Chapter 11

Disease Spreading

Infectious diseases spreading in human populations represent a growing global challenge, as we have experienced with the recent coronavirus disease (covid-19) pandemic (Fig. 11.1). An individual affected by an infectious disease can transmit it to several other individuals, who in turn become infected and can transmit the illness to many others, in an almost exponential progression. When the disease is severe and hospitalization or intensive care is needed, an uncontrolled spreading can seriously overwhelm any healthcare system. The logistic burden entails a practical impossibility to dispense the needed care to each affected individual, leading to an increase of the number of deaths. This poses several ethical questions and puts considerable stress on healthcare givers.

To choose the most effective policy to mitigate and contain outbreaks, it is very impor-

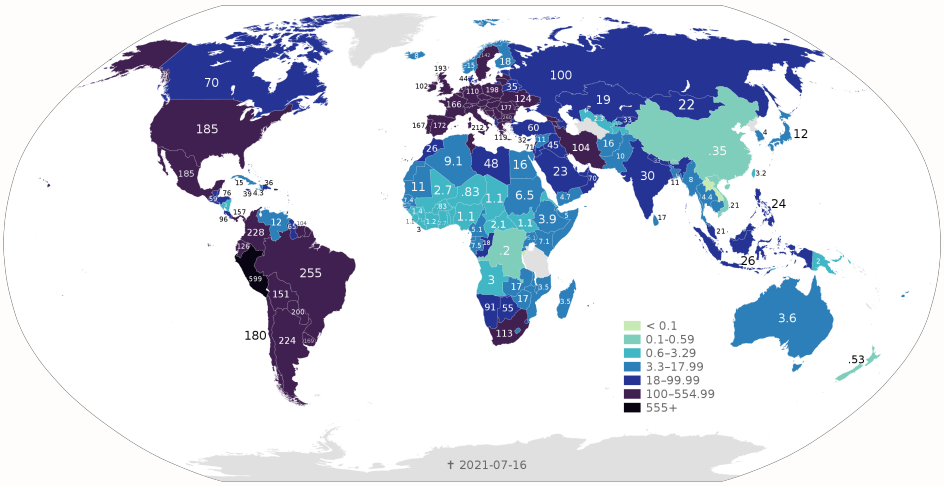

Figure 11.1: **World map of the total deaths per capita due to the coronavirus disease pandemic.** The coronavirus disease (covid-19) pandemic rapidly became one of the biggest global problems during 2020 and 2021. By July 2021, the virus had already spread to hundreds of millions of people and killed several millions in all countries. The total deaths per capita (updated to July 16, 2021) are shown in the figure. *Source: COVID-19_Outbreak_World_Map_Total_Deaths_per_Capita by Dan Polansky under CC BY-SA 4.0.*

tant to understand the mechanisms of diseases spreading. Infectious diseases often spread in a society through individuals' contact. This can take place through direct contact, via a sneeze or cough, or by exchange of bodily fluids. The dynamics of an infectious disease depends on mobility, infection probability, and recovery speed. The susceptible–infected–recovered model (*SIR model*, introduced by W. O. Kermack and A. G. McKendrick in 1927 [1], building on previous work by Sir Roland Ross and Hilda Hudson [2, 3, 4]) studies disease spreading mathematically, providing a series of ordinary differential equations (ODEs) that capture its essential properties. Lots of studies have built on this model, shining light on various aspects of disease spreading. Agent-based models are a natural next step from the simple ODE approach. They have become an important tool in understanding disease dynamics and developing countermeasures.

In this chapter, we show a simple agent-based SIR model that has been used in epidemiology to model the spread of various infectious diseases [5]. We start with the basic principles of the SIR model in order to numerically simulate the spreading of diseases in a finite environment using agents. Next, we introduce further parameters to develop more realistic versions of the SIR model, such as incubation time, mortality, and hospitalization. Finally, we analyze how lockdowns can contain the spreading of a disease.

