Appendix A
Stochastic simulation of epidemics

In this appendix, we discuss some algorithms for performing stochastic simulations and comment on some issues related to interpreting the resulting output.

A.1 Efficient simulations

We begin with techniques for simulating disease spread in networks. We consider two general algorithms: The Gillespie algorithm and an event-driven algorithm. The Gillespie algorithm is a well-known algorithm for simulating Markovian processes where objects change status. The algorithm calculates the time to the next event and then separately calculates what that event will be. It then jumps to that time, updates statuses and repeats. This is particularly efficient for processes where all that matters is the number of objects of each status, such as a chemical reaction in a well-mixed vessel or disease spread in a well-mixed, mass-action population. For these, the information update at each event simply adjusts the counts. In a network however, knowing the exact node changing status is important. Choosing which node changes status can be a computationally slow process.

An alternative event-driven approach involves a priority queue. Rather than calculating at each time what the next event might be (chosen from all available events), when a node is infected, we calculate when it will transmit to others and when it will recover. These events are placed into the priority queue, and then the next event is removed from the queue and processed. The computational time required to add and remove events is roughly proportional to the log of the number of events already in the queue. This significantly reduces the amount of processing per event, producing a more efficient algorithm. An implementation of these methods is available at

https://springer-math.github.io/Mathematics-of-Epidemics-on-Networks/

Although the implementations of the SIS and SIR event-driven algorithms are quite different from the Gillespie algorithms, they simulate the same stochastic processes.

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Thus, either could be used for the same purpose. In general, the event-driven algorithms are faster than the equivalent Gillespie algorithms and are more flexible in the case of non-Markovian transmission and recovery processes.

A.1.1 Gillespie algorithm

Input: Network G, per-edge transmission rate τ, recovery rate γ, set of index node(s) initial_infecteds, maximum time t_{max}.
Output: Lists times, S, I, and R giving number in each state at each time.

```
function Gillespie_network_epidemic(G, τ, γ, initial_infections, t_max)
    times, S, I, R ← [0], [|G|-len(initial_infections)], [len(initial_infections)], [0]
    infected_nodes ← initial_infections
    at_risk_nodes ← uninfected nodes with infected neighbours
    for each node u in at_risk_nodes do
        infection_rate[u] = τ × number of infected neighbours
    total_infection_rate ← ∑_{u∈at_risk_nodes} infection_rate[u],
    total_recovery_rate ← γ × len(infected_nodes)
    total_rate ← total_transmission_rate + total_recovery_rate
    time ← exponential_variate(total_rate)
    while time< t_max and total_rate> 0 do
        r = uniform_random(0,total_rate)
        if r <total_recovery_rate then
            u = random.choice(infected_nodes)
            remove u from infected_nodes
            reduce infection_rate[v] for u's susceptible neighbours v
        else
            choose u from at_risk_nodes with probability infection_rate[u] / total_infection_rate.
            remove u from at_risk_nodes
            add u to infected_nodes
            for susceptible neighbours v of u do
                if v not in at_risk_nodes then
                    add v to at_risk_nodes
                update infection_rate[v]
        update times, S, I, and R
        update total_recovery_rate, total_infection_rate, and total_rate
        time ← time + exponential_variate(total_rate)
    return times, S, I, R
```

Fig. A.1: Pseudocode for the Gillespie algorithm simulating an SIR epidemic in a network. Small changes are needed for simulating an SIS epidemic: when a node recovers, it needs to become susceptible and possibly needs to be placed into the at-risk node category.

Figure A.1 gives pseudocode adapting the well-known Gillespie algorithm [112, 113] (much of which was introduced earlier by Doob in [83]) to epidemics on networks. This algorithm uses iterative steps:

1. Find the rate of all possible events and compute the total rate of change occurring; this is done by finding the rate at which each infected node will recover and each at-risk susceptible node becomes infected;
2. Based on this rate of change, select the waiting time until the next event from an exponential distribution whose rate is the total rate of change;
3. Select which event occurs, with probability proportional to each event's rate; and
4. Update the rates based on which node changes status and repeat.

