Block 2.3
Stochastic Simulation Algorithms

NDMC Measles and Rubella Transmission Modelling Workshop

5-8 February 2024

The SIR Model

$$\frac{dS}{dt} = -\beta S \frac{I}{N}$$

$$\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

Recall that:

Rate of event is proportional to time until event

Here, rates depend on current states (number of S/I/R)

So, rates are constant ***until*** the states change

When the states change, the rates change

The SIR Model

$$\frac{dS}{dt} = -\beta S \frac{I}{N}$$

$$\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

Recall that:

For constant rate processes, with rate θ, the time until the event occurs can be reasonably modeled as an exponentially distributed random variable with mean 1/ θ

The SIR Model

$$\frac{dS}{dt} = -\beta S \frac{I}{N}$$

$$\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

For this simple SIR model:

Two kinds of events can happen

1. An infection can occur, which leads to
   S -> S – 1 and
   I -> I + 1
   This occurs at a rate $\beta S \frac{I}{N}$

2. An infected individual recovers, which leads to
   I -> I – 1 and
   R -> R + 1
   This occurs at a rate γI

The Gillespie Algorithm

Conditional on current numbers of S, I, R and current time T

1. Take a random draws from Exponential distribution for all possible state transitions

   X = random draw from exponential distribution with mean $1/(\beta S \frac{I}{N})$

   Y = random draw from exponential distribution with mean γI

2. Update States: IF

   X <= Y, then transmission occurs first: S -> S - 1, I -> I + 1, increment time T + X

   ELSE, recovery occurs first: I -> I - 1, R -> R + 1, increment time T + Y

3. Return to step 1

Interactive session 1: Run code

Questions:

What was R_0?

What did you notice about trajectories?

Gillespie Algorithm

Benefits

- Exact translation of stochastic ODE

Costs

- Computation scales with the number of state transitions (arrows in the SIR model) AND with the population size
- For this example, must draw ~2 random variables for every individual in the simulated population

Tau-leaping Algorithm

$$\frac{dS}{dt} = -\beta S \frac{I}{N}$$

$$\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

Recall that:

IF an event occurs at a constant rate θ, THEN the number of events that will occur in a time interval ΔT will be distributed as:

Poisson(θ* ΔT)

i.e. number of events will increase with the rate AND the duration of the interval

Tau-leaping Algorithm

$$\frac{dS}{dt} = -\beta S \frac{I}{N}$$

$$\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

So, for relatively small time steps, ΔT:

We can assume that the number of new infections that will occur will be distributed as:

$$\text{Poisson}(\beta S \frac{I}{N} * \Delta T)$$

And the number of recoveries that will occur will be distributed as:

$$\text{Poisson}(\gamma I * \Delta T)$$

Tau-leaping Algorithm

Conditional on current numbers of S, I, R and time step ΔT

1. Make random draws:

   New infections, dSI, are random draw from Poisson($\beta S \frac{I}{N}$* ΔT)

   New recoveries, dIR, are random draw from Poisson(γI* ΔT)

2. Update states

   S_{new} = S - dSI

   I_{new} = I + dSI – dIR

   R_{new} = R + dIR

   Update time by ΔT

3. Return to 1

Tau-leaping Algorithm

Conditional on current numbers of S, I, R and time step ΔT

1. Make random draws:

   New infections, dSI, are random draw from Poisson($\beta S \frac{I}{N}$* ΔT)

   New recoveries, dIR, are random draw from Poisson(γI* ΔT)

2. Update states

   S_{new} = S - dSI

   I_{new} = I + dSI – dIR

   R_{new} = R + dIR

   Update time by ΔT

3. Return to 1

Recall the definitions of **Incidence** and **Prevalence**,

Which of the terms at the left is the **Incidence**?

Which of the terms at the left is the **Prevalence**?

Is the number of children newly diagnosed for measles at clinic **Incidence** or **Prevalence**?

Tau-leaping Algorithm

Benefits

- Computation (number of random draws) is independent of population size

  (Note: while this makes a small difference in this code, it makes a ***large*** difference when simulating with births and deaths)

Costs

- Inexact. Requires assumption that rate is constant over ΔT, even though we know states are changing.

