Perfect Epidemics

Seminar at University College Dublin

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Warwick, York

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Introduction

Homage to Dublin
(Book of Kells, 9th century)

Work on perfect simulation (CFTP) for epidemics, now being written up.
WSK acknowledges the support of UK EPSRC grant EP/R022100.

Handout is on the web: use the `QR-code` or visit
`wilfridskendall.github.io/talks/PerfectEpidemics`.

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Plan of talk

Gregory: Is there any other point to which you would wish to draw my attention?
Holmes: To the curious incident of the dog in the night-time.
Gregory: The dog did nothing in the night-time.
Holmes: That was the curious incident.

from "The Adventure of Silver Blaze", Sir Arthur Conan Doyle (1892).

(a) Introduction to perfect simulation:
(b) A little theory about CFTP;
(c) Epidemics and the R-number;
(d) "Contact tracing" (inferring infection pattern if removals observed);
(e) Example with real data.

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1. A Visual Introduction to Perfect Simulation

1. Propp & Wilson (1996) invented exact simulation / Coupling from the Past (CFTP) / perfect simulation;
2. The term "perfect simulation" (WSK, 1998) was chosen to encourage you to be suspicious: perfection is never achieved!
3. Key ideas of "*classic CFTP*":
   - extend simulation *backwards* through time not forwards;
   - exploit monotonicity (*couple* maximal and minimal processes);
   - seek coalescence.
4. Simplest possible example: *random-walk-CFTP*
   (can boost to use Ising model to do simple image reconstruction).

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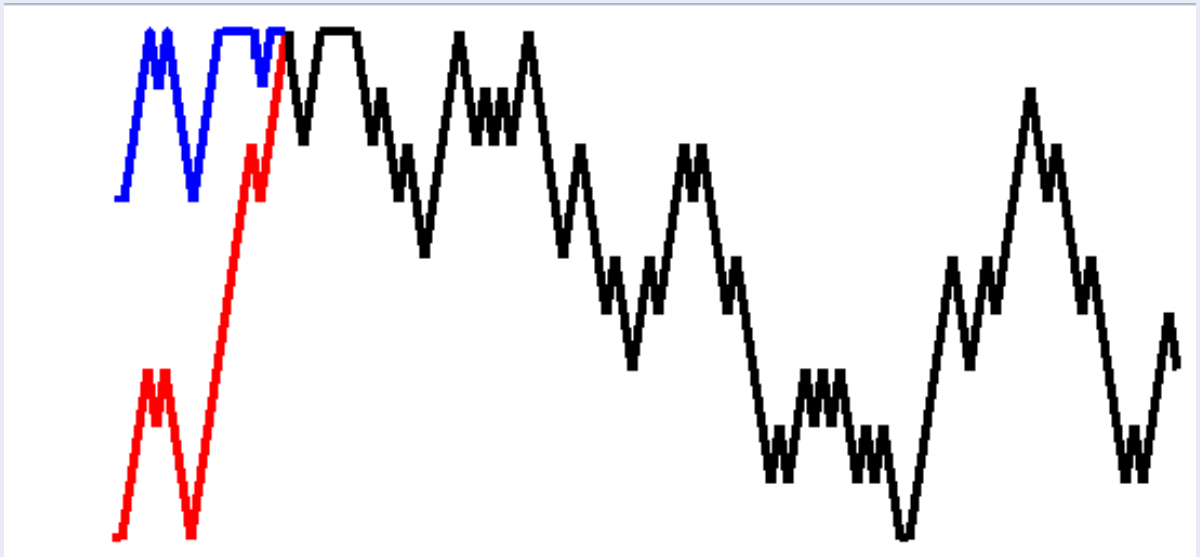
Classic CFTP for a simple random walk (I)

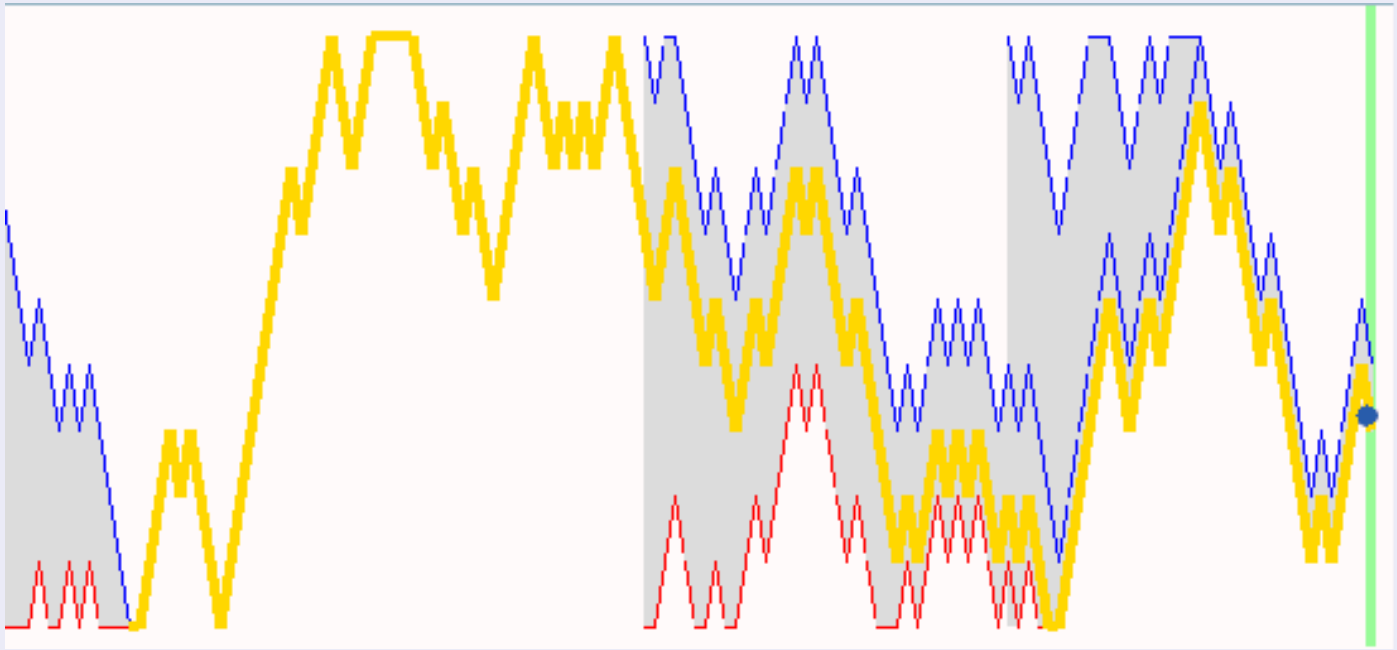
1. Consider a simple random walk on $0{:}9 = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$.
   - $\mathbb{P}[+1 \text{ jump}] = p \in (0, 1)$, while $\mathbb{P}[-1 \text{ jump}] = 1-p$, **except that**
   - at state 9 replace the $+1$ jump by "staying still", **and**
   - at state 0 replace the -1 jump by "staying still".
2. Conventional MCMC picks a starting point, then runs the simple random walk for long time till approximate equilibrium.