In more detail, these steps amount to determining the rate of infection of all susceptible nodes and the rate of recovery of all infectious nodes. Let these be denoted by r_u, where $u = 1,2,3,\ldots,N$ are the nodes. The infection rate of a susceptible node depends on how many infected neighbours it has, but the recovery rate of an infected node is independent of the network and status of neighbours. For example, Fig. A.2 illustrates the computation of some transition rates. Node 1 has one infected neighbour, so $r_1 = \tau$, and the two infected neighbours of node 3 yield $r_3 = 2\tau$. All infected nodes, e.g. nodes 5 and N have $r_5 = r_N = \gamma$. From this, the total rate of all transitions, denoted by T (total_rate in the pseudocode), is calculated from the current status of all individuals across the whole network. Therefore, $T = \sum_{u=1}^{N} r_u$, and the waiting time until the next event, t_{next}, is chosen from an exponential distribution with rate T. Because $r_u = \gamma$ if u is infected and 0 if u is susceptible and not in the at-risk nodes, we can write $T = \gamma[I] + \sum_{u \in \text{at\_risk\_nodes}} r_u$.

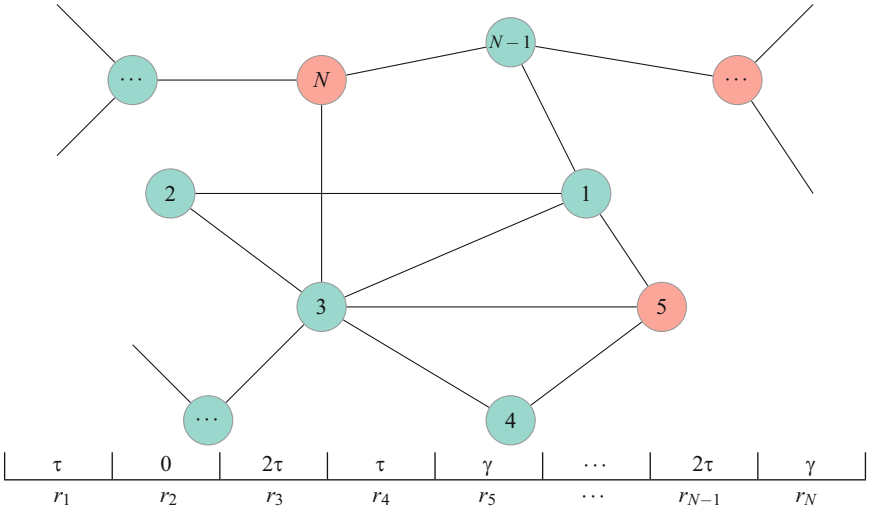

Fig. A.2: Illustrating the relation between the network, status of nodes and events rate vector used by the Gillespie algorithm. Susceptible nodes are denoted by (●) and infected nodes by (●).

Next, a single event is chosen with probability proportional to its rate. Because all recoveries occur with the same rate, γ, the total recovery rate is $\gamma[I]$. So the probability the event is a recovery is $\gamma[I]/T$. If so, we select a random infected node. If a recovery does not occur, we select a random at-risk node with probability proportional to its rate. Because not all at-risk nodes have the same rate, this step of selecting the node is more involved than simply choosing a random node. It can be done in several ways:

