

1 The epidemic lambda-coalescent model

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1 Introduction

Superspreading in infectious disease epidemiology (Lloyd-Smith et al. 2005). For example SARS-CoV-2 superspreading (Wang et al. 2020; Lemieux et al. 2021; Gómez-Carballa et al. 2021). Coalescent model (Kingman 1982a,b). Work by Li and Fraser (Li et al. 2017; Fraser and Li 2017). Lambda-coalescent models (Pitman 1999; Sagitov 1999; Donnelly and Kurtz 1999). Beta-coalescent (Schweinsberg 2003) is a specific type of Lambda-coalescent. Was used in (Hoscheit and Pybus 2019) and (Menardo et al. 2021). David’s paper on inference of multiple mergers while dating a pathogen phylogeny (Helekal et al. 2024).

2 General case

Discrete time t . Non-overlapping generations of infected individuals. At time t there are N_t infected individuals. Each of them creates a number $s_{t,i}$ of secondary infections at time $t + 1$, following the offspring distribution $\alpha_t(s)$. The mean of this distribution is the basic reproduction number R_t and the variance is V_t . We have:

$$N_{t+1} = \sum_{i=1}^{N_t} s_{t,i} \quad (1)$$

Let $p_{k,t}$ be the probability that k individuals at time $t + 1$ have the same infector at time t .

2.1 Inclusive coalescence probability

Inclusive coalescence probability $p_{k,t}(N_t, N_{t+1})$ is the probability that exactly k randomly-sampled individuals from generation $t + 1$ find a common ancestor in generation t (*conditioning on population sizes N_t and N_{t+1}*).

Given full information about offspring counts from individuals in generation t $\mathbf{s}_t = (s_{t,1}, \dots, s_{t,N_t})$, we have

$$\begin{aligned} p_{k,t}(\mathbf{s}_t, N_t) &= \sum_{i=1}^{N_t} \frac{\binom{s_{t,i}}{k}}{\binom{N_{t+1}}{k}} \\ &= \sum_{i=1}^{N_t} \frac{\Gamma(s_{t,i} + 1) \Gamma(N_{t+1} - k + 1)}{\Gamma(s_{t,i} - k + 1) \Gamma(N_{t+1})}. \end{aligned} \quad (2)$$

Full information $\{s_{t,i}\}$ yields the population size N_{t+1} but is not feasible to observe in practice. We can instead express the inclusive coalescence probability conditioning on the next population size N_{t+1} by summing over possible offspring counts $\mathbf{s}_t = (s_{t,1}, \dots, s_{t,N_t})$ conditional on the total generation size

33 To-do/To-discuss:

- 34 • Almost certainly should be an appendix not a main-body derivation, doesn't fundamentally
35 change anything but I think this looks horrific
- 36 • Sum subscripts over $\mathbf{s}_t \in \mathbb{N}_0^{N_t}$ rather than $\mathbf{s}_t : \dots$ (c.f. exclusive probability derivation)? We have
37 probability 0 if sum does not equal N_{t+1} anyway
- 38 • Change $\mathbf{s}_t \mapsto \mathbf{s}$ and $s_{t,i} \mapsto s_i$ for clarity/brevity? Should maintain $S_{t,i}$ etc. for consistent notation
39 ($S_{t,i} = s_i$ etc.)
- 40 • Define $S_t^{-(1)} = (S_{t,2}, \dots, S_{t,N_t})$ notation