3. How long? One way to *estimate* this is to run two (or several?) coupled copies till they meet. If probability of meeting by time T is high, then deviation of X_T from equilibrium is statistically small;
4. Generally not true that location *at* coupling is a draw from equilibrium.

Classic CFTP for a simple random walk (II)

1. Start at top (9) and bottom (0) at negative time $-T$, run to time 0.



2. If not coupled by time 0, than back-off to time $-2T$ and repeat.
   NB: re-use randomness!
3. May need to iterate back-off doubling several times.
4. When coupled, top and bottom yield a common value at time 0.
5. The common value (golden thread) is an exact draw from equilibrium!

Some more CFTP theory

1. What if monotonicity fails? or there isn't a sensible "maximal" process? Ideas (WSK, 1998):
   - cross-couple upper and lower envelope processes,
   - or dominate by amenable "dominating process" (time-reversible, can draw from equilibrium, can couple target processes below dominating process).
2. Theoretical limits: *in principle*
   - *Classical CFTP* equivalent to uniform ergodicity (Foss & Tweedie, 1998);
   - *Dominated CFTP* achievable under geometric ergodicity (WSK, 2004);
   - Dominated CFTP can work in some **non**-geometrically ergodicity cases (SBC & WSK, 2007a; *nb* corrigendum SBC & WSK, 2007b).
3. Dominated CFTP delivers perfect simulation for stable point processes (WSK & Møller, 2000);
4. Detailed expositions: WSK (2005), Huber (2015).
   (Want to implement CFTP in R? see WSK, 2015.)

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2. Perfect Epidemics: a challenge problem for CFTP

S-I-R deterministic epidemic: differential equation system for (s, i, r)

$$\begin{aligned}
\textbf{Susceptible:} \quad & s' &=& -\alpha\, s\, i\,, \\
\textbf{Infected:} \quad & i' &=& (\alpha\, s - \beta\,)\; i\,, \\
\textbf{Removed:} \quad & r' &=& \beta\, i\,.
\end{aligned}$$

Constant total population $s + i + r = n$.

S-I-R stochastic epidemic: Markov chain (S, I, R) with transitions

$$\begin{aligned}
\textbf{Infection:} \quad & S \to S - 1\,, & I \to I + 1 \quad & \text{at rate} & \alpha\, S\, I\,, \\
\textbf{Removal:} \quad & I \to I - 1\,, & R \to R + 1 \quad & \text{at rate} & \beta\, I\,.
\end{aligned}$$

Both models share an unrealistic assumption: homogeneous mixing.

In contrast, Fraser *et al* (2023) deploy a UK model with $N{=}10^6$ agents!

There are *many* important inferential questions (Cori & Kucharski, 2024).

The first question asked about a new epidemic

"What is the R-number?"

The R-number is $\alpha\ s_0/\beta$: mean number of new infectives produced per infective at *start* of epidemic with initially s_0 susceptibles.
Whittle (1955)'s threshold theorem: R-number $\gg 1$ implies strongly positive chance of epidemic infecting significant proportion of the population.

Wikipedia: "The British-registered *Diamond Princess* was the first cruise ship to have a major `[COVID-19]` outbreak on board, with the ship quarantined at Yokohama from 4 February 2020 for about a month. Of 3711 passengers and crew, around 700 people became infected and 9 people died."
Evidently $\alpha\ s_0/\beta \gg 1$ – as was sadly later confirmed, a sorrow for us all.

Inference on the R-number

Important, because the R-number controls severity of epidemic. However:

1. Modelling is tough. *Either* massive assumptions (homogeneous mixing) *or* very many parameters;
2. Inference is really tough: hard to get information about infection times;
3. It is all especially tough in early stages. Answers are most needed when hardly any information is available (a simplified example for a Warwick UG second-year statistics module shows how tough this can be);
4. Markov chain Monte Carlo (MCMC) can be used (see next slide) but what about burn-in?
5. Can we use perfect simulation?

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An easier question: "Contact Tracing"

The simplest possible variant of contact tracing:
"When did the infections occur, supposing we only observe removals?"
(Gibson & Renshaw, 1998; O'Neill & Roberts, 1999; Gibson & Renshaw, 2001)

Important first step: think about generation of an *unconditioned* epidemic.

1. Suppose n, α, β are known. Eventually removal times are observed, but unobserved infection times must be inferred.
2. Visualize n timelines, along which incidents are scattered:
   - potential removals, activated if timeline is infected;
   - potential infections, activated if timeline is infected *and* if designated target timeline is lowest uninfected timeline.
3. Poisson point processes *of appropriate rates* yield an S-I-R epidemic.
4. First step: evolve whole S-I-R trajectory in *algorithmic time* (alter potential infections and removals using immigration-death in discrete algorithmic time).
5. Result: *trajectory-valued chain*, unconditioned S-I-R as equilibrium.

