}^{y_{t}-2} \binom{|x_{s}-x'|+|y_{s}-y'|}{|x_{s}-x'|} \binom{|x_{t}-x'+1|+|y_{t}-y'-2|}{|x_{t}-x'+1|} + \sum_{x'=x_{s}}^{x_{t}-2} \sum_{y'=\max\{y_{s},2\}}^{\min\{y_{t}+1,\sqrt{n}\}} \binom{|y_{s}-y'|+|x_{s}-x'|}{|y_{s}-y'|} \binom{|y_{t}-y'+1|+|x_{t}-x'-2|}{|y_{t}-y'+1|} + \mathcal{B}(x_{s},x_{t}) \binom{|x_{t}+1-x_{s}|+|y_{t}-1-y_{s}|}{|x_{t}+1-x_{s}|} + \mathcal{B}(y_{s},y_{t}) \binom{|y_{t}+1-y_{s}|+|x_{t}-1-x_{s}|}{|y_{t}+1-y_{s}|},$$

$$(3.36)$$



Figure 3.5: Counting the 2nd shortest path  $l_2$  for 2D square lattice. Every 2nd shortest self-avoiding path must contain one and only one of the configurations (solid line): either "Z"-shape (a-b) or "L"-shape (c-f), then the rest connected by shortest paths (dashed lines).

where the boundary effect

$$\mathcal{B}(u,v) = \mathcal{B}(v,u) = \begin{cases} 0, & u = 1, v = \sqrt{n} \\ 1, & u = 1, v < \sqrt{n} \text{ or } u > 1, v = \sqrt{n} \\ 2, & u > 1, v < \sqrt{n} \end{cases}$$
(3.37)

(w.l.o.g.,  $u \leq v$ ) is taken into account. In particular, Eq. (3.36) is given by the fact that every 2nd shortest self-avoiding path in the square lattice, having length  $l_2 = |x_s - x_t| + |y_s - y_t| + 2$ , must contain one and only one of the configurations as shown in Figs. 3.5a-3.5f. The first and second terms in Eq. (3.36) account for the two "Z"-shape configurations (Figs. 3.5a and 3.5b), respectively; the third term for the two "L"-shape configurations (Figs. 3.5c and 3.5d); and the last term for the other two "L"-shape configurations (Figs. 3.5e and 3.5f).

#### **Piecewise Path Enumeration Algorithm**

For m > 2, it becomes difficult to write down a closed-form combinatorial expression like Eqs. (3.35) and (3.36) for  $N_{l_m}(s \to t)$ . A path enumeration algorithm is thus needed. We treat paths of length  $l_m$  with m > 2 as deviations from the 1st and 2nd shortest paths. For a given m, these deviations can only take a finite number of shapes. Once we have identified these primitive deviations, we must next identify positions in the lattice where these deviations can be placed. Finally, we count the total number of paths by counting the number of shortest paths between deviations using Eqs. (3.35) and (3.36).

For example, given source and target nodes s and t, all 3rd-shortest paths (m = 3)have either two single-step deviations or one double-step deviation from the 1st shortest path. For the case where we have two single-step deviations, we first identify two sets of points,  $D_1$  and  $D_2$ , where the first and second deviations can happen respectively. Then we calculate  $N_{s,D_1}$  (the number of shortest paths from s to every point in  $D_1$ ),  $N_{D_1,D_2}$  (the number of shortest paths from every point in  $D_1$  to every point in  $D_2$ ), and  $N_{D_2,t}$  (the number of shortest paths from every point in  $D_2$  to t). The total number of 3rd-shortest paths is then given by  $N_{l_2}(s \to t) = N_{s,D_1}N_{D_1,D_2}N_{D_2,t}$ . This algorithm, while significantly faster than a brute-force path enumeration, is still too involved for large m. We use this algorithm to calculate  $S_3$  exclusively.

#### Numerical Calculations

The final numerical results of  $C_{\rm SC}$ , calculated using the exact combinatorial expressions  $(S_1, S_2)$  and/or the piecewise path enumeration algorithm  $(S_3)$ , are shown in Fig. 3.6. From Fig. 3.6b we see that for large enough m or n, the numerical threshold  $\theta_{\rm th}$  levels out at constant values that are very close to those calculated using the star-mesh transform. For example, for  $n^2 = 8$  the Fast ConPT method yields  $\theta_{\rm th} = 0.4$ , compared to the value of  $\theta_{\rm th} = 0.416$  calculated using the star-mesh transform [49]. This suggests that our Fast ConPT calculation can yield a good approximation of the ConPT threshold. We can also see from Fig. 3.7 that the Fast ConPT computation is over 100 times faster than the star-mesh transform method.



Figure 3.6: Fast ConPT calculation on 2D square lattices. (a) Sponge-crossing concurrence  $C_{SC}$  as a function of link weight  $\theta$ , calculated under the  $S_1$ - $S_3$  approximations. Only the result of  $S_3$  is plotted. The results of  $S_1$  and  $S_2$  are nearly identical to  $S_3$ . (b) Numerical ConPT threshold  $\theta_{th}$  under the  $S_m$  approximation. As m increases,  $\theta_{th}$ approaches a constant value. (c)  $\theta_{th}$  for different size n. (d) Same as (c) but for larger n.  $S_3$  becomes too computationally intensive to calculate for  $n > 20^2$ . As n increases,  $\theta_{th}$  also approaches a constant value.



Figure 3.7: Computing time (in seconds) to calculate  $C_{st}$ , the *s*-*t* concurrence between two nodes *s* and *t*, on 2D square lattices with  $n^2$  nodes. We can see that the Fast ConPT method speeds up the calculation over the star-mesh transform method by two orders of magnitude.



Figure 3.8: The *s*-*t* concurrence  $C_{st}$  between two maximally separated nodes as a function of link weight  $\theta$  for (a) Erdős–Rényi (ER) with  $\langle k \rangle = 4$ and (b) Barabási–Albert (BA) networks with coordination number z = 2, calculated under the  $S_1$  approximation.

## 3.5.3 Complex Network Topologies

Unlike 2D square lattices, we cannot write down any analytical expressions for the path length distribution of complex networks. While techniques to enumerate paths, such as those presented in Ref. [70], give a good estimate of the total number of paths, they approximate the path-length distribution poorly. This means that we must enumerate paths through brute force methods and this restricts our analysis to sparse graphs.