- We can select a random number $r \in (0, T - \gamma[I])$. We iterate through the at-risk nodes, each time subtracting r_i until the result becomes negative. This is the node that recovers. This approach can be slow because, on average, half of the at-risk nodes will be processed in each iteration;
- We can *a priori* artificially inflate the transmission rates, treating all nodes as having the same infection rate $r^* \geq \max_{u \in \mathsf{at\_risk\_nodes}}\{r_u\}$. This increases T to $\gamma[I] + r^*|\mathsf{at\_risk\_nodes}|$. When a transmission is predicted to happen, we select a random at-risk node u whose true rate is $r_u \leq r^*$. We then correct for the fact that we have overestimated the risk of u by selecting an additional random number $p \in (0,1)$. If $p < r_u/r^*$, we "accept" the event: u is infected. Otherwise, we "reject" the event: no nodes change status, but the time t is increased. This can be slow if much processing time is spent on events in which nothing happens; and
- Alternately, we keep T as $T = \gamma[I] + \sum_{u \in \mathsf{at\_risk\_nodes}} r_u$. We track the maximum transmission rate r^*. When a transmission event is going to occur, we choose a random node u from the at-risk nodes. We select an additional random number $p \in (0,1)$. If $p < r_u/r^*$, we infect u. If not, we choose a new random node u' from the at-risk nodes and a new p' and repeat. This can be slow if some of these events require repeated selections before finding the newly infected node.

These last two options use a technique known as rejection sampling. Whichever option is chosen, this is generally the slowest step of the algorithm. Once the time to next event and the event itself have been found, necessary rate updates are performed and the process begins again. The Gillespie algorithm allows us to exactly simulate the process.

A.1.2 Event-driven algorithm

We now consider another efficient algorithm for simulating SIR and SIS epidemics. This uses event-based simulation techniques to improve on Gillespie-style algorithms by avoiding the slow step of finding which node becomes infected. An additional advantage of this approach is that it can be easily generalised for non-Markovian processes.

A key observation is that when a node is infected, nothing that any of its neighbours does will affect when it recovers, who it transmits to or the timing of those transmissions. Thus, as soon as a node is infected, we can calculate when it will recover and when it will transmit to its neighbours. These events are inserted into a priority queue ordered by event time.[1] At each step of the simulation, the next event in the list is removed and processed. If it is a transmission, new events will be added to the queue corresponding to the recovery of the node and any transmissions from that node. This process iterates until a time specified by the user or no events remain in the queue (in which case no infection remains).

Although we assume here that the algorithm is performed using constant rates τ and γ, it is straightforward to adapt event-based simulations to other rules. The key requirement is that when a node becomes infected, we can calculate transmission and recovery times without considering events that have not happened yet. Thus, this approach can handle a non-Markovian epidemic process, as in Chapter 9, by some relatively simple adjustments using a different calculation of the duration of infection and the waiting time before transmission.

SIR epidemics

We begin by describing an event-based algorithm for continuous-time SIR disease transmission in an arbitrary unweighted, undirected network. The algorithm is based on the use of a priority queue Q. The underlying structure of Q allows for efficient addition of new events and removal of the earliest remaining event in the queue. Pseudocode for the algorithm is given in Figs. A.3 and A.4.

The algorithm repeatedly removes the earliest remaining event in Q. If the event is a recovery, the node recovers. If the event is a transmission and the recipient of the transmission has not yet been infected, the node is infected. Now that it is infected, the time of its recovery and the times at which it transmits to its neighbours will not be influenced by any external event. Thus, we can determine the future recovery time and times at which it may transmit to its neighbours immediately, without regard to any events that may happen between now and those events. We add these to Q, unless we can immediately rule them out of consideration. Since only the first transmission to a node v has any effect, we can rule out any transmissions for which the recipient has already been infected or has an earlier scheduled transmission. Similarly, we do not add events that would occur after the user-specified $t_{\max}$ to Q.

[1] A "priority queue" is a data structure which allows for insertion of new events in such a way that we can easily remove the next event to occur. When implemented efficiently, the computational time required to add or remove events is logarithmic in the number of events in the queue [289].

```
Input: Network G, per-edge transmission rate τ, recovery rate γ, set of index node(s)
  initial_infecteds, and maximum time t_max.
Output: Lists times, S, I, and R giving number in each state at each time.

  function fast_SIR(G,τ, γ, initial_infecteds, t_max)
      times, S, I, R ← [0], [|G|], [0], [0]
      Q ← empty priority queue
      for u in G.nodes do
          u.status ← susceptible
          u.pred_inf_time ← ∞
      for u in initial_infecteds do
          Event ← {node: u, time: 0, action: transmit}
          u.pred_inf_time ← 0
          add Event to Q                                   ▷ ordered by time
      while Q is not empty do
          Event ← earliest remaining event in Q
          if Event.action is transmit then
              if Event.node.status is susceptible then
                  process_trans_SIR(G, Event.node, Event.time, τ, γ, times, S, I, R, Q, t_max)
          else
              process_rec_SIR(Event.node, Event.time, times, S, I, R)
      return times, S, I, R
```

