

# MCMC 2: Lecture 1

## Simulation

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- 2. Simulating Markov models
- 3. Example: General epidemic model
- 4. Simulating non-Markov models
- 5. Example: Non-Markov SIR model



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# 1. Introducing simulation

- Suppose we have a stochastic epidemic model

(e.g. the general stochastic epidemic

= Susceptible-Infective-Removed model

= SIR model)

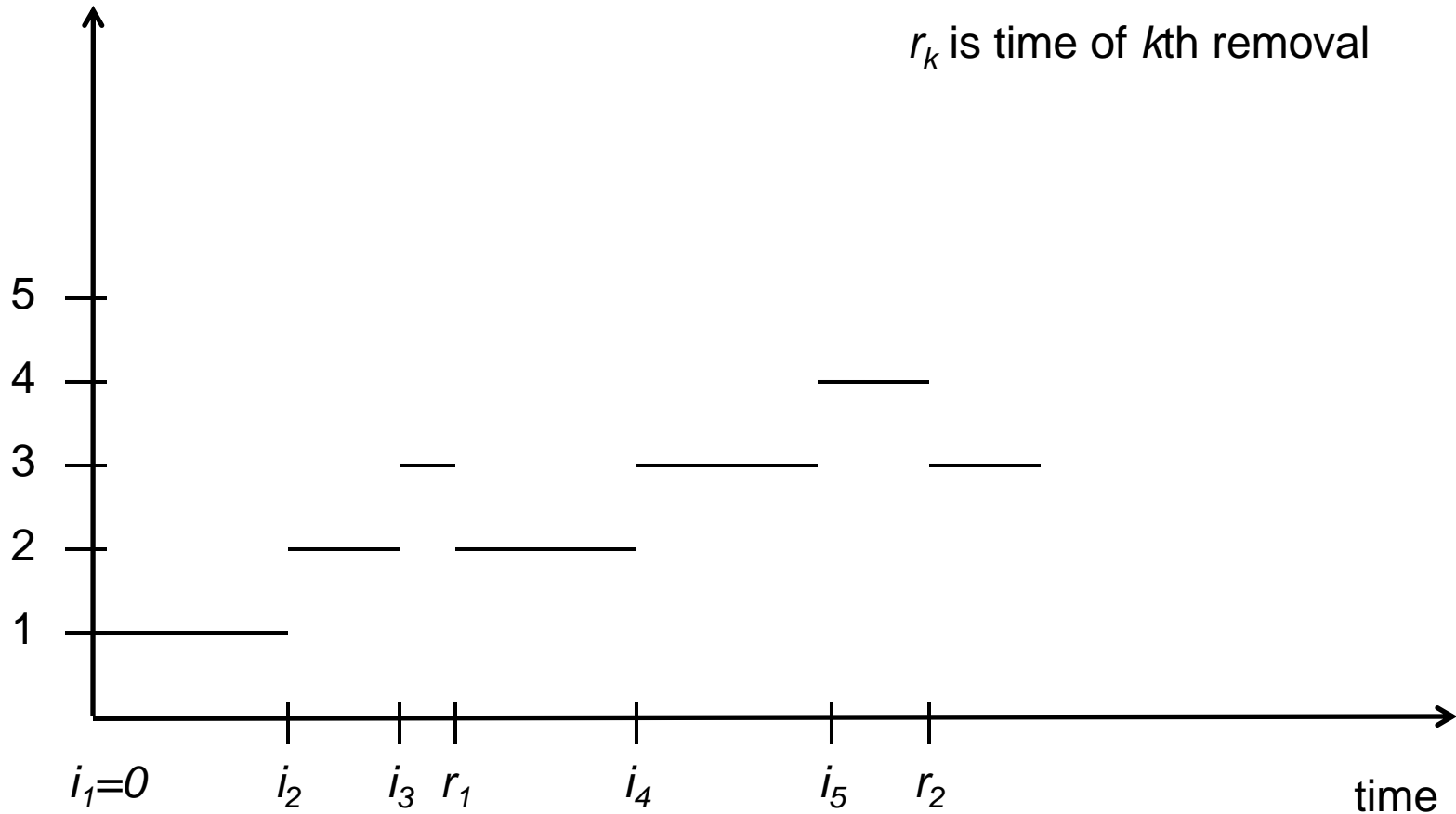
- By simulation we mean “producing a realisation of the model”, i.e. a possible outcome.