For complex networks, we simply define the sponge-crossing concurrence as the  $C_{st}$  between two nodes s and t which means that  $S = \{s\}$  and  $T = \{t\}$ . We choose s and t such that the shortest path between them is equal to the diameter of the network. In general there might be multiple choices for s and t that meet this criteria, and we randomly choose one of these pairs.

We randomly generate 100 networks of a given size and degree distribution and average the concurrence percolation threshold of each of these networks. These results are reported in Tab. 3.1 along with the standard error,  $\sigma/\sqrt{N}$ , where  $\sigma$  is the standard deviation and N = 100 is the number of samples of each random graph.

#### Erdős–Rényi Network

Results for Erdős–Rényi (ER) networks [3] are shown in Figs. 3.8a, 3.9a, and 3.9b. The concurrence is calculated under the  $S_6$  approximation for different settings of network sizes and average degrees. The results are averaged over 100 network realizations for each



Figure 3.9: (a) The behavior of  $\theta_{th}$  for ER networks with  $\langle k \rangle = 4$  and  $\langle k \rangle = 8$ under the  $S_1$  approximation with increasing network size. (b) The behavior of  $\theta_{th}$  for ER networks with n = 500 and n = 1000 as a function of  $\langle k \rangle$  for the  $S_1$  approximation. The circles are the simulated values of the percolation threshold and the dotted lines are a power-law fit with  $\theta_{th} \propto \langle k \rangle^{-0.5}$  (c) The behavior of  $\theta_{th}$  on BA networks with z = 1 and z = 2 under the  $S_1$  approximation with increasing network size. (d) The behavior of  $\theta_{th}$  for BA networks with n = 500 and n = 1000 as a function z under the  $S_1$ approximation.



Figure 3.10: The behavior of  $\theta_{th}$  with increasing m in the  $S_m$  approximation for ER networks. The relationship can be approximated with a power law with exponent  $\phi$ .

setting. Fig. 3.9a shows that the value of  $\theta_{\rm th}$  converges with increasing network size for smaller values of the average degree, e.g.  $\langle k \rangle = 4$ . For larger values of the average degree, such as  $\langle k \rangle = 8$ , we do not see the value of the threshold converging for the same network size.

The calculation of the number of paths becomes increasingly computationally intensive for larger values of the average degree and we must restrict our analysis to small values of m. Fig. 3.9b shows how the concurrence percolation threshold changes as a function of average degree under the  $S_1$  approximation.

For small values of m, the behavior of the concurrence for ER networks can be approximated with a power-law fit, as shown in Fig. 3.10. These results are also shown in Table 3.1.

### Barabási–Albert Network

Many real-world networks show power-law degree distribution, such as the Internet, WWW, scientific collaboration networks, protein-protein interaction networks, and actor networks [2], [73]. Barabási–Albert (BA) model [5] is the first model to describe the structure property of such networks, using preferential attachment. In this model, every new node in the graph is assigned z edges, where z is known as the coordination number, and nodes with higher degrees are more likely to be selected. The classical bond percolation threshold for a BA network with z > 1 and  $n \to \infty$  is  $p_c = 0$  [74], [75].

Results for BA networks are shown in Figs. 3.8b, 3.9c, and 3.9d. For z = 1 there are no loops in the network and the relatively small number of paths connecting any two nodes allows us to calculate the concurrence for up to  $10^4$  nodes, shown in 3.9c. We also look at smaller networks with higher coordination numbers, up to z = 25, shown in Fig. 3.9d. Unlike ER networks, the value of  $\theta_{\rm th}$  decreases with the increasing network size.

#### Comparison with Classical Entanglement Percolation (CEP)

As a baseline comparison, we numerically calculate  $\theta_{th}^{CEP}$ , the percolation threshold associated with Classical Entanglement Percolation (CEP) for ER networks. As before we define the percolation threshold on random networks as the minimum entanglement necessary for the existence of a path between two nodes s and t, where s and t are a randomly selected pair of nodes with the property that their distance is the diameter of the network. We



Figure 3.11: A comparison of  $\theta_{\text{th}}^{\text{CEP}}$ , the entanglement percolation threshold calculated under CEP, with  $\theta_{\text{th}}$ , the approximate concurrence percolation threshold for different network sizes and different values of m. The black line represents x = y and is added for comparison.

generate 100 random networks and eliminate edges with probability 1 - p, where  $p = 2 \sin^2 \theta$ is the singlet conversion probability. For each network we perform 1000 simulations and calculate  $\theta_{\text{th}}^{\text{CEP}}$  as the average minimum value of  $\theta$  such that the probability of the existence of a path between s and t is 0.5. We also calculate  $\theta_{\text{th}}(m)$  for these networks. The results are shown in Fig. 3.11. We can see that for all our samples  $\theta_{\text{th}}(1) < \theta_{\text{th}}^{\text{CEP}}$ . Since CEP represents the naive, baseline measurement strategy it is encouraging that our approximate ConPT threshold always lies below it even when we restrict ourselves to m = 1. Therefore  $\theta_{\text{th}}$  heuristically approaches a lower-bound on the true concurrence and even for low values of m it predicts a lower concurrence percolation threshold than that predicted by CEP.

## **3.6** Discussion and Conclusions

Table 3.1 summarizes the numerical results of our fast concurrence percolation theory (Fast ConPT) computation compared with previously known results [49]. The algorithm we have presented in this report utilizes two approximations to allow for numerical calculations of ConPT. Where available, our results are in good agreement with the analytical values of

the concurrence percolation. We have also extended the analysis of the ConPT threshold to complex networks and demonstrated that our method could be applied to square lattices of 200<sup>2</sup> nodes and complex networks of 300 nodes. Combining our method with more efficient path-counting algorithms would allow us to probe a more significant fraction of the total paths of a network for the ConPT calculation and provide a more robust estimate for the ConPT threshold. We believe that this work is an important step towards understanding the structural and communication properties of large-scale quantum networks.