$$\begin{aligned}
p_{k,t}(N_t, N_{t+1}) &= \sum_{\mathbf{s}_t : \sum_{i=1}^{N_t} s_{i,t} = N_{t+1}} \mathbb{P} \left[\mathbf{S}_t = \mathbf{s}_t \middle| \sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right] p_{k,t}(\mathbf{s}_t, N_t) \\
&= \sum_{\mathbf{s}_t : \sum_{i=1}^{N_t} s_{i,t} = N_{t+1}} \mathbb{P} \left[\mathbf{S}_t = \mathbf{s}_t \middle| \sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right] \sum_{i=1}^{N_t} \frac{\binom{s_{t,i}}{k}}{\binom{N_{t+1}}{k}} \\
&= \sum_{i=1}^{N_t} \sum_{\mathbf{s}_t : \sum_{i=1}^{N_t} s_{i,t} = N_{t+1}} \frac{\binom{s_{t,i}}{k}}{\binom{N_{t+1}}{k}} \mathbb{P} \left[S_{t,1} = s_{t,1}, \mathbf{S}_t^{-(1)} = \mathbf{s}_t^{-(1)} \middle| \sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right] \\
&= \frac{N_t}{\binom{N_{t+1}}{k}} \sum_{\mathbf{s}_t : \sum_{i=1}^{N_t} s_{i,t} = N_{t+1}} \binom{s_{t,1}}{k} \mathbb{P} \left[S_{t,1} = s_{t,1} \middle| \sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right] \\
&\quad \times \mathbb{P} \left[\mathbf{S}_t^{-(1)} = \mathbf{s}_t^{-(1)} \middle| S_{t,1} = s_{t,1}, \sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right] \\
&= \frac{N_t}{\binom{N_{t+1}}{k}} \sum_{s_{t,1}=0}^{N_{t+1}} \binom{s_{t,1}}{k} \mathbb{P} \left[S_{t,1} = s_{t,1} \middle| \sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right] \\
&\quad \times \underbrace{\sum_{\mathbf{s}_t^{-(1)} : \sum_{i=2}^{N_t} s_{i,t} = N_{t+1} - s_{t,1}} \mathbb{P} \left[\mathbf{S}_t^{-(1)} = \mathbf{s}_t^{-(1)} \middle| \sum_{i=2}^{N_t} S_{t,i} = N_{t+1} - s_{t,1} \right]}_{=1} \\
&= \frac{N_t}{\binom{N_{t+1}}{k}} \mathbb{E} \left[\binom{S_{t,1}}{k} \middle| \sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right] \tag{3}
\end{aligned}$$

41 The falling factorial moments $\mathbb{E} \left[\frac{S_{t,1}!}{(S_{t,1}-k)!} \middle| \sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right]$ in (3) can be readily obtained by
42 differentiating the probability generating function of $S_{t,1} | (\sum_{i=1}^{N_t} S_{t,i} = N_{t+1})$.

43 2.2 Exclusive coalescence probability

44 Generally, we observe a sample of individuals from each generation rather than the entire population.
45 In this case, we are interested in the exclusive coalescence probability $p_{nkt}(N_t, N_{t+1})$ that exactly k

46 individuals from a sample of n arose from a common ancestor one generation in the past given knowledge
 47 of the total population sizes N_t and N_{t+1} .

48 Given full information about offspring counts of the parents of sampled individuals at the present,
 49 $\mathbf{x}_t = (x_{t,1}, \dots, x_{t,N_t})$, we have

$$\begin{aligned} p_{nkt}(\mathbf{x}_t, N_t) &= \sum_{i=1}^{N_t} \frac{\binom{x_{t,i}}{k}}{\binom{n}{k}} \mathbb{I}\{x_{t,i} = k\} \\ &= \sum_{i=1}^{N_t} \frac{x_{t,i}!}{(x_{t,i} - k)!} \frac{(n - k)!}{n!} \mathbb{I}\{x_{t,i} = k\}. \end{aligned} \quad (4)$$

50 Similarly to the exclusive coalescence probability, we can use this to evaluate the exclusive probability
 51 given N_t and N_{t+1} by summing over possible parent offspring configurations (for $k \leq n$),