Interactive session 2: Run code

Questions:

How well do projections of Gillespie and Tau-leaping match?

Tau-leaping Algorithm

Benefits

- Computation (number of random draws) is independent of population size

  (Note: while this makes a small difference in this code, it makes a ***large*** difference when simulating with births and deaths)

Costs

- Did anyone get “warning” errors?

There were 50 or more warnings (use warnings() to see the first 50)

Tau-leaping Algorithm

Conditional on current numbers of S, I, R and time step ΔT

1. Make random draws:

   New infections, dSI, are random draw from Poisson($\beta S \frac{I}{N}$* ΔT)

   New recoveries, dIR, are random draw from Poisson(γI* ΔT)

2. Update states

   S_{new} = S - dSI

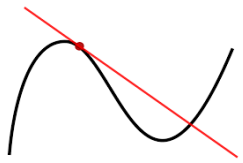
   I_{new} = I + dSI – dIR

   R_{new} = R + dIR

   Update time by ΔT

3. Return to 1

Tangent



It is possible to make a random draw of dIR that is greater than I, which makes I_{new}<0

This can be addressed by disallowing negative outcomes in code, or using binomial draws

Tau-leaping Algorithm

$$\frac{dS}{dt} = -\beta S \frac{I}{N}$$

$$\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

ALSO, for relatively small time steps, ΔT:

Rate in Poisson process can be translated to probability of event and modeled as a Binomial random variable.

The number of new infections that will occur will be:

Binomial(S, 1-exp($-\beta \frac{I}{N}$* ΔT))

And the number of recoveries that will occur will be:

Binomial(I,1-exp(-γ * ΔT))

Tau-leaping Algorithm

$$\frac{dS}{dt} = -\beta S \frac{I}{N}$$

$$\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

ALSO, for relatively small time steps, ΔT:

Rate in Poisson process can be translated to probability of event and modeled as a Binomial random variable.

The number of new infections that will occur will be:

Binomial(S, 1-exp($-\beta \frac{I}{N}$* ΔT))

And the number of recoveries that will occur will be:

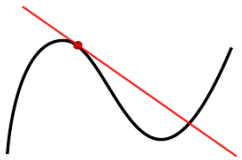
Binomial(I, 1-exp(-γ * ΔT))

Recall that this expression turns **rate** ($\beta S \frac{I}{N}$ or γ) measured over time into **risk,** which is measured per population.

ODEs, Gillespie, Tau-leaping

- An implicit assumption of the standard ODE representation the SIR model, the difference equation representation, AND both the Gillespie and Tau-leaping algorithms is that the rate of recovery (γ) is constant across time for each infected individual.
- This means that an individual is just as likely to recover after 1 day as after 10 days or 20 day (if they haven't already recovered)

Tangent



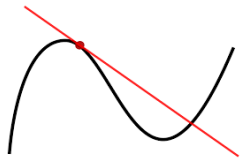
Some elegant approaches to overcome this:
http://alun.math.ncsu.edu/static/alun/tpb_01.pdf

ODEs, Gillespie, Tau-leaping

- An implicit assumption of the standard ODE representation the SIR model, the difference equation representation, AND both the Gillespie and Tau-leaping algorithms is that the rate of recovery (γ) is constant across time for each infected individual.
- This means that an individual is just as likely to recover after 1 day as after 10 days or 20 day (if they haven't already recovered)

One simple approach to overcome this is to use a time step, ΔT, that is equal to the average infectious period, $1/\gamma$

Tangent



Some elegant approaches to overcome this:
http://alun.math.ncsu.edu/static/alun/tpb_01.pdf

Chain Binomial Algorithm

Conditional on current numbers of S, I, R and time step equal to $1/\gamma$

1. I_{new} is a binomial draw from all current susceptibles

   I_{new} ~binomial(S, 1 – exp(- $\beta \frac{I}{N}$))

2. $S_{new} = S - I_{new}$
3. Return to 1

Note that magnitude of β will be different than for Gillespie and Tau-leaping algorithms.