We believe that ConPT is a promising tool for practically designing and analysing quantum networks. It offers crucial insights into how entanglement strength, viewed as a costly resource, should be distributed throughout a network to ensure resilient communication. In full-optical quantum communication networks, for example, entanglement strength is usually expressed as a function of the number of entangled photons shared between nodes [76]. Current methods used in simulations to determine the entanglement strength necessary for the emergence of a giant-component in quantum networks or the connectivity of two random nodes implicitly assume the CEP measurement strategy, i.e., they assume that the topology of the quantum network is immutable like that of a classical network [76], [77]. The numerical methods we have presented in this paper allow concurrence percolation theory to be practically useful in the analysis of large complex networks, providing a lower bound on the entanglement strength necessary for communication between distant nodes, therefore allowing the cost associated with establishing communication channels of a certain strength in these networks to be lowered. As we showed in our comparison with CEP, even for m = 1 the Fast ConPT method already predicts a lower entanglement percolation than CEP, demonstrating its effectiveness for determining how close any given measurement strategy is to being optimal.

Still, the critical behaviors of ConPT near  $\theta_{\rm th}$  remain an interesting and open question. Previous studies have indicated that some critical phenomena, such as the emergence of subgraphs, are drastically different in quantum random networks than in classical networks [26]. While Meng et al. has provided a finite-size analysis of the critical behaviors of Bethe lattices, their analysis of 2D lattices is limited by the size of the lattices they could investigate [49]. Their initial results indicate that the critical exponent  $\nu$  associated with ConPT on 2D lattices are the same as those of classical percolation theory. This can now be investigated more thoroughly using the algorithm presented in the present work.

# CHAPTER 4 MODELING EPIDEMIC SPREAD IN CITIES USING PUBLIC TRANSPORTATION AS A PROXY FOR GENERALIZED MOBILITY TRENDS

## 4.1 Introduction

Long-range mobility, such as traveling between cities, can cause a disease to spread through case importation across large distances [78], [79]. Short-range mobility, such as usage of city buses or trams, has been correlated with a higher risk of contracting acute respiratory infections [80] and with the number of cases of COVID-19 within cities [81], [82]. Accordingly, restrictions on human mobility, either directly by shutting down public transportation [83], [84] or indirectly by restricting public and private gatherings [85], which were highly effective in stopping the spread of COVID-19. We hypothesize that alongside being a high-risk medium for infections, public transportation usage is also a good indicator for the level of short-range mobility for the entire population of a city.

## COVID-19 in New York City

When it became clear that the COVID-19 virus is highly infectious, New York City (NYC) imposed restrictions that included shutting-down non-essential businesses and forbidding large gatherings, but kept public transportation [86] and schools open [87]. The usage of NYC's sprawling subway system was found to be correlated with the spread of COVID-19 [81], [82], [88] and mobility patterns in general were correlated with the spread of COVID-19 within regions of the city [89], [90]. There are various models of disease spread that incorporate human mobility patterns, such as a recent disease transmission model inspired by collision theory gas-phase chemistry [91], or a metapopulation model that allows for the movement of individuals between subpopulations [92]. We propose a model based on SIR dynamics where we explicitly model human mobility as a parameter and treat the infection rate as a function of the mobility of a region. To effectively model the spread of COVID-19 in NYC, we focus on data from the NYC subway. We hypothesize that trends in

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Figure 4.1: (a) The red line shows the daily reported cases of COVID-19 in New York City. The blue line shows the total daily number of trips taken on the subway, with entries related to the Port Authority Trans-Hudson (PATH) removed. The dotted line indicates the start of the NY PAUSE Program, (b) The fraction of total weekly cases reported on each day of the week, averaged over 44 weeks. While the weekdays remain largely consistent, there is a significant drop in reporting on weekends.

subway usage are correlated with the usage of other modes of transport, such as buses, taxis etc. We therefore treat subway usage as an indicator for broader human mobility patterns in the city.

# 4.2 Data

### New York City Subway Turnstile Data

Unlike pedestrian traffic, private automobiles, and to some extent taxis, public transportation, and in particular the subway, has detailed records of passenger traffic such as the total number of entries and exits from a station collected in real time. This enables us to extract some important statistics regarding passenger traffic using publicly available data on subway usage published by the Metropolitan Transportation Authority (MTA) [93]. As awareness of the pandemic grew in early 2020 the Governor of New York announced a state of emergency on March 7 2020, followed shortly by the passage of an executive order, known as 'New York State on PAUSE', that shutdown all non-essential businesses in the state [94], [86]. New York City saw a decline in subway usage alongside various other modes of public transport, including bikeshares [95], [96], and taxis [97]. As restrictions were slowly eased in the later half of the year, there was a corresponding increase in the usage of public transport, although some modes were preferred over others at different rates than before the pandemic. Bikehares, for example, had recovered to their 2019 levels by September 30, 2020 while subway ridership was at 30% of pre-pandemic levels [95]. Despite the different rates at which different modes recovered, both bikeshares and the subway saw increases in usage in the latter half of 2020. We believe that this increase in both modes of transport corresponds to the underlying increase in human mobility as restrictions were loosened after June 8, 2020. This motivates us to use this directly measurable traffic as a proxy for all traffic in the city.

We collected and analyzed the subway turnstile data of New York City for 12 consecutive months, starting from January 2020 to December 2020. The MTA publishes turnstile data on a weekly basis, which includes administrative information such as the control area, unit number, station name and line name, as well as the counts of the entries and exits at a specific time for a particular turnstile [93]. The system collects these counts every four hours, each of which is a cumulative register value. The data were first converted into dataframes and then into a combination of control area code, remote unit, subunit channel position (SCP), as well as the time of the observation that serves as a unique ID to identify and remove duplicate records. We removed entries related to Port Authority Trans-Hudson (PATH) trains, since they do not represent the mobility among NYC boroughs. The absolute difference between the first and last counts at a turnstile on a particular day defines the number of subway riders passing through that particular turnstile. The geographic coordinates of the station and the borders of each borough allow us to place each station in its corresponding borough. We calculated the total number of borough-level subway riders by summing the numbers of riders at all the turnstiles of all subway stations located within each borough. To estimate the mobility between boroughs, we used a survey that was conducted among subway riders regarding the origin and destination of their trips [98]. Given the number of departures at a given station, we used probabilities extracted from the survey to determine the destinations of those trips.