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From incidents to unconditioned epidemic trajectories (1/3)

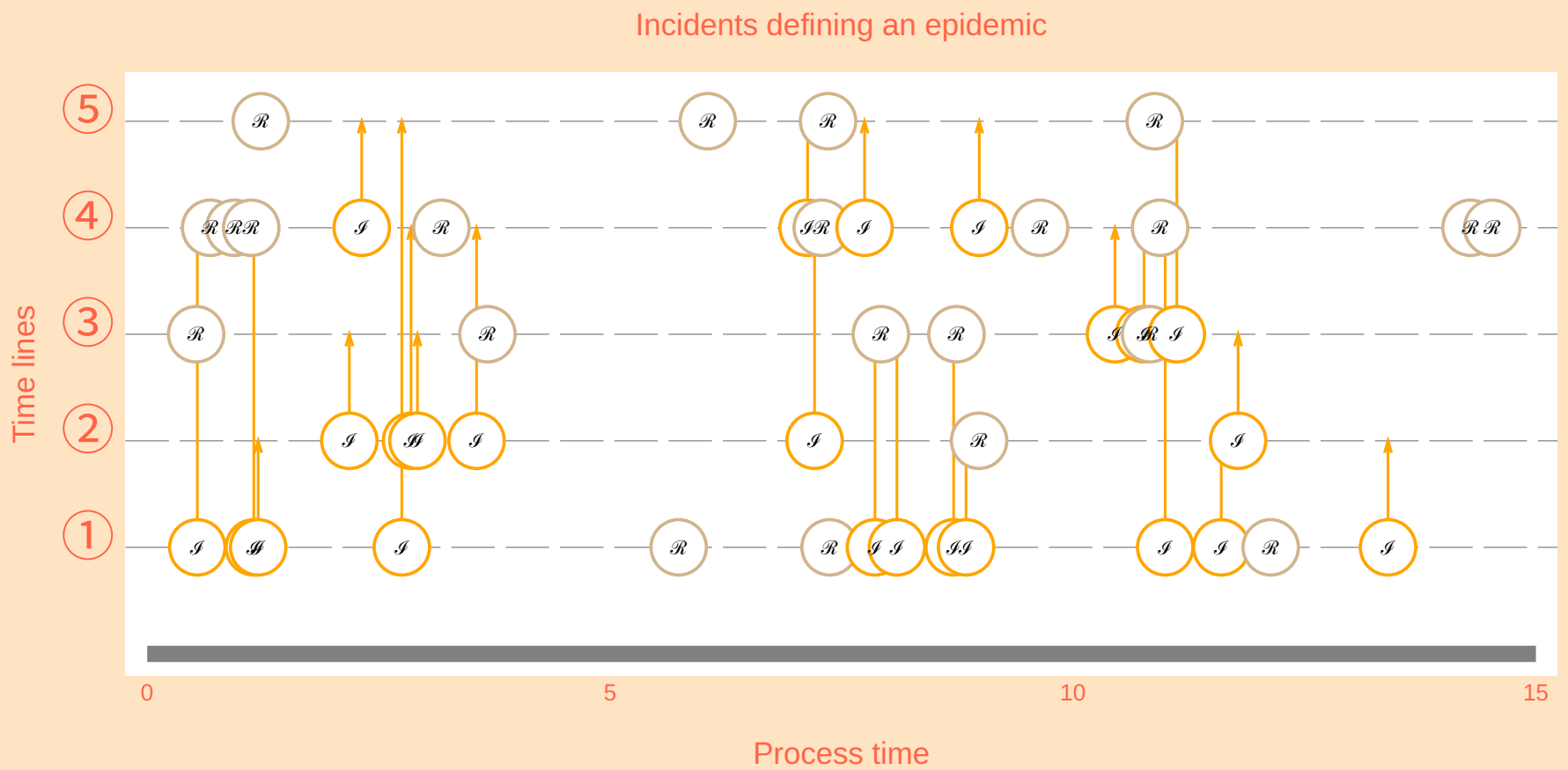

Figure 1: Light-orange circles denote potential infections (arrows point upwards to targets); light-brown circles denote potential removals.

From incidents to unconditioned epidemic trajectories (2/3)