Example codes: Example Python scripts related to this chapter can be found on:
https://github.com/softmatterlab/SOCS/tree/main/Chapter%5F11%5FDisease%5FSpreading
Readers are welcome to participate in the discussions related to this chapter on:
https://github.com/softmatterlab/SOCS/discussions/20

11.1 Agent-based SIR Model

We will first consider the three-compartment model known as SIR, where each individual is either Susceptible (S) to the disease, Infected (I), or has Recovered (R) and is immune. Infected individuals infect the susceptible they meet with rate β and recover with rate γ. In the original model [1], the problem is solved using an ODE approach while considering that the infection is a continuous process. In such a version of the model, only the ratio $k = \beta/\gamma$ matters for the behavior of the model. With an agent-based model, it is also possible to examine what happens when we take into account spatial effects.

This is a description of the series of steps to implement the agent-based SIR model:

1. On a finite arena (e.g., a square grid lattice), at $t = 0$ initialize N agents at random locations and make a small fraction of the agents infected.

2. Model the movements of the agents as random walks on the arena: Every time step each agent either sits still with some probability $1-d$, or moves to a random neighboring tile (e.g., von Neumann neighborhood, orange boxes in Fig. 11.2a) with probability d, where d sets the diffusion rate.

3. For every infected agent, check if there are any susceptible agents that are sitting in the same lattice site. Every time step, each infected should have a probability β of infecting all susceptible individuals at its current site, as shown in Fig. 11.2b.

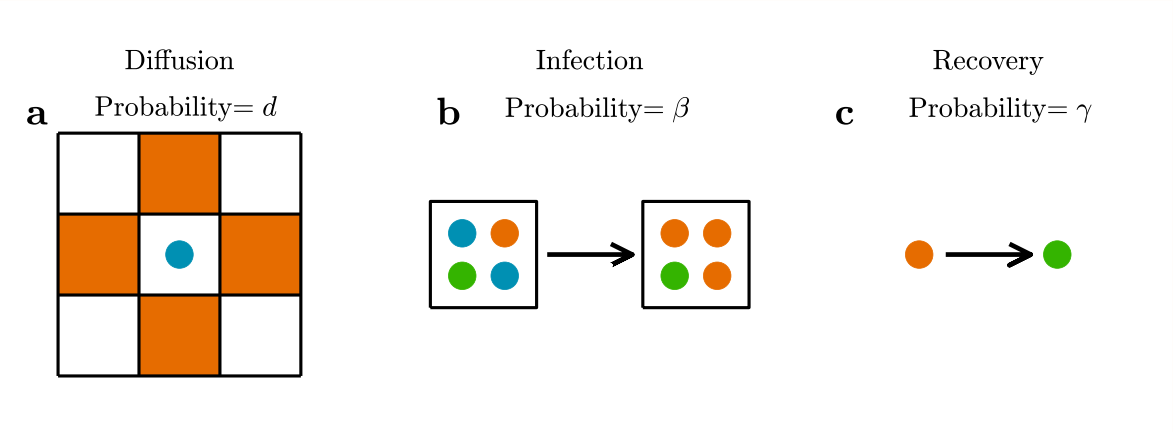

Figure 11.2: **Agent-based SIR model.** In each time step: **a.** Every agent (blue dot) moves to a random neighboring site (von Neumann neighborhood, orange boxes) with a probability d. **b.** Every infected agent (orange dot) has probability β of infecting all the susceptible agents (blue dots) that are in the same site. The recovered agents (green dot) remain unaffected by the infection as they are immune. **c.** Every infected agent (orange dot) recovers (green dot) with probability γ.