#### COVID-19 Data

We used publicly available data published by the NYC government about the number of new COVID-19 cases reported for each day and for each of the five boroughs [99]. Fig 4.1a shows that this data has a clear weekly cyclical pattern. Fig 4.1b shows that this pattern arises because of the much smaller numbers of cases that were reported on weekends than on weekdays. We remove this pattern by using a running 7-day average of the number of daily cases.

We also chose to restrict our analysis to 2020, since the introduction of vaccines in early 2021 decreases the number of people susceptible to infection. To account for this decrease on the spread of epidemics would require the introduction of another parameter that might change the quantitative effect of mobility on the spread of the disease.

## **Population Data**

All population data for New York City were taken from the 2020 census conducted by the US Census Bureau and published on their website [100].

# Model

We start with the well-established SIR model [2],[?]. While more powerful models for modelling disease spread exist, such as the SEIR model [101], we picked the SIR model in order to reduce the number of parameters and avoid overfitting. The COVID-19 hospitalization data that we use only reports daily newly infected cases and we do not believe this data is fine-grained enough to justify the use of a more complex model. The SIR model divides the total population (N) into susceptible (S), infected (I), and recovered or dead (R) compartments. The equations governing the spread of the disease are

$$\frac{d}{dt}S(t) = -\beta \frac{S(t)I(t)}{N},\tag{4.1}$$

$$\frac{d}{dt}I(t) = \beta \frac{S(t)I(t)}{N} - \gamma I(t), \qquad (4.2)$$

$$\frac{d}{dt}R(t) = \gamma I(t), \tag{4.3}$$

where  $\beta$  and  $\gamma$  are the infection and recovery rate, respectively.



Figure 4.2: (a) Schematic representation of the mobility-based SIR model. Each region j has an associated infection rate  $\beta_j$  and mobility parameters  $f_{jj'}$  and  $f_{j'j}$ , which represent individuals from region jvisiting region j' and vice versa. (b) The enhanced model that includes a public transportation node without a permanent population. Inter-region mixing still occurs as in the basic model, but the visiting populations of every region pass through the transportation node for the duration of their commute time during which they are exposed to the higher infection rate associated with using public transportation. The effective population of region jthat is commuting is given by  $f_{jT}$  while the effective population of all other regions that are visiting region j are given by  $f_j^+$ .

We modify the model by dividing the total population into subpopulations called regions, each with a fraction of the population  $p_j$  living in region j, thus  $\sum_j p_j = 1$ . When we apply the model to New York City the different  $p_j$  represent the populations of the five boroughs of New York City, normalized by the total population of the city, which was 8,804,190 in 2020 [100]. Within a region, people will have different infection rates based on their activity. The infection rate for individuals working from home and following strict quarantine protocols will be lower than the rate for frontline workers. Each activity-based cohort has an associated infection rate  $\beta_{jc}$ . Additionally, people may also have access to different quality of healthcare, which may impact the frequency of testing and the likelihood of visiting a doctor. Both of these parameters influence the recovery rate of a patient. Each healthcarebased cohort has an associated recovery rate  $\gamma_{je}$ . The fraction of the total population in region j with behavior c and healthcare e is denoted as  $p_{jce}$ . For parameters representing the population fractions, an omitted index indicates a sum over all values of this index, so  $p_{jc} = \sum_e p_{jce}$  and  $p_j = \sum_{c,e} p_{jce}$  etc.

Each cohort within each region follows SIR dynamics. The equations governing the population fractions of susceptible, infected and recovered individuals are given by:

$$s_{jce}(t + \Delta t) = s_{jce}(t) \left(1 - \beta_{jc} i_{jce}(t) \Delta t\right), \qquad (4.4)$$

$$i_{jce}(t + \Delta t) = i_{jce}(t) + \left(\beta_{jc}s_{jce}(t)i_{jce}(t) - i_{jce}(t)\gamma_{je}\right)\Delta t, \tag{4.5}$$

$$r_{jce}(t + \Delta t) = r_{jce}(t) + i_{jce}(t)\gamma_{je}\Delta t, \qquad (4.6)$$

where  $s_{jce}(t)$ ,  $i_{jce}(t)$  and  $r_{jce}(t)$  are the population fractions of susceptible, infected and recovered individuals, respectively at time t.

## Inter-region Mixing

So far our model follows straightforward SIR dynamics. We now want to introduce inter-region mixing through a mixing parameter that tells us the population fraction of one region that is visiting another region at a given time. In order to calculate this quantity, we need to know the origin, destination, and trip duration for every rider using the subway. From the data, we only know the borough of departure. We do not know an individual rider's destination based just on the borough they departed from. Using an MTA survey on the use of the NYC subway, we can determine the probabilities of a trip departing and terminating at different boroughs [98].

In order to determine the average time spent visiting a borough, we also need to know the borough of origin of riders arriving at a station. From the survey, we know  $P(o_j)$ , the probability of any trip originating in borough j,  $P(d_j)$ , the probability of any trip terminating in borough j, and  $P(d_{j'}|o_j)$ , the probability that a trip originating in borough j terminates in borough j' [98].

It will be helpful to define a fractional time,  $\tau$ , which measures the time of day as the fraction of the day that has passed since midnight. So, for example, 3 PM corresponds to a fractional time of  $\tau = 0.625$ . In order to determine the average duration that residents of one borough spend in another borough, we start by treating NYC as a closed system where individuals do not travel into or out of the city, and all residents of a borough return to it at the end of the day. If a rider k leaves borough j at fractional time  $\tau_{A_k}$  and returns at  $\tau_{D_k}$ , then the fraction of the day spent away from the borough is  $\tau_{A_k} - \tau_{D_k}$ .