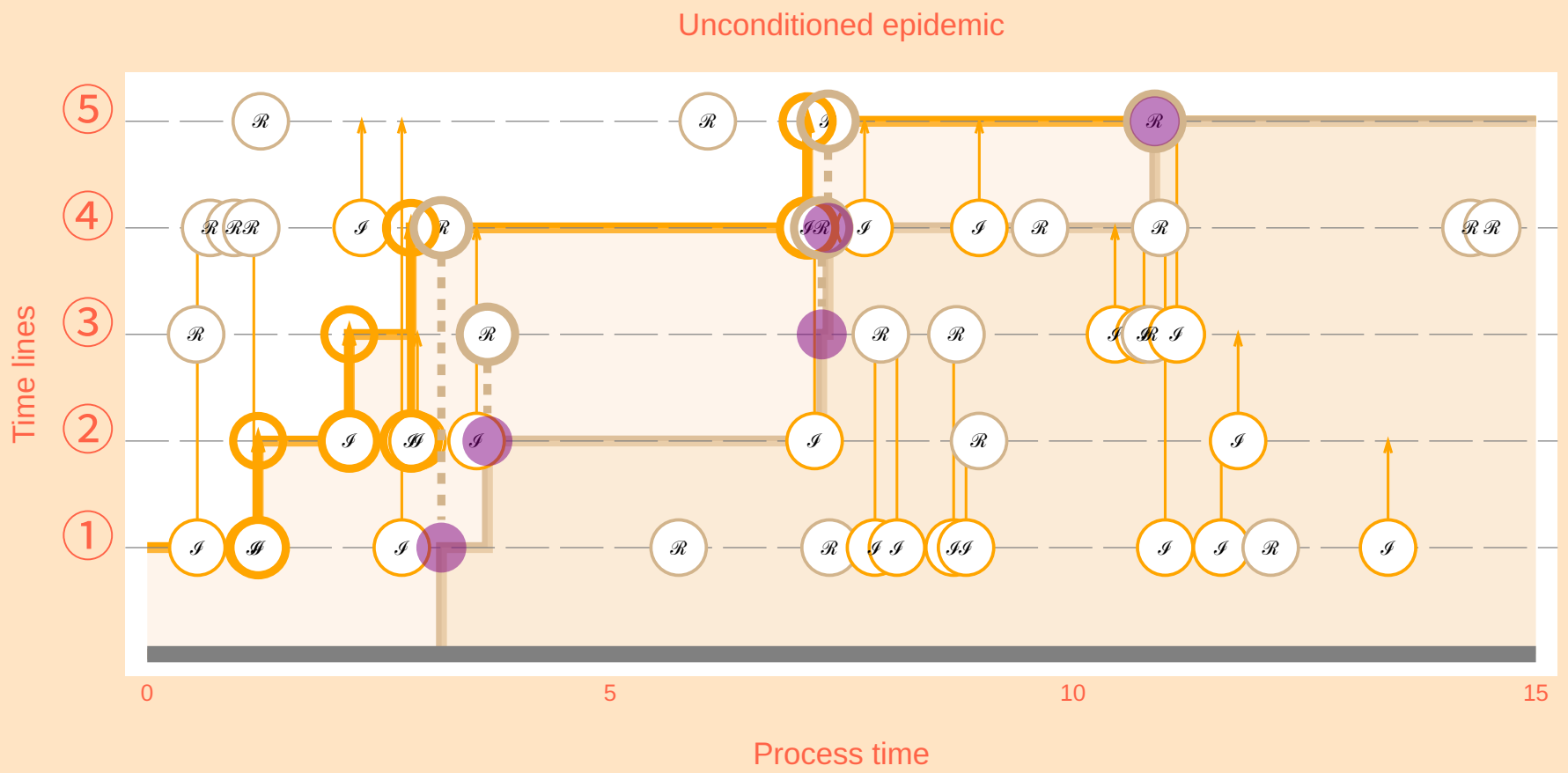

Figure 2: (a) *Infections* activate if on infected timeline and pointing to lowest uninfected timeline; (b) *Removals* activate if on infected timeline; remove lowest infected (purple disk).

From incidents to unconditioned epidemic trajectories (3/3)

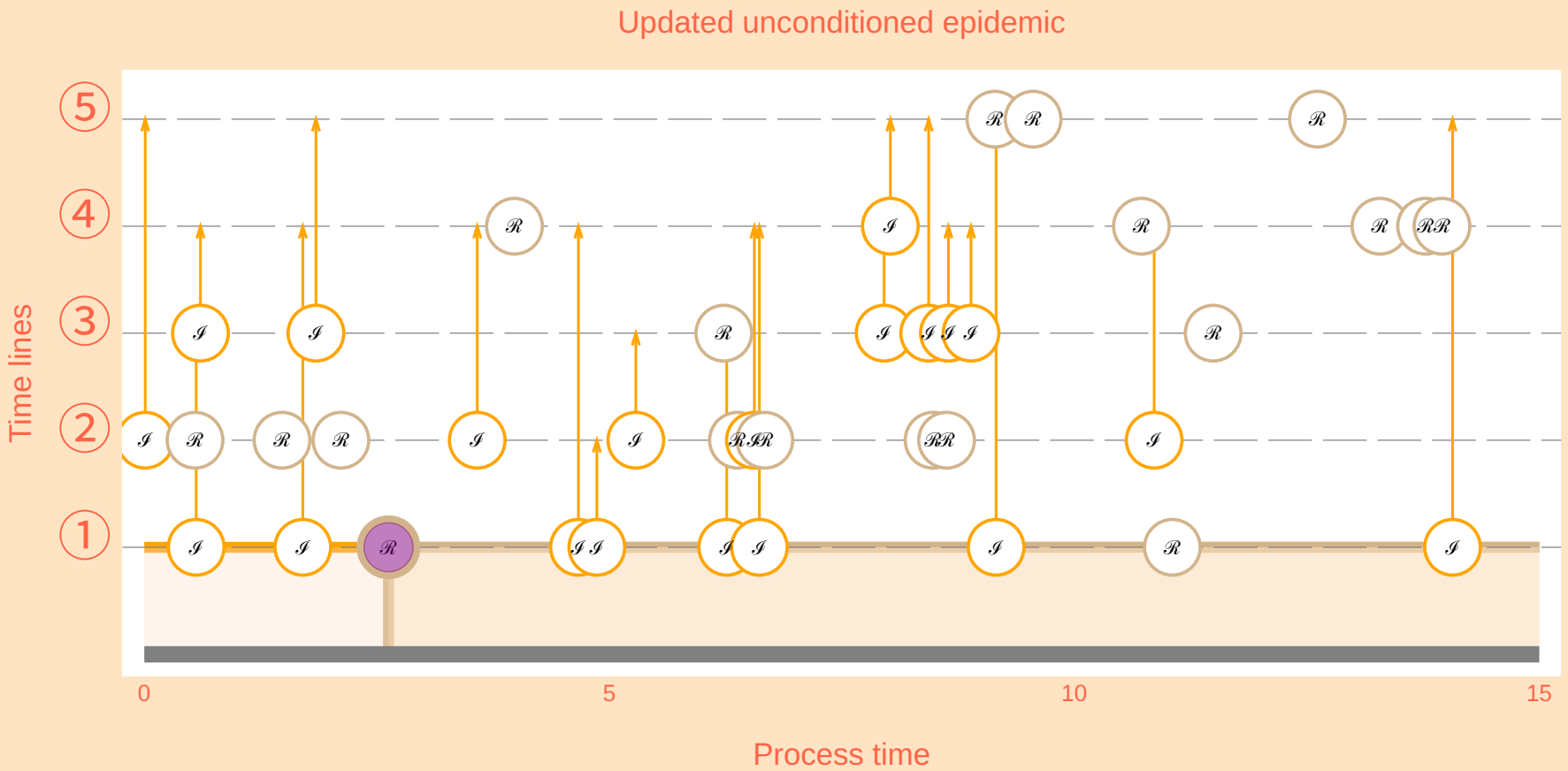

Figure 3: A step in algorithmic time for the unconditioned epidemic simply involves replacing all original incidents by an entirely new set of incidents.