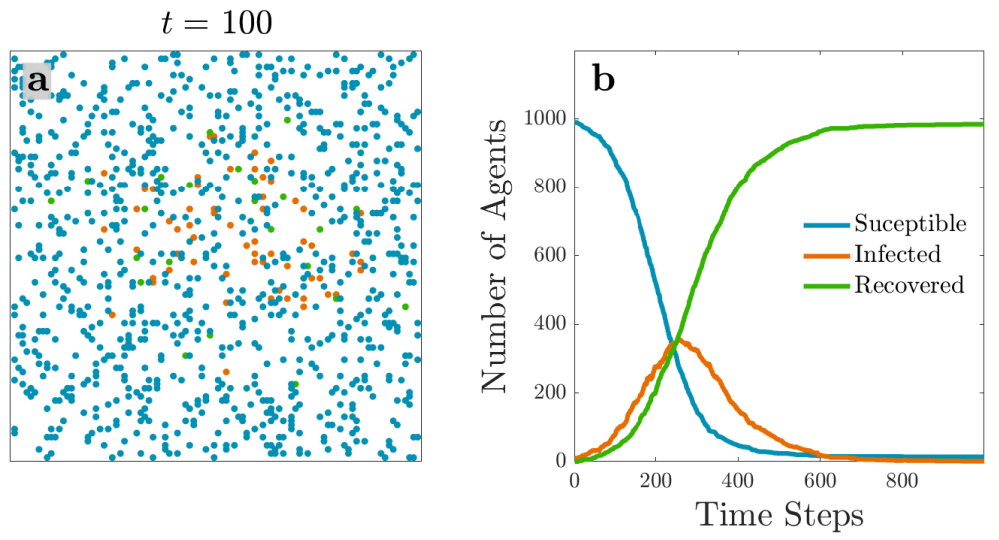

Figure 11.3: **Modeling disease spreading on a square lattice. a** Screenshot of SIR-agents on a lattice after 100 time steps. Blue dots represent susceptible, orange dots represent infected, and the green dots represent recovered agents. **b** Number of susceptible (blue), infected (orange), and recovered (green) individuals as a function of time step in the agent-based SIR model. The parameters used for this simulation are $d = 0.8$, $\beta = 0.6$, $\gamma = 0.01$. At $t = 0$, 1% of the total number of agents (10 out of 1000) are initialized infected.

4. Every time step, each infected agent has a probability of recovery γ, as shown in Fig. 11.2c.

5. The disease dynamics evolves until the number of infected agents reaches zero. This fact can be used as a stopping criterion for the simulations.

A screenshot of an agent-based SIR simulation is shown in Fig. 11.3a. Every simulation starts with zero recovered agents and ends zero infected agents, as shown in Fig. 11.3b. In the first exercise, we will simulate this simple agent-based SIR model.

Exercise 11.1: Simulation of the SIR model. Implement the basic model as explained above and visualize it. Start with just a few agents and make sure they perform the random walk, infection and recovery correctly. Then, test some small number of agents to check that the disease dynamics seems reasonable. Choose parameters $\gamma = 0.01$ and $d = 0.8$. Use β as the varying parameter.

a. Scale the simulation up (e.g., 1000 agents on a 100×100 lattice, as shown in Fig. 11.3a). Use an initial infection rate of 1%.

b. Show that the model has two regimes, i.e., that there are parameters for which the disease spreads to a large proportion of the population and values for which it does not. *[Hint: For fixed values of γ and d, find out what is the critical β value that makes the disease spread to a majority of the population.]*

c. Plot the number of susceptible (S), infected (I), and recovered (R) agents as a function of time (as shown in Fig. 11.3b).

d. Repeat the simulations for various values of β and γ. Comment on your results.

11.2 Disease spreading as a function of the infection rate

In the SIR model, the reach of a pandemic can be measured by the final number of recovered agents, which is denoted as R_∞. In fact, at the end of a simulation, the population is divided into agents that have never been infected and agents that have been infected and recovered. Naturally, R_∞ depends strongly on the infection rate β. This dependence is demonstrated in Fig. 11.4 for $\gamma = 0.01$ (blue dots) and $\gamma = 0.02$ (green dots). Interestingly, in the original ODE model, the values of R_∞ only depends on the ratio β/γ. However, when we take into account of the movement of each individual within the agent-based model, this is no longer true.

Exercise 11.2: Dependence of the final number of recovered agents on the infection rate. Simulate the agent-based SIR model with $d = 0.8$ and $N = 1000$. Use 1% initial infection rate. For all the questions in this exercise, repeat the simulation several times to obtain the average R_∞.

a. Set the recovery rate $\gamma = 0.01$ and plot R_∞ as a function of β, as shown in Fig. 11.4.

b. Set $\gamma = 0.02$ and compare the results. Convert the figure into R_∞ vs β/γ for both γ values, and show that the results do not only depend on β/γ but also on the value of