# 1. Introducing simulation

Infectives

$i_k$  is time of  $k$ th infection

$r_k$  is time of  $k$ th removal



# 1. Introducing simulation

- For the SIR model, simulation means producing a set of infection and removal times according to the correct distributions inherent in the model.
- In general, it means producing an outcome from the model according to the correct distribution of all possible outcomes.

# 1. Introducing simulation

## Why is simulation useful?

- 1. In general it helps us understand model behaviour.
- 2. For inference it is useful for testing our inference procedure. Specifically we can validate our method against data from simulations, where we know the “truth”.

# 1. Introducing simulation

## Why is simulation useful?

- Specifically, suppose we perform  $N$  simulations (e.g.  $N=1000$ ) from a model with parameter vector  $\theta$  fixed at  $\theta_T$ , say. For each simulation we estimate the model parameters to get estimates  $\theta_1, \dots, \theta_N$  (e.g. estimates might be posterior means).



# 1. Introducing simulation

## Why is simulation useful?

- Then the average of  $\theta_1, \dots, \theta_N$  should be close to the true value  $\theta_T$ .
- If it is not, then our method (or its implementation) might be wrong.

# 1. Introducing simulation

## Why is simulation useful?

- 3. Simulation is also useful for model checking.
- Suppose we estimate a parameter  $\alpha$ . Here  $\alpha$  might be a fixed value (e.g. posterior mean), or we might have a sample from the posterior density of  $\alpha$ .

# 1. Introducing simulation

## Why is simulation useful?

- Next, for each value of  $\alpha$  we can perform a (large) number of simulations.
- For each simulation, we see whether or not the output is “similar” to the actual data.
- In other words: if I put my best guess(es) for  $\alpha$  back into the model and simulate it, do I get something like the data or not?

# 1. Introducing simulation

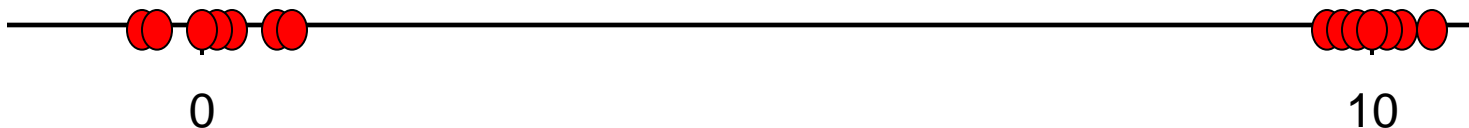
## Why is simulation useful?

- Example: Observe  $x_1, x_2, \dots, x_n$  from a mixture model:

$x_k \sim N(0, 1)$  with probability 0.5

$\sim N(10, 1)$  with probability 0.5

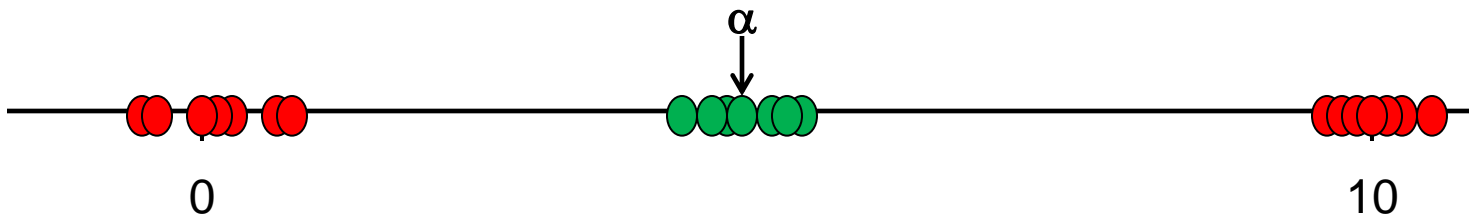
Data might look like this:



# 1. Introducing simulation

## Why is simulation useful?

- If we fit a  $N(\alpha, 1)$  model we would estimate  $\alpha = (x_1 + x_2 + \dots + x_n) / n$
- Simulations from our model using our best guess for  $\alpha$  would never look like the data.



# 1. Introducing simulation

## Why is simulation useful?

- 4. Simulation can be used for prediction.
- Example - suppose we estimate parameters of an epidemic model based on observations up to time  $T$ .