If there are  $M_t$  total riders on day t, then the average fraction of the day spent away from the borough on that day is  $\frac{\sum_{k=1}^{M_t} (\tau_{A_k} - \tau_{D_k})}{M_t}$ . This average can be rewritten by collecting all the arrival and departure times separately rather than tracking each rider's individual arrival and departures so that  $\frac{\sum_{k=1}^{M_t} \tau_{A_k} - \sum_{k=1}^{M_t} \tau_{D_k}}{M_t}$ . The subway turnstile data does not track the arrival and departure of individual riders. Instead, it provides a number of snapshots everyday of the cumulative arrivals and departures. So, the data instead provides us with the number of arrivals,  $A_{t,j}(\tau_k)$ , and departures,  $D_{t,j}(\tau_k)$ , at fractional time  $\tau_k$ , where the index k no longer refers to riders, but to the different times at which the number of entries and exits are recorded. We can then write the average fractional time spent by residents of borough j away from their home borough

$$\Delta \tau_j = \frac{1}{t_{\text{tot}}} \sum_{t=1}^{t_{\text{tot}}} \frac{\sum_k \tau_k \left( A_{t,j}(\tau_k) - D_{t,j}(\tau_k) \right)}{M_t},$$
(4.7)

where  $t_{tot}$  is the total number of days. It should be noted that the sum over k is no longer over the number of riders, but over the number of snapshots of total entries and exits taken that day.

For a variety of reasons, such as travel into and out of the city and the usage of multiple modes of transport, the number of arrivals and departures at a station will not match exactly. In order to account for this, we match the number of arrivals and departures at a given snapshot in time in the data, and any discrepancy is added to the next time bin. Once all time periods have been accounted for, any unmatched arrivals or departures are ignored. The equation then becomes

$$\Delta \tau_j = \frac{1}{t_{\text{tot}}} \sum_{t=1}^{t_{\text{tot}}} \frac{\sum_k \tau_k \min\left(\tilde{A}_{t,j}(\tau_k), \tilde{D}_{t,j}(\tau_k)\right)}{\tilde{M}_t},$$
(4.8)

where

$$\tilde{A}_{t,j}(\tau_k) = A_{t,j}(\tau_k) + U_t^A(\tau_k), \qquad (4.9)$$

$$\tilde{D}_{t,j}(\tau_k) = D_{t,j}(\tau_k) + U_t^D(\tau_k),$$
(4.10)

$$U_t^D(\tau_k) = \max\left(0, \tilde{D}_{t,j}(\tau_{k-1}) - \tilde{A}_{t,j}(\tau_{k-1})\right),$$
(4.11)

$$U_t^A(\tau_k) = \max\left(0, \tilde{A}_{t,j}(\tau_{k-1}) - \tilde{D}_{t,j}(\tau_{k-1})\right),$$
(4.12)

$$U_t^D(\tau_0) = U_t^A(\tau_0) = 0, (4.13)$$

$$\tilde{M}_t = \min\left(\sum_k A_{t,j}(\tau_k), \sum_k D_{t,j}(\tau_k)\right),\tag{4.14}$$

where  $U_t^A(\tau_k)$  and  $U_t^D(\tau_k)$  are the unmatched arrivals and departures from the previous time period. An example of the matching process is shown in Tab 4.1. We can now write our mixing parameter

$$f_{jj'}(t) = \Delta \tau_j P(d_{j'}|o_j) \sum_k \frac{D_{t,j}(\tau_k)}{N}.$$
 (4.15)

On any given day we could estimate the number of people, expressed as a fraction of the total population, that travel from borough j to borough j' by  $P(d_{j'}|o_j) \sum_k \frac{D_{t,j}(\tau_k)}{N}$ . This would give us an estimate of how many of the people leaving borough j are heading towards j'. However, we do not have detailed temporal resolution on the movement of riders within a borough and we do not know when any individual rider returns to their home borough. We define an effective population of visitors by multiplying this quantity with  $\Delta \tau_j$ , the estimate of the average time fraction spent away from borough j, that spend the entire day in borough j'. The mixing parameter represents this effective visiting population.

The population fraction that leaves region j for all other regions is  $f_j^- = \sum_{j' \neq j} f_{jj'}$ , while the population fraction that arrives at region j from all other regions is  $f_j^+ = \sum_{j' \neq j} f_{j'j}$ . The resulting total population fraction in region j becomes  $p_j + f_j^+ - f_j^-$ .

We must now keep track of the part of the susceptible and infected populations of region j that do not leave the region, which we call 'stationary', given by

$$s_{jce}^{S} = s_{jce} \frac{p_j - f_j^-}{p_j}, \tag{4.16}$$

$$i_{jce}^{S} = i_{jce} \frac{p_j - f_j^-}{p_j}.$$
(4.17)

It should be noted that while this 'stationary' population does not leave the borough, the individuals that constitute this population may still be mobile within their borough. This will be addressed later in this section. We also keep track of infected individuals visiting region j from other regions. These are given by

$$i_{jce}^{+} = \sum_{j' \neq j} i_{j'ce} \frac{f_{j'j}}{p_{j'}}.$$
(4.18)

We can now write down the equations for the stationary susceptible and infected populations for region j:

$$s_{jce}^{S}(t + \Delta t) = s_{jce}^{S}(t)(1 - \beta_{jc}i_{jce}^{S}(t)\Delta t - \beta_{jc}i_{jce}^{+}(t)\Delta t).$$
(4.19)

We also need to track individuals from region j who are visiting region j'. These are given by

$$s_{jce}^{V} = \sum_{j' \neq j} s_{jce}^{j'} = \sum_{j' \neq j} s_{jce} \frac{f_{jj'}}{p_j}.$$
(4.20)

These individuals will interact with stationary infected individuals from other regions. We can now write the equations for the individuals from region j visiting all other regions

$$s_{jce}^{V}(t + \Delta t) = \sum_{j' \neq j} s_{jce}^{j'}(t)(1 - \beta_{j'c}i_{jce}^{+}(t)\Delta t - \beta_{j'c}i_{j'ce}^{S}(t)\Delta t),$$
(4.21)

We can combine the equations for the stationary and visiting populations by introduc-

ing a flow parameter

$$\lambda_{jce} = s_j^S \beta_{jc} \left[ i_{jce}^S + i_{jce}^+ \right] + \sum_{j' \neq j} s_j^{j'} \beta_{j'c} \left[ i_{jce}^+ + i_{j'ce}^S \right].$$
(4.22)

The flow parameter lets us compactly write the dynamics of region j

$$s_{jce}(t + \Delta t) = s_{jce}(t) - \lambda_{jce}(t)\Delta t, \qquad (4.23)$$

$$i_{jce}(t + \Delta t) = i_{jce}(t) + (\lambda_{jce}(t) - i_{jce}(t)\gamma_{je})\Delta t, \qquad (4.24)$$

$$r_{jce}(t + \Delta t) = r_{jce}(t) + i_{jce}(t)\gamma_{je}\Delta t.$$
(4.25)

Since the data provided by the NY government tracks the number of newly reported cases and does not report the number of active cases (i(t) in our model) we construct the quantity

$$i_{jce}^{\text{new}}(t) = \sum_{t'=t}^{t+1-\Delta t} \lambda_{jce}(t')\Delta t, \qquad (4.26)$$

where t is in units of days. In other words,  $i_{jce}^{\text{new}}(t)$  represents the number of new cases reported on day t and this is the quantity that we will fit to the data. Fig 4.2a shows a schematic representation of our mobility-based SIR model.