Expected value of binomial(N,p) is N*p.
Here, the expected value of I_{new} is
$E[I_{new}] = S * 1\text{-}\exp(-\beta \frac{I}{N}) \cong \beta * S * \frac{I}{N}$

Chain Binomial Algorithm

Conditional on current numbers of S, I, R and time step equal to $1/\gamma$

1. I_{new} is a binomial draw from all current susceptibles

   I_{new} ~binomial(S, $1 - \exp(-\beta \frac{I}{N})$)

2. $S_{new} = S - I_{new}$
3. Return to 1

Note that magnitude of β will be different than for Gillespie and Tau-leaping algorithms.

Expected value of binomial(N,p) is N*p.
Here, the expected value of I_{new} when I=1 and S=N is

$E[I_{new}] = S * 1\text{-}\exp(-\beta \frac{I}{N}) \cong \beta * S * \frac{I}{N}$

$= N * 1\text{-}\exp(-\beta \frac{1}{N}) = N * 1\text{-}\exp(-\frac{\beta}{N})$

$\cong N * \frac{\beta}{N}$

$\cong \beta$ -> $\beta = R_0$

Chain Binomial Algorithm

Benefits

- Computation (number of random draws) is independent of population size
- Only need 1 random draw per time step
- Natural translation to methods for inference …

Costs

- Inexact. Requires assumption that rate is constant over ΔT, even though we know states are changing.

Interactive session 3: Run code

Questions:

How well do projections of Chain Binomial match Gillespie and Tau-leaping?

Chain Binomial Algorithm

If each infectious individual is expected to be infectious, for on average, a time equal to $1/\gamma$, then we can use a time step ΔT that is equal to $1/\gamma$.

Chain Binomial Algorithm

If each infectious individual is expected to be infectious, for on average, a time equal to $1/\gamma$, then we can use a time step ΔT that is equal to $1/\gamma$.

Why? … well, this means that everyone is infected for the same amount of time (Gillespie and Tau-leaping technically allow some to be infected for very short or very long times, analogous to continuous aging that Emilia mentioned yesterday.)

Chain Binomial Algorithm

If each infectious individual is expected to be infectious, for on average, a time equal to $1/\gamma$, then we can use a time step ΔT that is equal to $1/\gamma$.

Why? … well, this means that everyone is infected for the same amount of time (Gillespie and Tau-leaping technically allow some to be infected for very short or very long times, analogous to continuous aging that Emilia mentioned yesterday.)

And … each case recovers at the end of each time step, so the number of Is in time step t is ***BOTH*** the prevalence ***AND*** the incidence. So this more naturally matches to observed time series of incident cases.

Chain Binomial Algorithm

Conditional on current numbers of S, I, R and time step equal to $1/\gamma$

1. I_{new} is a binomial draw from all current susceptibles

   I_{new} ~binomial(S, 1 – exp(- $\beta \frac{I}{N}$))

2. $S_{new} = S - I_{new}$
3. Return to 1

Note that magnitude of β will be different than for Gillespie and Tau-leaping algorithms.

Expected value of binomial(N,p) is N*p.
Here, the expected value of I_{new} is

$E[I_{new}] = S * 1\text{-}\exp(-\beta \frac{I}{N}) \cong \frac{\beta}{N} * S * I$

β is ~ R_0

Chain Binomial Algorithm

Benefits

- Computation (number of random draws) is independent of population size
- Randomness is limited only to the infection
- Individuals all remain infectious for the same amount time

Costs

- Inexact. Requires assumption that rates are constant over the entire epidemic

Chain Binomial Algorithm – with births

Conditional on current numbers of S, I, R and time step equal to $1/\gamma$

1. I_{new} is a binomial draw from all current susceptibles

   I_{new} ~binomial(S, 1 – exp(- $\beta \frac{I}{N}$))

2. $S_{new} = B + S - I_{new}$
3. Return to 1

Note that magnitude of β will be different than for Gillespie and Tau-leaping algorithms.

Expected value of binomial(N,p) is N*p.
Here, the expected value of I_{new} is

$E[I_{new}] = S * 1\text{-}\exp(-\beta \frac{I}{N}) \cong \frac{\beta}{N} * S * I = \hat{\beta} * S * I$

B = birth in each time step