We can then simulate the epidemic model, using the estimates as model parameters, to see what the model predicts after time  $T$ .

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## 2. Simulating Markov models

### Continuous-time Markov Chain

Define a continuous-time Markov chain as follows.

Let the state-space be denoted

$$S = \{1, 2, 3, \dots, n\}.$$

S is the set of states that the MC can visit.

Note each “state” might be multi-dimensional.



## 2. Simulating Markov models

Let  $X(t)$  denote the position (= state) of the chain at time  $t$ , where  $t \geq 0$ .

For  $i, j \in S$ , define  $q_{ij}$  as the “rate” at which the chain jumps from state  $i$  to state  $j$ .

This means:

$$P(X(t+dt) = j \mid X(t) = i) = q_{ij} dt + o(dt)$$

## 2. Simulating Markov models

### Important facts

1. The chain stays in state  $i$  for time  $T_i$ , where

$$T_i \sim \text{Exp}(\sum_{j \neq i} q_{ij})$$

(  $\text{Exp}(a)$  denotes exponential distribution with mean  $1/a$  )

So e.g.  $P(T_i > t) = \exp(- \sum_{j \neq i} q_{ij} t)$

## 2. Simulating Markov models

2. When it leaves state  $i$ , the chain jumps to state  $j$  with probability

$$q_{ij} / (\sum_{j \neq i} q_{ij})$$

3. The time spent in state  $i$  and the choice of where to jump to are independent, and they are also independent of the same quantities in other states and at other times.



## 2. Simulating Markov models

### Next Event Simulation (Gillespie Algorithm)

These facts lead naturally to a method of simulating a continuous-time Markov chain.

All that is needed is to generate the time spent in a state, and the next state that is visited.

## 2. Simulating Markov models

### Algorithm

Initialise ( $t=0, X(0) = x_0$  )

## 2. Simulating Markov models

Loop:      Current state is  $i$ , say.  
Set  $L = \sum_{j \neq i} q_{ij}$   
Generate  $T_i \sim \text{Exp}(L)$   
Generate  $u \sim U(0,1)$   
if  $u < ( \sum_{j \leq 1, j \neq i} q_{ij} )/L$  then  $k = 1$   
else if  $u < ( \sum_{j \leq 2, j \neq i} q_{ij} )/L$  then  $k = 2$   
else .....(etc)

## 2. Simulating Markov models

...

Update current time:  $t = t + T_i$

Record  $t$  and  $k$

End loop

Note that Time of next event =  $t + T_i$

State jumped to is  $k$

## 2. Simulating Markov models

The output of the algorithm is a sequence of times  $t_0, t_1, t_2, \dots$  and a corresponding sequence of states  $x_0, x_1, x_2, \dots$

Here  $t_k$  is the time of the  $k$ th event, and  $x_k$  is the state of the Markov chain at that point (i.e. immediately after the jump).





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# 3. General epidemic model

## Model Definition

- Population of  $N$  individuals

- At time  $t$  there are:

$S_t$  susceptibles

$I_t$  infectives

$R_t$  recovered / immune individuals

Thus  $S_t + I_t + R_t = N$  for all  $t$ .

Initially  $(S_0, I_0, R_0) = (N-1, 1, 0)$ .

# 3. General epidemic model

- Each infectious individual remains so for a length of time  $T_i \sim \text{Exp}(\gamma)$ .
- During this time, infectious contacts occur with each susceptible according to a Poisson process of rate  $\beta / N$ .
- Thus overall infection rate is  $\beta S_t I_t / N$ .
- Two model parameters,  $\beta$  and  $\gamma$ .

# 3. General epidemic model

- Viewed as a Markov Chain, the epidemic can be thought of as the bivariate process  $\{ (S(t), I(t)) : t \geq 0 \}$ ,  
where  $(S(0), I(0)) = (N-1, 1)$ .
- If chain currently at  $(s, i)$ , then it can jump to  
 $(s-1, i+1)$  (infection) at rate  $\beta s i / N$   
 $(s, i-1)$  (removal) at rate  $\gamma i$

# 3. General epidemic model

- Thus time spent in  $(s,i)$  is

$$T_{(s,i)} \sim \text{Exp}([\beta s i / N] + \gamma i)$$

- When chain leaves  $(s,i)$  it jumps to  
 $(s-1, i+1)$  with prob  $[\beta s i] / [\beta s i + N\gamma]$   
 $(s, i-1)$  with prob  $[N\gamma] / [\beta s i + N\gamma]$