$$\begin{aligned} p_{nkt}(N_t, N_{t+1}) &= \sum_{\mathbf{x}_t \in \mathbb{N}_0^{N_t}} \mathbb{P}\left[\mathbf{X}_t = \mathbf{x}_t \mid \sum_{i=1}^n X_{t,i} = n\right] p_{n,k,t}(\mathbf{x}_t, N_t) \\ &= \sum_{\mathbf{x}_t \in \mathbb{N}_0^{N_t}} \mathbb{P}\left[\mathbf{X}_t = \mathbf{x}_t \mid \sum_{i=1}^n X_{t,i} = n\right] \sum_{i=1}^{N_t} \frac{\binom{x_{t,i}}{k}}{\binom{n}{k}} \mathbb{I}\{x_{t,i} = k\} \\ &= \frac{N_t}{\binom{n}{k}} \sum_{\mathbf{x}_t \in \mathbb{N}_0^{N_t}} \binom{x_{t,1}}{k} \mathbb{P}\left[\mathbf{X}_t = \mathbf{x}_t \mid \sum_{i=1}^{N_t} X_{t,i} = n\right] \mathbb{I}\{x_{t,1} = k\} \\ &= \frac{N_t}{\binom{n}{k}} \sum_{\mathbf{x}_t^{-(1)} : \sum_{i=2}^n x_{t,i} = n-k} \binom{k}{k} \mathbb{P}\left[X_{t,1} = k, \mathbf{X}_t^{-(1)} = \mathbf{x}_t^{-(1)} \mid \sum_{i=1}^{N_t} X_{t,i} = n\right] \\ &= \frac{N_t}{\binom{n}{k}} \mathbb{P}\left[X_{t,1} = k \mid \sum_{i=1}^{N_t} X_{t,i} = n\right] \sum_{\mathbf{x}_t^{-(1)} : \sum_{i=2}^n x_{t,i} = n-k} \mathbb{P}\left[\mathbf{X}_t^{-(1)} = \mathbf{x}_t^{-(1)} \mid \sum_{i=1}^{N_t} X_{t,i} = n, X_{t,1} = k\right] \\ &= \frac{N_t}{\binom{n}{k}} \mathbb{P}\left[X_{t,1} = k \mid \sum_{i=1}^{N_t} X_{i,t} = n\right]. \end{aligned} \quad (5)$$

52 2.3 Complementarity of exclusive coalescence probabilities

53 Note that for any offspring distribution we have:

$$\sum_{k=1}^n p_{nkt} \binom{n-1}{k-1} = 1 \quad (6)$$

$$\sum_{k=1}^n \binom{n-1}{k-1} p_{nkt} = \sum_{k=1}^n \binom{n-1}{k-1} \frac{N_t}{\binom{n}{k}} \mathbb{P}[X_1 = k | \sum_{i=1}^{N_t} X_i = n] \quad (7)$$

$$= \sum_{k=1}^n N_t \frac{k}{n} \mathbb{P}[X_1 = k | \sum_{i=1}^{N_t} X_i = n] \quad (8)$$

$$= \frac{N_t}{n} \sum_{k=0}^n k \mathbb{P}[X_1 = k | \sum_{i=1}^{N_t} X_i = n] \quad (\text{lower limit } k=0 \text{ makes no difference overall})$$

$$= \frac{N_t}{n} \mathbb{E}[X_1 | \sum_{i=1}^{N_t} X_i = n] \quad (9)$$

$$= p_{1,t}(N_t, n) = 1 \quad (\text{see below})$$

54 Taken from stackexchange (link)

$$\begin{aligned} \mathbb{E}[X_1 | \sum_{i=1}^{N_t} X_i = n] &= \frac{1}{N_t} \sum_{i=1}^{N_t} \mathbb{E}[X_i | \sum_{i=1}^{N_t} X_i = n] && (X_i \text{ i.i.d.}) \\ &= \frac{1}{N_t} \mathbb{E}[\sum_{i=1}^{N_t} X_i | \sum_{i=1}^{N_t} X_i = n] && (\text{Swap expectation, sum (possibly questionable?)}) \\ &= \frac{n}{N_t} && (10) \end{aligned}$$

55 3 Poisson case

56 Here the offspring distribution is $\alpha_t = \text{Poisson}(R_t)$. In this case, we have

$$\sum_{i=1}^{N_t} S_{t,i} \sim \text{Poisson}(N_t R_t), \quad (11)$$

57 and conditional distribution

$$\mathbb{P}\left[S_{t,1} = s \mid \sum_{i=1}^{N_t} S_{t,i} = N_{t+1}\right] = \frac{\mathbb{P}\left[S_{t,1} = s, \sum_{i=1}^{N_t} S_{t,i} = N_{t+1}\right]}{\mathbb{P}\left[\sum_{i=1}^{N_t} S_{t,i} = N_{t+1}\right]} \quad (12)$$

$$= \frac{\alpha_t(s) \mathbb{P}\left[\sum_{i=2}^{N_t} S_{t,i} = N_{t+1} - s\right]}{\mathbb{P}\left[\sum_{i=1}^{N_t} S_{t,i} = N_{t+1}\right]} \quad (13)$$

$$= \frac{\frac{R_t^s e^{-R_t}}{s!} \cdot \frac{((N_t - 1)R_t)^{N_{t+1}-s}}{(N_{t+1} - s)!}}{\frac{(N_t R_t)^{N_{t+1}} e^{-N_t R_t}}{N_{t+1}!}} \quad (14)$$

$$= \binom{N_{t+1}}{s} \left(\frac{1}{N_t}\right)^s \left(1 - \frac{1}{N_t}\right)^{N_{t+1}-s}, \quad (15)$$

that is

$$S_{t,1} \left| \left(\sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right) \right. \sim \text{Binomial} \left(N_{t+1}, \frac{1}{N_t} \right). \quad (16)$$