#### Introducing a Public Transportation Node

While our model accounts for the spread of disease through the transit of infected individuals between regions, it does not take into account that use of public transportation poses a higher risk of infection [80]. To account for this effect, we introduce a public transportation node, denoted by the index T. The fraction of the population permanently residing on this node is 0 ( $p_T = 0$ ). We modify our model so that all riders travelling to another borough spend some part of their time at node T. This duration is taken from the average commute time reported by riders of each borough [98]. The mixing parameter from node j to node Tbecomes Table 4.1: An example of the matching process using real data. The columns labelled ENTRIES, EXITS, and TIME are from the turnstile data. We calculate the number of arrivals,  $A_{t,j}(\tau)$ , by subtracting successive values of the running total of entries. These arrivals are assigned a fractional time,  $\tau$ , corresponding to the midpoint of successive time snapshots. The departures,  $D_{t,j}(\tau)$ , are calculated in the same way.

ENTRIES	EXITS	TIME	τ	$A_{t,j}(\tau)$	$D_{t,j}(\tau)$	$U_t^A(\tau)$	$U_t^D(\tau)$	$\tilde{A}_{t,j}(\tau)$	$\tilde{A}_{t,j}(\tau)$
0007328037	0002483731	03:00:00							
0007328044	0002483742	07:00:00	0.208	7	11	0	0	7	11
0007328075	0002483781	11:00:00	0.375	31	39	0	4	31	43
0007328193	0002483821	15:00:00	0.542	118	40	0	11	118	51
0007328375	0002483878	19:00:00	0.708	182	57	67	0	249	57
0007328499	0002483910	23:00:00	0.875	124	32	192	0	316	32

$$f_{jT}(t) = \Delta \tau_{jT} \sum_{j' \neq j} P(d_{j'}|o_j) \sum_k \frac{D_{t,j}(\tau_k)}{N},$$
(4.27)

where  $\Delta \tau_{jT}$  is the commute time for riders in node t, expressed as a fraction of the day. Due to the introduction of a transport node we must also modify our expression for the inter-borough mixing parameter, which becomes

$$f_{jj'}(t) = (\Delta \tau_j - \Delta \tau_{jT}) P(d_{j'}|o_j) \sum_k \frac{D_{t,j}(\tau_k)}{N}.$$
 (4.28)

Fig 4.2b shows a schematic depiction of the model with the public transportation node. The introduction of such a node allows us to independently model the infection rate during rides on public transportation systems,  $\beta_T$ , for individuals using public transportation. Since our model does not track individual interactions but rather only the infection rate at the population level we introduce the transport node to model the different risks of infection experienced by the fraction of the population that uses the subway where they interact with a different mixture of populations than the mixture that they encounter in the borough in which they live.

#### Mobility-dependent Infection Rate

While inter-region mixing and the introduction of a public transportation node account for mobility between regions, we also need to account for mobility within a region. To do this, we introduce a mobility parameter for each region,  $m_j(t)$ , which represents the extent to which individuals are moving within the region. We then write our infection rate as

$$\beta_{jce}(t) = \beta_{jce}^0 m_j(t), \qquad (4.29)$$

where  $\beta_{jce}^0$  is the static infection rate. This is similar to the mobility-informed approach used in [91]. For the particular case of the NYC subway,  $m_j(t)$  is calculated by taking a 7-day moving average of the total trips that start in borough j and rescaling this quantity by dividing it by the maximum number of trips taken in one day in borough j in this training period, thereby scaling it between 0 and 1. A plot of the average mobility parameter, defined as  $m_{\text{avg}}(t) = \sum_j p_j m_j(t)$ , is plotted in Fig. 4.4b. We are using the level of subway usage as a stand-in for all short-range mobility. We found that the number of bike-share rides taken during the pandemic was correlated with the number of subway trips [96]. We assume that subway usage is correlated with all mobility within the city, even as subway usage fell during the pandemic across cities around the world [102].

## 4.3 Results

While our model is able to incorporate complex demographic information such as healthcare status, access to testing, and public policies regarding gathering sizes and mask usage, we are limited by the data to which we have access. Since we only have public transportation data and the daily case count, we will assume that each region in our model, corresponding to one of the five boroughs of NYC, has a uniform demographic distribution. This means that we will be ignoring the c and e indices in our model.

In order to model the effect of different policies, we pick March 22, 2020, the official start day of the NY PAUSE Program, as the beginning of the lockdown. We assume that there are *two different* infection rates, one before and the other after this date. This assumption is made because the PAUSE program marks the start of the implementation of widespread mask usage and social distancing. These are non-mobility factors which impact the overall infection rate.



Figure 4.3: (a) The best-fit model output of the daily number of new cases in NYC. The black line shows the model's output. The red line is the 7-day running average of the total daily reported cases in NYC as a fraction of the total population of the city. The dotted line indicates the start of the NYC Pause Program. (b) Fitting results for the model *without* the mobility-dependent infection rate given by Eq. 4.30. As the plot demonstrates, we cannot fit NYC's COVID-19 spread without modifying the infection rate by the mobility term.