Fig. A.3: An efficient algorithm simulating continuous-time SIR epidemics in static networks with rates τ and γ. It relies on functions given in Fig. A.4. Events are stored in a priority queue Q, and the first is executed. If the event is a transmission and the recipient is susceptible, it becomes infected, its recovery is added to Q and transmissions to its neighbours may be added. If the event is a recovery, the node recovers.

SIS epidemics

With some modest alterations, we can adapt the event-driven SIR disease algorithm to SIS disease. Figures A.5 and A.6 show the pseudocode. The major change is that we must consider the possibility of successful transmissions to a node after its first infection because it may recover to a susceptible state in between. This involves some changes to the algorithm to find the next transmission, and whenever we encounter a transmission event, after checking its effect, we have to consider the possibility that the original source may transmit again.

```
function process_trans_SIR(G, u, t, τ, γ, times, S, I, R, Q, t_max)
    append times, S, I, and R with t, S.last−1, I.last+1, and R.last
    u.status ← infected
    u.rec_time ← t+exponential_variate(γ)
    if u.rec_time< t_max then
        newEvent ← {node: u, time: u.rec_time, action: recover}
        add newEvent to Q
    for v in G.neighbours(u) do
        find_trans_SIR(Q, t, τ, u, v, t_max)
function find_trans_SIR(Q, t, τ, source, target, t_max)
    if target.status is susceptible then
        inf_time ← t+exponential_variate(τ)
        if inf_time < minimum(source.rec_time, target.pred_inf_time, t_max) then
            newEvent ← {node: target, time: inf_time, action: transmit}
            add newEvent to Q
            target.pred_inf_time ← inf_time
function process_rec_SIR(u, t, times, S, I, R)
    append times, S, I, and R with t, S.last, I.last−1, and R.last+1
    u.status ← recovered
```

Fig. A.4: Auxiliary functions for fast_SIR in Fig. A.3. process_rec_SIR handles a recovering node. process_trans_SIR takes a newly infected node u and creates a recovery event for u if the recovery happens before $t_{\max}$. For each neighbour v of u, it calls find_trans_SIR to determine when u would transmit to v, adding a transmission event to Q if the event might occur (u still infected and v not known to be already infected by then).

A.2 Time shifting of simulation results

We now consider a technical issue related to comparing deterministic models with stochastic simulations. When a stochastic simulation begins with a small number of infections, it may die out, it may have unusually fast early growth or it may take a long time before successfully becoming established and growing. The deterministic models do not have this variability.

When we use a simulation to study epidemics, we must account for these stochastic delays and the fact that some realisations die out. If our goal is to predict the future spread of an epidemic that has already established itself, we should obviously discard the outbreaks that died out stochastically.

It is natural to consider the average of the simulations that do not die out. However, there is an additional issue. The stochastic effects that may accelerate or delay the onset of the epidemic mean that simulated epidemics become large at different times. In Fig. A.7, the epidemics are effectively time translations of one another. Thus, the peaks occur with some stochastic delay. If the population model and the

```
Input: Network G, transmission rate per edge τ, recovery rate γ, set of index node(s)
  initial_infecteds, and maximum time t_max.
Output: t: list of times and I: list containing number infected at each time.

  function fast_SIS(G,τ, γ, initial_infecteds, t_max)
      initialise Q, node statuses and return variables as in fast_SIR, but include a source for
  infections with recovery time 0.
      while Q is not empty do
          Event ← earliest remaining event in Q
          if Event.action is transmit then
              if Event.node.status is susceptible then
                  process_trans_SIS(G, Event.node, Event.time, τ, γ, times, S, I, Q, t_max)
              find_next_trans_SIS(Q, Event.source, Event.node, t)    ▷ needed for SIS model
          else
              process_rec_SIS(Event.node, t, S, I)
      return times, S, I
```