Crucial technical point

- Updates in algorithmic time τ are then (algorithmic-)*time-reversible*: so restriction to a subset S of state-space (*activated* / *conditioned* removals must occur precisely at the specified set of times) implies a new equilibrium which is the old equilibrium conditioned to lie in S.
- For later purposes it is convenient to stage the replacement as follows:
  1. Replace removals ($\mathcal{R}$s);
  2. Re-sample timelines (though not times) of $\mathcal{R}$s;
  3. Replace infections ($\mathcal{I}$s).
- Re-express using *continuously varying* τ. Process time runs over $[0, T]$.
  1. For $2nT < \tau < (2n{+}1)T$, update old $\mathcal{R}$s with times in $(0, \tau - 2nT)$;
  2. For $\tau = (2n{+}1)T$, resample timelines (not times) of $\mathcal{R}$s;
  3. For $(2n{+}1)T < \tau < (2n{+}2)T$, update old $\mathcal{I}$s in $((2n{+}2)T - \tau, T)$.
- Thus the original update is expressible as a (continuous) composition of updates, each of which satisfies detailed balance in equilibrium.
- The connection "restriction=conditioning" still holds.
- Crucially, re-sampling step 2 ensures composite evolution is irreducible over S! (So equilibrium under conditioning is unique.)

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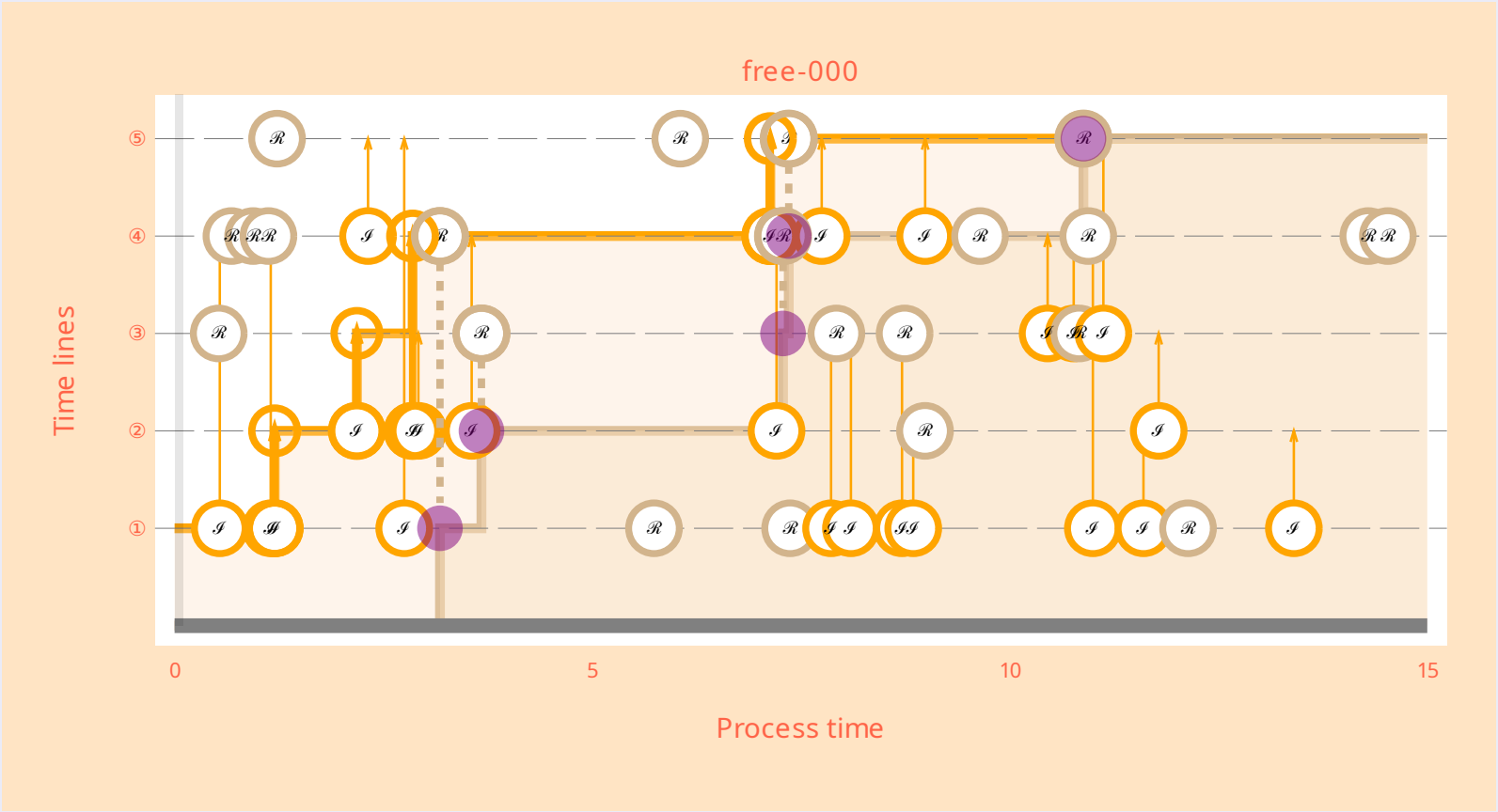
Free evolution evolving in continuous algorithmic time



GIF MP4

3. Conditioning on observed removals

- The trajectory-valued chain is *dynamically reversible*, in *continuous algorithmic time*.
- Irreducibility is *vital* (otherwise equilibrium depends on starting point). Consequently:
  - conditioned removals must be able to change timeline (but not time of occurrence);
- Forbidding removal of observed removals, and forbidding creation of new activated removals, yields a modified chain whose invariant probability measure conditions on observed pattern of removals.
  Implications:
  - a removal can be introduced only if it doesn't activate;
  - a conditioned removal timeline can be altered only if it doesn't de-activate;
  - an infection cannot be removed if that action loses a conditioned removal;
  - an infection can be introduced only if no new observed removals result.
- Does this produce a *feasible* and suitably *monotonic* algorithm?
- Housekeeping details used to establish that monotonicity still works: *laziest feasible epidemic* (LFE) and *no-fly zone* (NFZ).