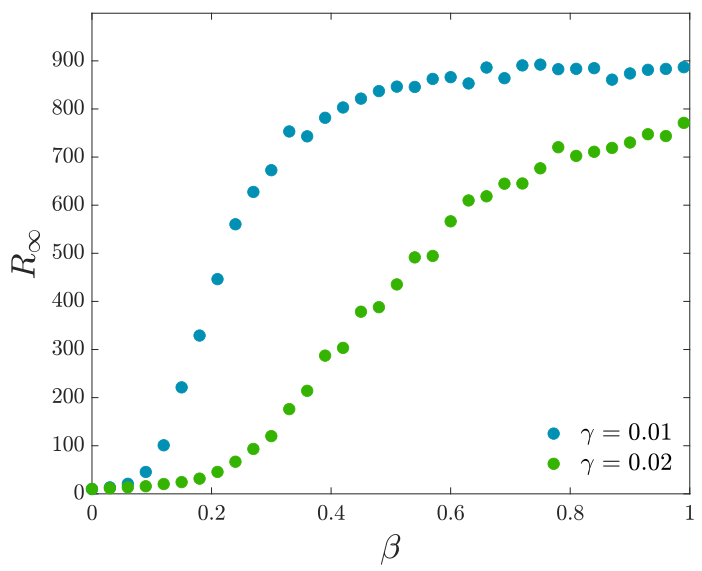

Figure 11.4: **Final number of recovered agents as a function of the infection rate.** Average number of recovered agents at the end of the simulation (R_∞) as a function of the infection probability β for $\gamma = 0.01$ (blue dots) and for $\gamma = 0.02$ (green dots). The results for each dot are averaged over 100 repetitions of the simulation ($d = 0.8$, $N = 1000$, and 1% initial infection rate).

the infection rate β.

c. Plot the phase diagram of R_∞ as a function of β and β/γ. Show that the output depends not only on β/γ but also β itself, as shown in Fig. 11.5.

11.3 Extended SIR Models

Although being a very powerful minimalist model, the SIR model does not fully describe the underlying behavior of every possible pandemic. In fact, there are many assumptions underlying the SIR model, which might not reflect real-world conditions. The list of the main oversimplifications that the agent-based SIR model makes can be listed as follows:

- We assume that the infection is immediate and people can infect others as soon as they get infected. However, in real life, there is a delay between the time when an individual gets exposed to the virus and the time when they develop the infection themselves and become capable of infecting others (in fact, these latter two times might not even coincide).

- We assume that all cases are asymptomatic, which means that the mobility of infected agents does not change at all. This is not true as in real life sick individuals tend to move less.

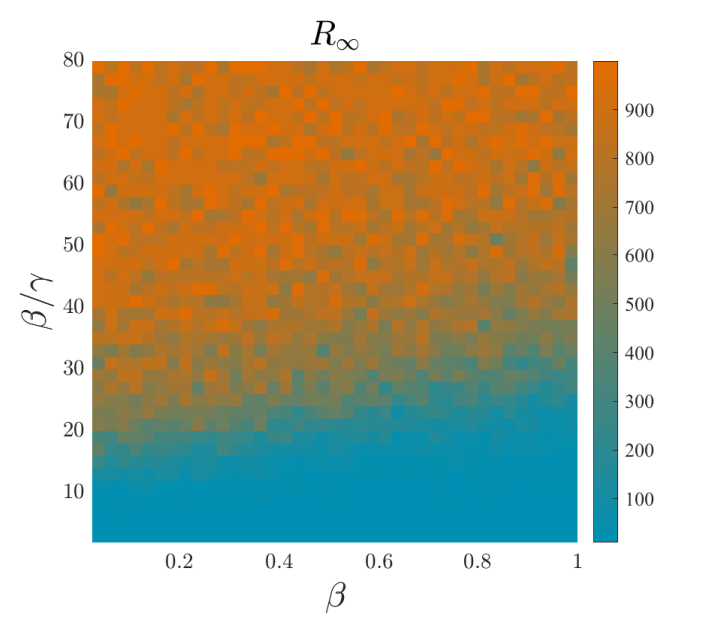

Figure 11.5: **Final number of recovered agents as a function of β and β/γ.** Average number of recovered agents at the end of the simulation (R_∞) as a function of the infection probability β and β/γ. The results are averaged over 3 repetitions of the simulation ($d = 0.8$, $N = 1000$, and 1% initial infection rate).