Fig. A.5: An efficient event-based algorithm simulating continuous-time SIS epidemics in static networks. It relies on functions given in Fig. A.6. It is similar to the algorithm in Fig. A.3. When nodes recover, they become susceptible again. An important change compared to the SIR version is that when a transmission event occurs, we check the possibility that the source of that transmission might cause another transmission later. This requires that we include the source in every transmission event.

disease model accurately represent the real-world epidemic, we would expect the real epidemic to have the same shape, with some stochastic delay. If we try to capture this by taking the average of many simulations, the result will have a different shape. By averaging many peaks that do not align, we get a lower, wider peak which does not resemble any single realisation.

Thus, we have two options to align trajectories:

- We can take many simulations and shift time so that $t = 0$ corresponds to the prevalence crossing some threshold size; or
- We can initialise our simulations with a large number of infections such that the stochastic noise is negligible.

Both of these assume that the epidemic is in a large enough population so that it is reasonable to talk about the deterministic phase of an epidemic.

```
function process_trans_SIS(G, u, t, τ, γ, times, S, I, Q, t_max)
    append times, S, and I with t, S.last−1, and I.last+1
    u.status ← infected
    u.rec_time ← t+exponential_variate(γ)
    if u.rec_time < t_max then
        newEvent ← {node: u, time: u.rec_time, action: recover}
        add newEvent to Q
    for v in G.neighbours(u) do
        find_next_trans_SIS(Q, t, τ, u, v, t_max)
function find_next_trans_SIS(Q, t, τ, source, target, t_max)
    if target.rec_time < source.rec_time then
        transmission_time = max(t, target.rec_time)+exponential_variate(τ)
        if transmission_time < source.rec_time then
            newEvent ← {node: target, time: transmission_time, action: transmit, source:
source}
            push(Q, newEvent)
function process_rec_SIS(u, times, S, I)
    append times, S, and I with t, S.last+1, and I.last−1
    u.status ← susceptible
```

Fig. A.6: Auxiliary functions for event-based SIS simulation. Recovery is handled as in the SIR case except that the node becomes susceptible again. Each transmission is handled similarly, but when finding the next transmission event, there are fewer events we can exclude from adding to Q. We find the first transmission from the source to the recipient and add it to Q unless the recipient is infected and will not recover prior to the transmission or the source will recover prior to the transmission. Since multiple transmissions from a source to a target may cause infection, after each transmission event, fast_SIS also calls find_next_trans.

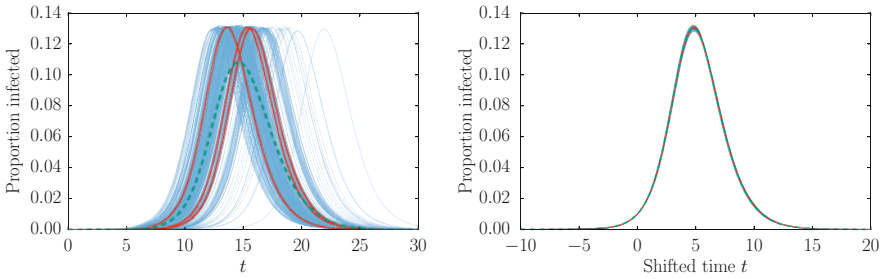

Fig. A.7: (Left) SIR simulations in a 10^6 node Configuration Model network with $P(2) = P(3) = P(4) = P(5) = 1/4$ and $\tau = \gamma = 1$. Simulations were run until 200 epidemics occurred, using the algorithm in Fig. A.3. These epidemics are shown: three are highlighted, and the average of all 200 is dashed. The average does not resemble individual realisations. (Right) Shifting time so that $t = 0$ when 1% of the population is infected aligns individual realisations and the average.

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