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Initial conditioned epidemic

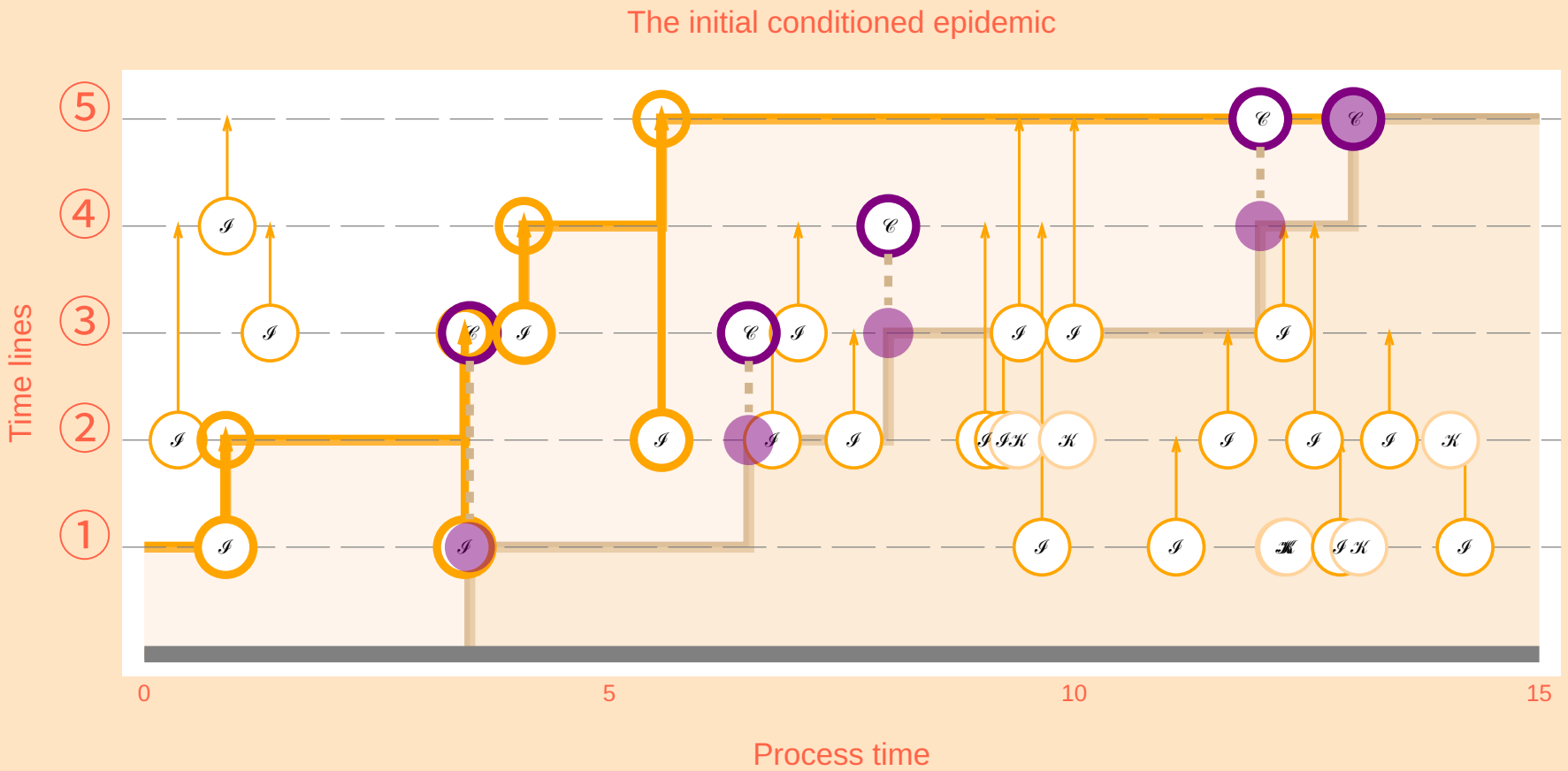


Figure 4: Initial conditioned epidemic, with conditioned removals indicated using purple circles (and purple disks when non-target timelines are infected).