- We assume that the immunity is permanent. However, the immunity often reduces over time after the recovery, and reinfection is often possible.
- We assume that the disease does not cause hospitalization or death. This may not always be the case. In fact, lots of global pandemics, including the covid-19 pandemic, caused millions of deaths.

Depending on the purpose of the simulation model, these assumptions can be relaxed by implementing extended versions of the SIR model. Although these extended SIR models have increased computational complexity, they capture a wider range of outputs in the spreading of a disease. Therefore, to make our SIR model more realistic, we are now going to make it more complex and relax some of the assumptions mentioned above.

Exercise 11.3: SIR model with mortality. Simulate the agent-based SIR model adding a probability μ for infected agents to die at each time step. Denote the number of dead agents at the end of the simulation as D_∞. In each time step, simulate infection, recovery, and death. Start with 1% initial rate of infected agents.

a. Show that the number of final casualties does not monotonically depend on μ. Show that both for very low and very high values of μ, the final number of casualties is minimal. Demonstrate the range of μ where the pandemic becomes most severe.

b. Analyze and plot the dependence of D_∞ on μ for different values of β and γ. Play

with the parameters and identify the most dangerous value of μ for different values of β and γ.

Exercise 11.4: SIR model with temporary immunity. Simulate the agent-based SIR model adding a probability α to become again susceptible for recovered agents.

a. Simulate this model and plot the number of susceptible and infected agents as a function of time. What happens at long times?

b. Play with the parameters α, β and γ. For which parameters does the disease die out? And for which ones does it become endemic? Does this depend on the number and distribution of the initial infected agents?

11.4 Lockdown strategies

If a disease with a high mortality rate gets out of control and spreads to the general public, it can disrupt society. For example, the Antonine plague destroyed the social fabric of the Roman Empire during the 2$^{\text{nd}}$ century AD, eventually causing 30% of its population to lose their life. Another example is the bubonic plague, which killed more than 30% of the European population in the 14$^{\text{th}}$ century. Because of the ever-increasing population density and global travel, major pandemics in modern ages, such as the Spanish flu and the covid-19 pandemic, have spread worldwide.

An ideal strategy to quash a pandemic would be to identify and isolate all infected individuals. However, this is often logistically impossible due to difficulties in a timely diagnosis. Therefore, often lockdowns have been imposed as a practical strategy to minimize the overall damage caused by these pandemics. However, lockdowns themselves also entail serious social, financial, and psychological damages. Therefore, it is very important to identify the optimum strategies to impose an effective partial lockdown during a pandemic.

In the next exercise, we will implement a lockdown strategy that will limit the spread of the disease. To realistically model this behavior, we will only be allowed to hold the lockdown in place for a limited amount of time.

Exercise 11.5: Simulation of the simple SIR model with lockdown. Simulate the simple SIR model with parameters, $\gamma = 0.01$, $\beta = 0.5$, and $d = 1$, starting with 1000 agents and 1% initial infected agents. Assume that we are only allowed to operate a lockdown of 200 steps.

a. Start the lockdown at different time steps and observe the resulting R_∞. Plot the number of susceptible, infected, and recovered individuals as a function of time for each case and comment on your results. Decrease the diffusion coefficient by one order of magnitude to $d = 0.1$ while the lockdown is in place.

b. Calculate the optimum lockdown time and identify the best strategy, i.e., that resulting in a minimum number of R_∞.

11.5 Further readings

Ref. [5] is an excellent source to study the SIR model based on ODE, providing both the theoretical relations and their application to historical data. Ref. [6] is another article that presents three different ODE-based epidemiological models. Ref. [7] is a great book that explains in detail the theory of the standard epidemiological models, as well as case studies analyzing data from real outbreaks.

Ref. [8] is an excellent study showing that targeted lockdown strategies reduce the spread of the disease. The authors show that the optimal strategy can be found by differently targeting age and risk groups.

Ref. [9] uses techniques from optimization theory and machine learning to conduct optimizations over alternative disease policies.

Ref. [10] demonstrates a machine-learning approach to analyze the initial confirmed cases to provide strategies for targeted testing and lockdown. These machine-learning-based strategies are shown to contain the outbreak more effectively than the standard approaches.

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