The inclusive probability of coalescence for k lines is given by (3) with the falling factorial moments

$$\mathbb{E} \left[\binom{S_{t,1}}{k} \left| \sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right. \right] = \frac{1}{k!} \mathbb{E} \left[\frac{S_{t,1}!}{(S_{t,1} - k)!} \left| \sum_{i=1}^{N_t} S_{t,i} = N_{t+1} \right. \right] = \frac{1}{k!} \frac{N_{t+1}!}{(N_{t+1} - k)!} \left(\frac{1}{N_t} \right)^k, \quad (17)$$

taken from Potts (1953).

Consequently, the inclusive probability of coalescence for two lines is

$$p_{2,t} = \frac{1}{N_t}, \quad (18)$$

and more generally the inclusive probability of coalescence for k lines is

$$p_{k,t} = \frac{1}{N_t^{k-1}}. \quad (19)$$

The inclusive probability of coalescence for two lines is exactly analogous to the Wright-Fisher model, with each individual at generation $t + 1$ selecting a parent uniformly at random from generation t .

The exclusive probability of coalescence for two lines from a sample of n ($n \geq 2$) is

$$p_{n,2,t} = \frac{(N_t - 1)^{n-2}}{N_t^{n-1}}, \quad (20)$$

and more generally the exclusive probability of coalescence for k lines from a sample of n ($n \geq k$) is

$$p_{n,k,t} = \frac{(N_t - 1)^{n-k}}{N_t^{n-1}}. \quad (21)$$

4 Negative-Binomial case

Here the offspring distribution is Negative-Binomial with mean R_t and variance V_t . The parameters of this distribution are $r = R_t^2/(V_t - R_t)$ and $p = R_t/V_t$.

The inclusive probability of coalescence for two lines is:

$$p_{2,t} = \frac{r + 1}{N_t r + 1} \quad (22)$$

71 The inclusive probability of coalescence for k lines is:

$$p_{k,t} = \prod_{i=1}^{k-1} \frac{r+i}{N_t r + i} = \frac{B(N_t r + 1, r + k)}{B(r + 1, N_t r + k)} \quad (23)$$

72 where $B(x, y)$ denotes the Beta function defined as $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x + y)$.

73 The exclusive probability of coalescence for k lines is:

$$p_{nkt} = \frac{N_t B(k + r, n - k + N_t r - r)}{B(r, N_t r - r)} \quad (24)$$

74 5 Example

75 Let the offspring distribution have a mean of $R_t = 2$. In the Poisson case the offspring distribution
 76 is Poisson(2). We consider NegBin cases with the same mean and varying dispersion parameters r .
 77 When r is high the dispersion is low and the NegBin behaves almost like a Poisson. See Figure 1.

78 6 Lambda-coalescent

79 A lambda-coalescent model is defined by a probability measure $\Lambda(dx)$ on the interval $[0, 1]$, from which
 80 we can deduce the rate $\lambda_{n,k}$ at which any subset of k lineages within a set of n observed lineages
 81 coalesce:

$$\lambda_{n,k} = \int_0^1 x^{k-2} (1-x)^{n-k} \Lambda(dx) \quad (25)$$

82 The Beta($2 - \alpha, \alpha$)-coalescent model (Schweinsberg 2003) has a single parameter $\alpha \in [0, 2]$ and is
 83 defined as:

$$\Lambda(dx) = \frac{x^{1-\alpha} (1-x)^{\alpha-1}}{B(2-\alpha, \alpha)} dx \quad (26)$$

84 from which we can deduce that:

$$\lambda_{n,k} = \frac{B(k - \alpha, n - k + \alpha)}{B(2 - \alpha, \alpha)} \quad (27)$$