Conditional epidemic update

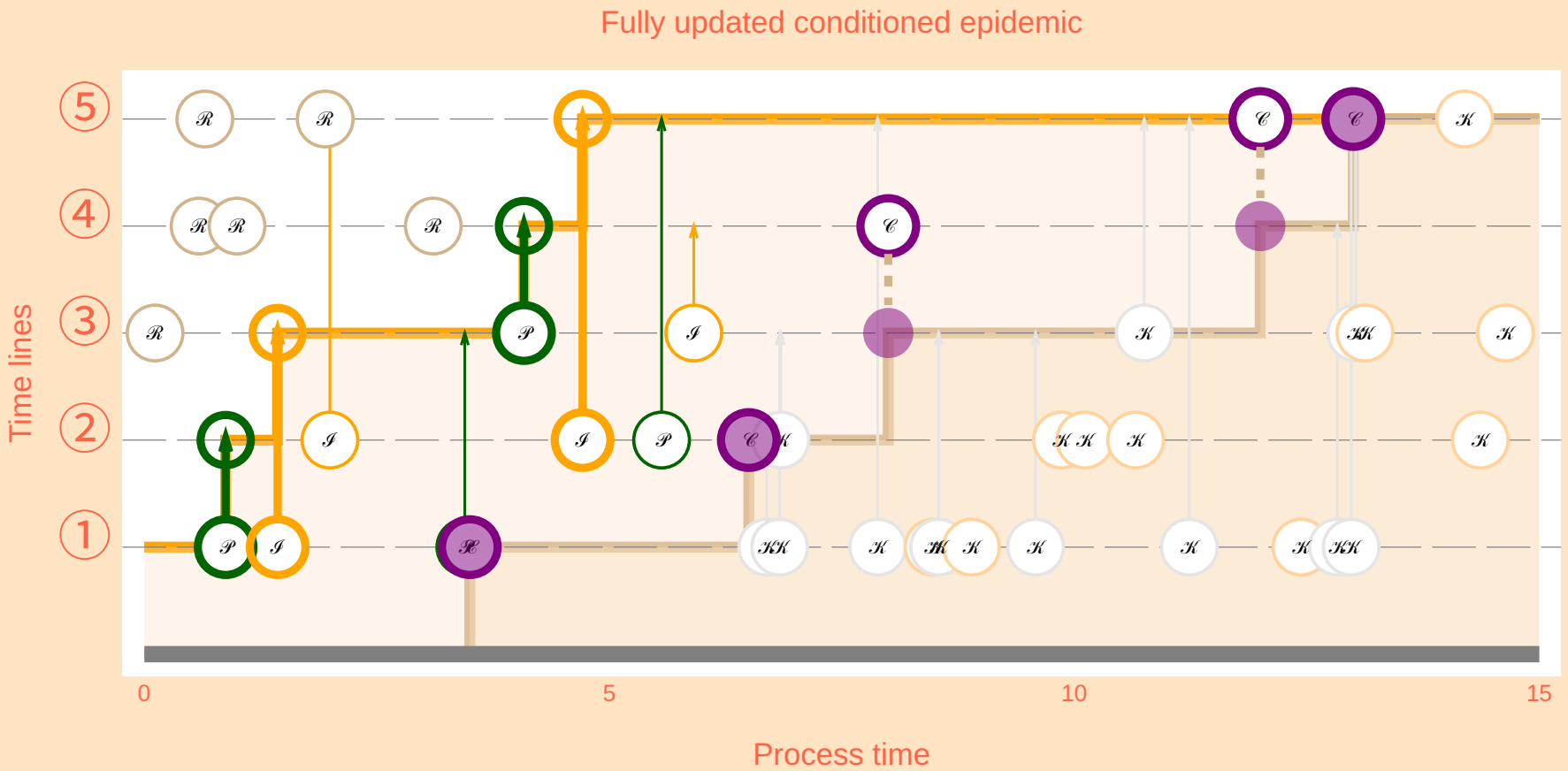


Figure 5: Epidemic updated under restriction: all conditioned removals remain activated, no new removals are activated. Green infections have been "perpetuated".

Laziest feasible epidemic (LFE)

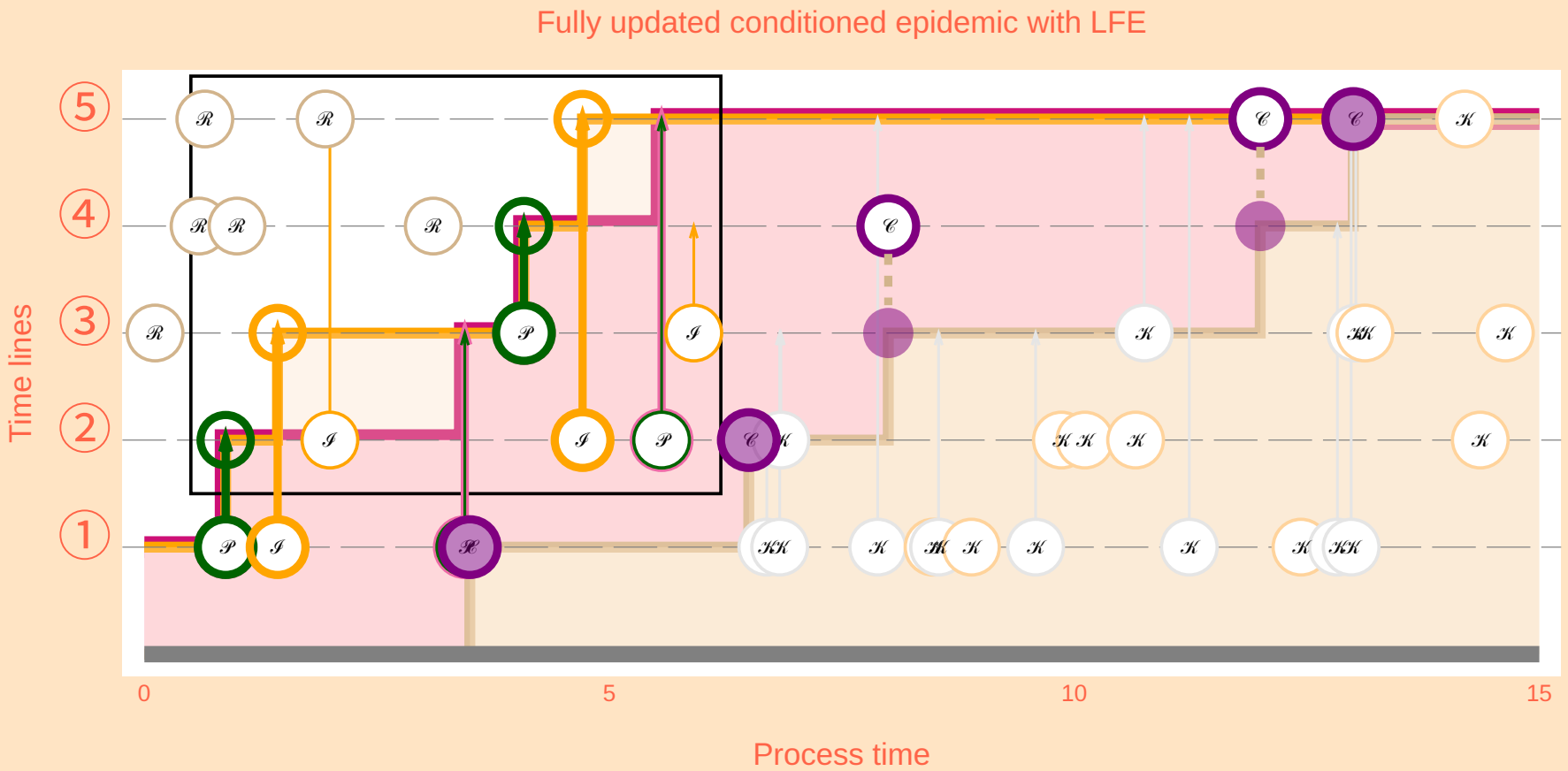
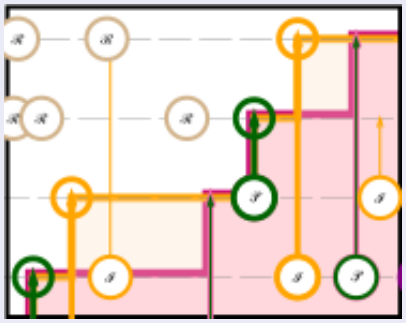


Figure 6: LFE computed recursively working right-to-left: slowest sequence of infections (and perpetuated infections) generating all conditioned removals. Can be used to identify perpetuated infections.