# 3. General epidemic model

## Algorithm

Input parameters are  $N, \beta, \gamma$

Initialise  $s = N-1, i = 1, t = 0$

# 3. General epidemic model

```
while (i > 0) do {  
    T ~ Exp( [β s i / N] + γ i )  
    u ~ U(0,1)  
    if u < [β s ] / [β s + Nγ] then  
        s = s-1, i = i+1  
    else i = i-1  
    t = t + T  
    record (s,i), t }  
}
```

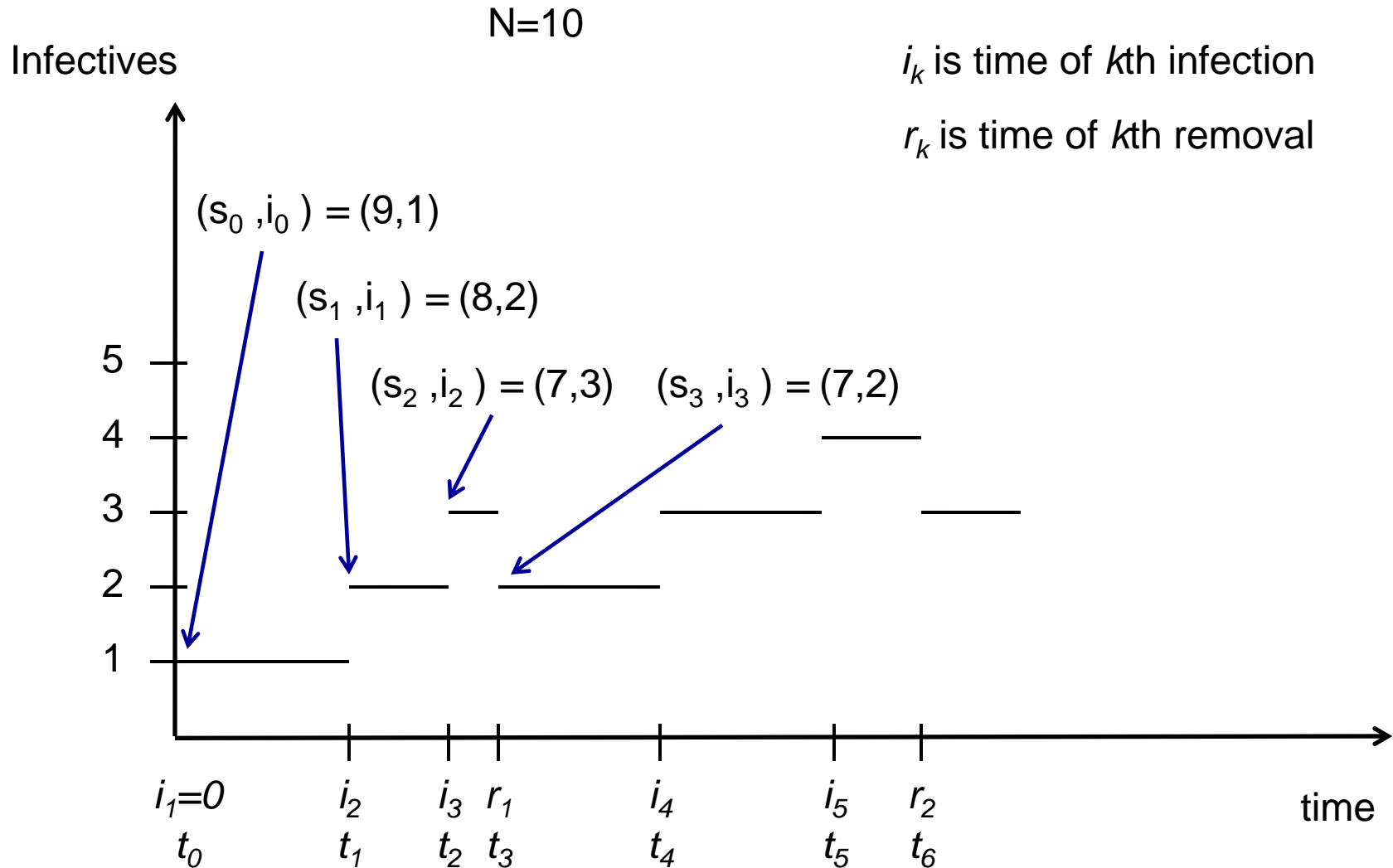
# 3. General epidemic model

Output of the algorithm is a sequence of times  $t_0, t_1, t_2, \dots$  and a corresponding sequence of states  $(s_0, i_0), (s_1, i_1), \dots, (s_m, i_m)$ , where  $m$  is the first event where  $i$  reaches zero.