We also assume that the intensity of usage of public transportation is correlated with the infection rate. The infection rate for borough j then becomes

$$\beta_i(t) = \beta^{\mathrm{p}}(t)m_i(t-t_D), \qquad (4.30)$$

where  $\beta^{p}(t) = \beta^{h}$  before the start of the NY PAUSE Program on March 22 2020, and  $\beta^{p}(t) = \beta^{l}$  afterwards. The second term,  $m_{j}(t - t_{D})$ , represents the normalized daily number of trips taken on the subway within a region. The parameter  $t_{D}$  accounts for the population level delay between subway usage and the subsequent increase in Covid-19 cases. We also average  $\beta_{j}(t)$  over a 7 day moving window in order to smooth out abrupt changes due to both noise in  $m_{i}(t)$  and the discontinuous transition in  $\beta^{p}(t)$ .

We have the values of  $f_{jj'}(t)$  and  $m_j(t)$  from the data, Using these two values, we can construct  $f_{jT}$ . We need to learn the values of  $\beta^{\rm h}, \beta^{\rm l}, \gamma$  and  $\tau_D$ . We also need to learn the values of  $\beta^{\rm h}_T$  and  $\beta^{\rm l}_T$ , the infection rate on the subway before and after the start of the PAUSE
program. Fig. 4.3a plots the results of fitting the model by minimizing the mean squared error (MSE). We fit our model by sweeping over a million values for these parameters, with our search guided by existing literature on the infection and the recovery rates [103]. By contrast, we can see from 4.3b that an SIR model that does not take into account mobility cannot explain the infection trend.

#### Forecasting

We also masked the last three weeks of data and trained our model without this period. First, we do a parameter sweep to find the values of the parameters that best fit the training data. Next, we use the end of the training period,  $i_{data}^{new}(t_{train})$  (where  $t_{train}$ , is the last day of the training data) as the initial condition for the testing period. However, we cannot directly use the number of daily new cases as the initial condition. Instead, the model requires knowledge of the active infected and total recovered cases,  $i(t_{train})$  and  $r(t_{train})$ , at the end of the training period as the initial conditions for the testing period. This was not a concern when we were fitting our model for the training period since we assumed that i(0) = 1/N and r(0) = 0. In order to predict the spread of the disease in the testing period, however, we need to know these quantities to serve as the initial conditions for our model. While data are available for the number of active and recovered cases for New York state, they are not available for New York City. We estimate the total recovered population by dividing the cumulative deaths reported in New York City by the state-wide case mortality rate [104]

$$r_{\rm est}(t) = \frac{\text{Cumulative deaths reported in NYC on day }t}{N * \text{Case mortality rate on day }t},$$
(4.31)

where  $r_{\text{est}}(t)$  is the estimated total recovered population (which includes both individuals who have died as well as those who have recovered from the disease) expressed as a fraction of the total population of New York City. We also need to know  $i_{\text{est}}(t)$ , the estimated total active number of infected cases. Specifically, we only need to estimate  $i_{\text{est}}(t_{\text{train}})$ , the total number of active cases on the last day of the training data. We do this by searching for a value of  $i_{\text{est}}(t_{\text{train}} - 1)$  such that using  $i_{\text{est}}(t_{\text{train}} - 1)$  and  $r_{\text{est}}(t_{\text{train}} - 1)$  as the initial condition for our model and predicting the daily number of cases for the next day gives us Table 4.2: The results from fitting the data with and without the last three weeks masked.  $E_{in}$  refers to the MSE of fitting the data, while  $E_{out}$ shows the MSE of the model's prediction during the testing period. While we minimize the MSE during the fitting process, the table also reports the in-sample and out of sample  $R^2$  score of the best fit. We use  $\Delta t = 10^{-2}$  for all our simulations.

Parameter Values	Data fitting	Data fitting with
	without testing period	three-week testing period
$\beta^{\mathrm{h}}$	1.55	1.59
$\beta^{\mathrm{l}}$	0.55	0.53
$eta_T^{ m h}$	4	4
$eta_T^{ m l}$	4	4
$\gamma$	0.04	0.04
$t_D$	21 days	21 days
$E_{ m in}$	$4.46 * 10^{-9}$	$2.98 * 10^{-9}$
$E_{\mathrm{out}}$	-	$2.44 * 10^{-10}$
$R_{\rm in}^2$	0.82	0.88
$R_{\rm out}^2$	-	0.43

$$i^{\text{new}}(t_{\text{train}}) = i^{\text{new}}_{\text{data}}(t_{\text{train}}), \qquad (4.32)$$

where  $i^{\text{new}}(t_{\text{train}})$  are the daily number of new cases output by our model on the last day of the training data. The corresponding values of  $i_{\text{est}}(t_{\text{train}})$  and  $r_{\text{est}}(t_{\text{train}})$  become the initial conditions for the model at the start of the testing period. The model's prediction is shown in Fig. 4.4a. Tab. 4.2 shows the parameters that minimize the MSE with and without a testing period.

## 4.4 Discussion

Fig. 4.1a shows that the total number of cases in NYC rapidly increased after the discovery of the first recorded case, followed by a decline and then a second rise. This trend seems to follow the usage of the subway: initially, the usage of the subway declines precipitously and then it slowly and partially recovers to about 2/3 of the previous usage.

By scaling our infection parameter with subway usage, we are simultaneously capturing two effects. The first is the rise in infections directly due to the use of the subway, either



Figure 4.4: (a) The predicted number of daily cases in NYC normalized by the total population of the city. The red line is the 7-day running average of the total daily reported cases in NYC as a fraction of the total population of the city. The dashed black line shows the best-fit output of the model in the training period, and the solid black line shows the model's prediction for the testing period. The vertical dotted line marks the beginning of the three-week testing period. The inset figure shows the testing period in more detail. (b) The ratio of the average infection rate,  $\beta_{avg}(t) = \sum_j p_j \beta_j(t)$ , over the recovery rate,  $\gamma$  as a function of time. The second axis shows the average mobility parameter,  $m_{avg}(t) = \sum_j p_j m_j(t)$ .

through higher infection rate or through case importation between regions. The second is taking subway usage as a proxy for broader mobility trends, which in turn depend upon public policy that governs the infection rate. As more people went back to work and as restrictions on public gatherings, schools etc. were eased, we assume that there was a corresponding increase in human mobility proportional to the increase in subway usage, even though this usage is just one form of the total population mobility in the city.