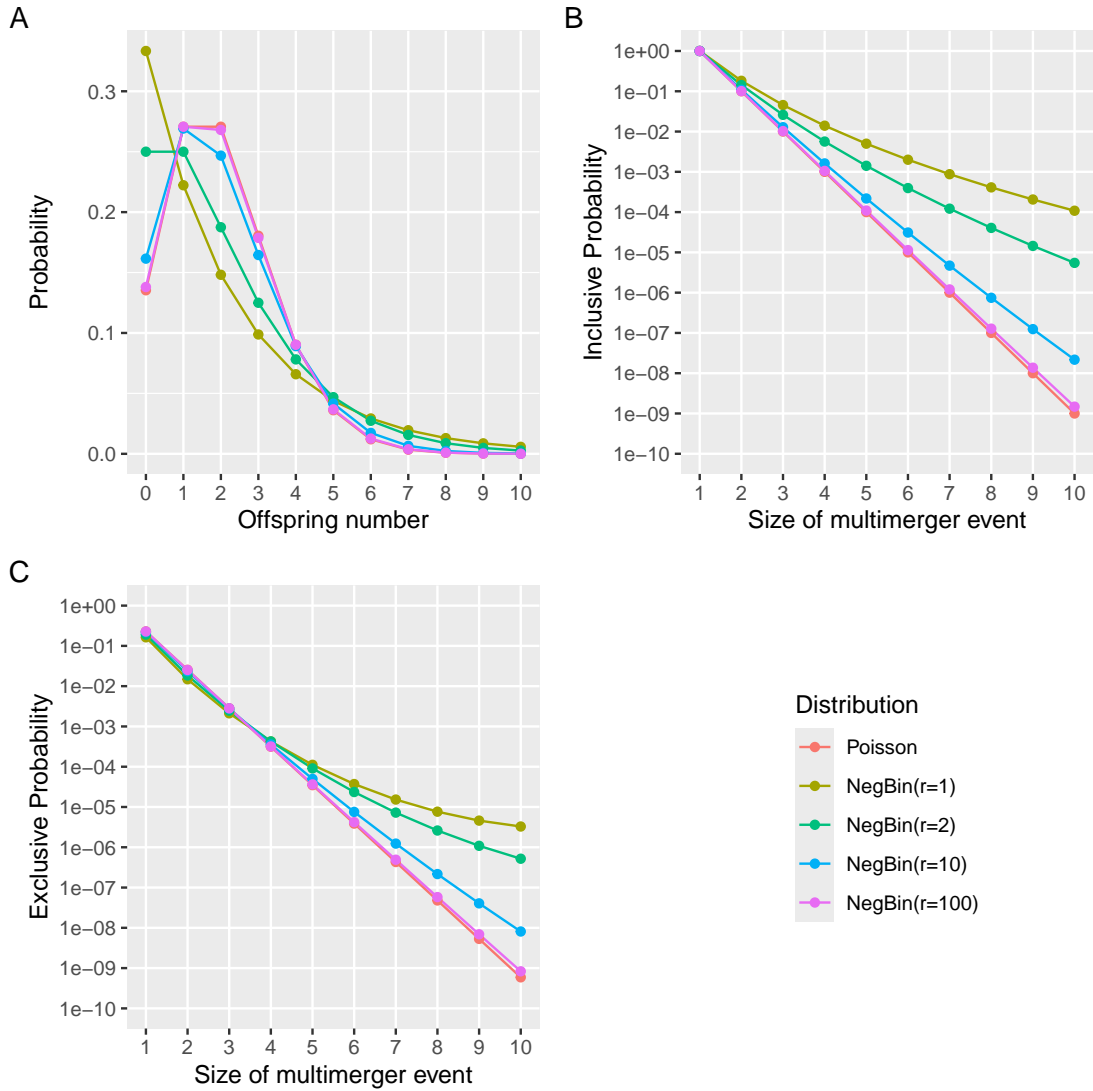


Figure 1: (A) Offspring distribution. (B) Inclusive probability of coalescence. (C) Exclusive probability of coalescence.

Special cases include $\alpha = 2$ corresponding to the Kingman coalescent, $\alpha = 1$ which is known as the Bolthausen-Sznitman coalescent and $\alpha = 0$ for which the phylogeny is always star-shaped.

7 Implementation

We implemented the analytical methods described in this paper in a new R package entitled *EpiLambda* which is available at <https://github.com/xavierdidelot/EpiLambda> for R version 3.5 or later. All code and data needed to replicate the results are included in the “run” directory of the *EpiLambda*

91 repository.

92 **8 Discussion**

93 **Acknowledgements**

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