It is usually also useful to keep track of the type of each event, i.e. whether it is an infection or a removal.



# 3. General epidemic model





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# 4. Non-Markov simulation

Same basic idea as before!

For non-Markov processes, we again simulate by generating the time until the next event.

However, in general the nice independence properties of the Markov case are lost and so we need to explicitly generate the times of future events as the algorithm evolves.

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# 5. Non-Markov epidemic model

In the Markov SIR model,

- infections occur according to a Poisson process of rate  $\beta S_t I_t / N$ .
- each infective remains so for a period of time  $T_i \sim \text{Exp}(\gamma)$ .

A common generalisation is to let the infectious period distribution  $T_i$  be some other distribution (e.g. constant, Gamma, ...)

# 5. Non-Markov epidemic model

## Model Definition

- Population of  $N$  individuals

- At time  $t$  there are:

$S_t$  susceptibles

$I_t$  infectives

$R_t$  recovered / immune individuals

Thus  $S_t + I_t + R_t = N$  for all  $t$ .

Initially  $(S_0, I_0, R_0) = (N-1, 1, 0)$ .

# 5. Non-Markov epidemic model

- Each infectious individual remains so for a length of time  $T_i$  drawn from some specified distribution with parameter vector  $\theta$
- During this time, infectious contacts occur with each susceptible according to a Poisson process of rate  $\beta / N$ .
- Thus overall infection rate is  $\beta S_t I_t / N$ .
- Two model parameters,  $\beta$  and  $\theta$ .

# 5. Non-Markov epidemic model

To simulate this epidemic:

- Generate removal time of each individual as they become infected
- This means that the time of next removal is known – as is the identity of the removed individual



# 5. Non-Markov epidemic model

To simulate this epidemic:

- Generate possible time-to-next-infection  
 $T \sim \text{Exp}(\beta s i / N)$
- If  $T <$  time of next removal, infection occurs
- Otherwise, the next removal occurs

# 5. Non-Markov epidemic model

Example: (Fixed infectious periods)

- Set  $T_i = c$ , a constant
- We will need  $r$ , which is a vector containing the removal times of all the current infectives

# 5. Non-Markov epidemic model

## Algorithm

Input parameters are  $N$ ,  $\beta$

Initialise  $s = N-1$ ,  $i = 1$ ,  $t = 0$

Initialise  $r = (c)$  (= removal time of initial infective)

# 5. Non-Markov epidemic model

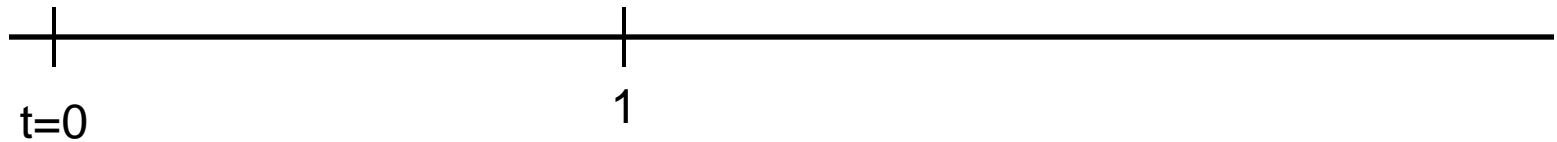
```
while (i > 0) do {  
    T ~ Exp(  $\beta s i / N$  )  
    R = min ( r )    # time of next removal  
    if (t + T < R)  # infection occurs  
        s = s - 1, i = i + 1  
    add new removal time (t + T + c) to r  
    t = t + T
```

## 5. Non-Markov epidemic model

```
else                # t + T > R: removal
i = i - 1
remove the minimal element of r from r
t = R
}                  # end of the i-loop
```