The fact that our model is able to accurately capture both the first wave of infections as well as the second one indicates that our assumption that subway usage is an indicator for broader human mobility trends (and for public policies regarding restrictions more generally) within the city is correct. While our model does predict a higher infection rate for the subway than for the boroughs, infection trends are much less sensistive to inter-region mobility compared to intra-region mobility.

If we set  $\beta_j(t) = \beta^p(t)$  and the dependence on  $m_j(t)$  is removed, the reduced model is unable to capture the second wave of infections towards the end of the year as shown in Fig 4.3b.

#### Limitations

The turnstile data that we use imposes some limitations on our model. The most crucial assumption in our work is that subway usage is correlated to all mobility within the city and can therefore be used as a proxy for all mobility. This assumption is supported by the fact that the usage of both bikeshares and taxis dropped at the same time as that of the subway [96], [97], and bikeshare usage increased in the same period as subway usage, although at a much faster rate [95]. Additional data on other forms of mobility, specially in the latter half of 2020, would allow us to construct the mobility parameter that encapsulates multiple modes of transport.

We also assume that the residents of a borough that leave it using the subway return to the home borough using the subway on the same day. This assumption impacts our interregion mixing parameter through the calculation  $\Delta \tau_j$ , the average time spent away from the home borough.

Finally, we assume that the fraction of cases that were reported remained constant throughout 2020. While we have adjusted for the drop in reporting on the weekends by taking a 7-day moving average, the fraction of cases that were reported may have changed over the course of the year due to other factors as well. A possible effect of this variation in the reporting rate is the very high ratio of the average infection rate, defined as  $\beta_{\text{avg}}(t) = \sum_{j} p_{j} \beta_{j}(t)$ , to the recovery rate,  $\gamma$ , that our model predicts during the beginning of the infection, shown in Fig. 4.4b. The precipitous rise in cases at the start of the pandemic may represent a slew of people getting tested in a short amount of time as awareness of the epidemic spread and widespread testing became available, rather than accurately representing the true spread of the disease. After this initial period our  $\beta_{avg}(t)/\gamma$  ratio has a minimum of 1.43 and a maximum of 5.25. While an initial estimate for the reproduction number was reported to be 2.2 in Wuhan [105], other studies using SIR models have reported a much higher reproduction number ranging from a global estimate of 4.5 [106] to some regions having a value as high as 7.8 [107]. While the ratio  $\beta_{avg}(t)/\gamma$  is not equivalent to the reproduction number and should be seen only as a crude estimate, it is encouraging that the ratio predicted by our model falls within the range of estimates reported in the literature.

## 4.5 Conclusion

The main contribution of this chapter is the introduction of a mobility-based model of epidemic spread that uses a mobility-dependent infection rate. Based only on fitting the data, our model confirms that subway usage is correlated with the usage of other forms of public transportation because using it as a proxy for the short-range mobility parameter allows us to predict the two peaks in the NYC infection rate in 2020. Using this model and the turnstile data from the NYC subway, we predict the trend of daily infections in NYC for a three-week period. Our model accounts for inter-region mixing of populations, and uses an infection rate that is dependent on the short-range mobility within a region.

While we have used NYC as a test case, it would be interesting to verify the model with data from other cities. We believe that by incorporating data from other public transportation services, such as taxis, ride- and bike-sharing services etc., our model can offer more accurate predictions about the spread of an epidemic disease. Thus, it can be a useful tool in guiding public policies to tame the spread of pandemics.

# CHAPTER 5 CONCLUSION AND FUTURE WORK

In this thesis we have presented three different topics under the broad category of spreading processes on complex networks.

For diffusive persistence on disordered networks we showed the emergence of a novel power-law exponent associated with local persistence at the percolation threshold on 2dlattices of  $\theta = 0.141 \pm 5.3 * 10^{-5}$ , as well as the emergence of a new scaling exponent,  $z \approx 2.56 \pm 2.3 * 10^{-3}$ , associated with the limiting value of persistence on finite lattices. It remains an open question how these quantities change for intermediate values of  $\phi$  above the percolation threshold.

While we have considered the persistence of a diffusive field where the field obeys the heat equation, it would be interesting to observe the behavior of the discretized Schrödinger equation on disordered lattices, where the field corresponds to the wavefunction. In this case persistence can be defined as a first-passage time for the probability (defined as the norm-squared value of the field) rather than the field itself. Since the probability is bounded between 0 and 1, persistence cannot be defined as the first-passage time when the field crosses 0 at a given node. Instead, we would have to pick a different threshold and track the nodes where the corresponding probability never crosses that threshold. While a natural choice for this threshold might be 1/N, persistence in this situation would not be symmetrical above and below this threshold. It might therefore be helpful to track the nodes that always stay above this threshold and those that always stay below this threshold separately.

For our work on numerical methods for concurrence percolation theory we introduced the parallel approximation, where we treat all paths connecting the source and target node as parallel. We showed that the total concurrence calculated under this approximation is an upper bound to the true concurrence on all series-parallel networks and we can greatly speed up the calculation of concurrence by avoiding the costly computation of the star-mesh transform. We combined this approximation with the  $S_m$  approximation, where we only consider the *m*-th shortest paths in the networks since shorter paths contribute more per path to the concurrence than longer paths. Taken together, these approximations greatly speed up the process of calculating concurrence and allow us to estimate the concurrence percolation threshold of complex networks of up to  $10^4$  nodes for the first time. However, we still rely on brute-force path-counting methods and in future work the approximation may be improved by replacing path-counting with approximating the number of paths of a given length. It will also be interesting to extend the study to concurrence based on mixed states.

For the work on the mobility-based SIR model we showed how data on public transportation can be used to forecast the spread of COVID-19 by making the infection rate a function of the mobility within a city, with the mobility parameter being calculated from public transportation usage. Specifically, we used data on the NYC subway as a proxy for all mobility within NYC and were able to show that our mobility based SIR model was able to capture both peaks in the number of cases of COVID-19 in NYC in 2020. While our model was able to successfully forecast three weeks of new daily COVID-19 infections, it can be enriched by combining it with demographic information about the different boroughs of NYC, as well as by using additional data on public transportation from taxis, ride-shares, and bike-shares. It will also be interesting to see how the model performs in other cities.

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