# 5. Non-Markov epidemic model

## Example



$$N=10, s=9, i=1, \beta = 1.5, c = 1$$

$$t = 0, r = (1)$$

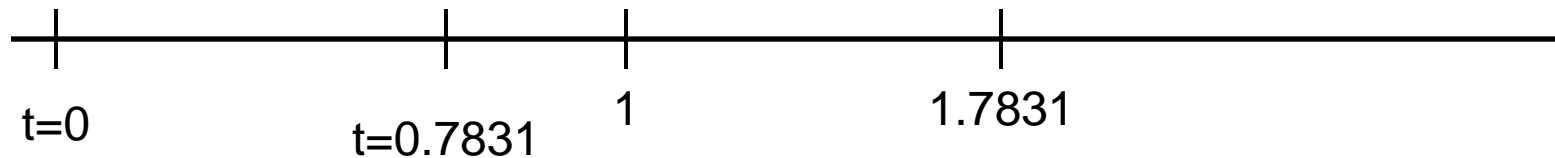
$$T \sim \text{Exp}(\beta s i / N) = 0.7831$$

$$R = \min(r) = 1$$

$$t + T = 0 + 0.7831 < R = 1 : \text{infection occurs}$$

# 5. Non-Markov epidemic model

## Example



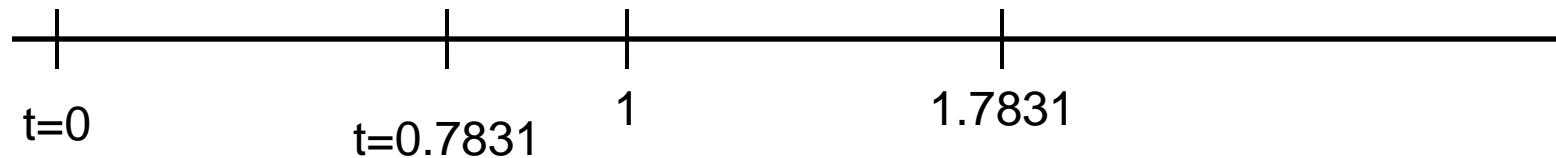
$$s = s - 1 = 8, i = i + 1 = 2$$

$$r = (1, 1.7831)$$

$$t = t + T = 0.7831$$

# 5. Non-Markov epidemic model

## Example



$$T \sim \text{Exp}(\beta s i / N) = 0.6110$$

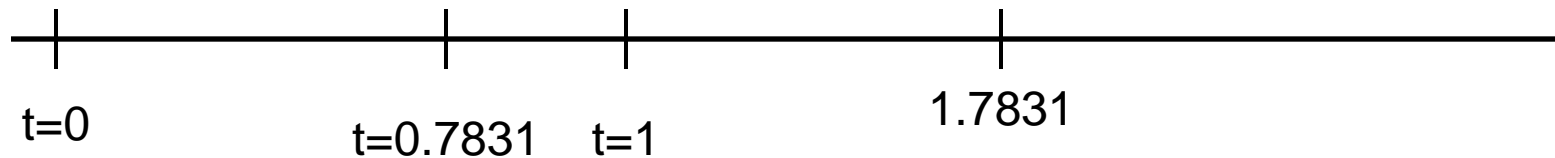
$$R = \min(r) = 1$$

$$t + T = 0.7831 + 0.6110 > R = 1 : \text{removal}$$



# 5. Non-Markov epidemic model

## Example



$$i = i - 1 = 1$$

Remove “1” from  $r$ , so now  $r = (1.7831)$

$$t = R = 1$$

etc.....

# 5. Non-Markov epidemic model

## Non-constant infectious period

- If  $T_i$  is not constant then simply need to generate a random sample from the distribution of  $T_i$  for the infectious period of an individual who has just become infected.

# 5. Non-Markov epidemic model

```
while (i > 0) do {  
    T ~ Exp(  $\beta s i / N$  )  
    R = min ( r )    # time of next removal  
    if (t + T < R)  # infection occurs  
        s = s - 1, i = i + 1  
    add new removal time (t + T + c) to r  
    t = t + T
```

↑

# 5. Non-Markov epidemic model

```
while (i > 0) do {  
     $T \sim \text{Exp}(\beta s i / N)$   
     $R = \min(r)$  # time of next removal  
    if ( $t + T < R$ ) # infection occurs  
         $s = s - 1, i = i + 1$   
    → generate  $c \sim T_i$   
    add new removal time ( $t + T + c$ ) to  $r$   
     $t = t + T$ 
```