LFE: construction details



1. Recursive definition of LFE: working over $[0, T)$ with $s_{N+1} = T$ and

$$\text{Choose (maximally) } s_i \text{ with } \mathcal{P}_{s_i}^{j<i+1} / \mathcal{I}_{s_i}^{j<i+1}$$
$$\text{and } s_i \leq \min\left\{ s_{i+1}, \inf\{ s \ : \ \text{there is a } \mathcal{C}_s^i \} \right\} .$$

2. Intrinsic definition of LFE:
   Slowest/lowest epidemic activating all re-marked $\mathcal{C}$s, amongst epidemics (varying I_{0-}) formed from *subsets* of the union of
   - the set of new potential $\mathcal{I}$s,
   - and $\mathcal{I}$s from the *old* epidemic history (supplies $\mathcal{P}$s).
3. Comparisons based on intrinsic definition show monotonic dependence of LFE on old epidemic history.

No-fly zone (NFZ)

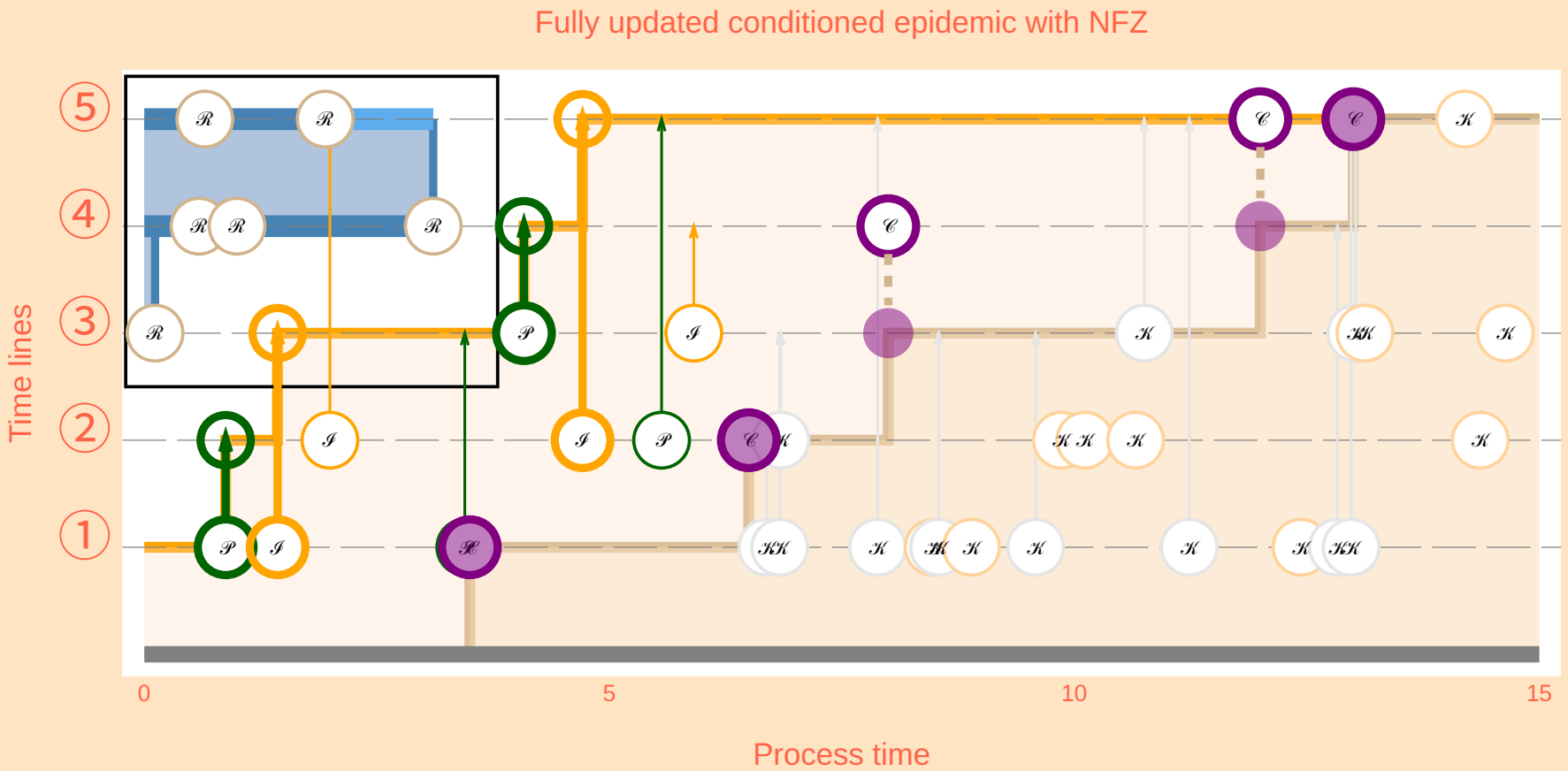
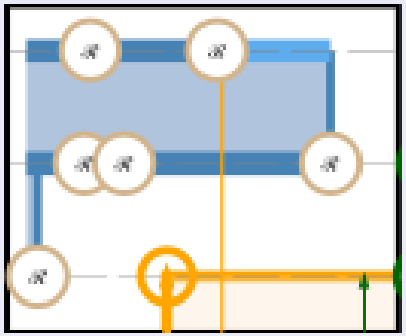


Figure 7: NFZ computed recursively working right-to-left: it traces a region of timelines such that unobserved removals are not activated if region not infected.

NFZ: construction details

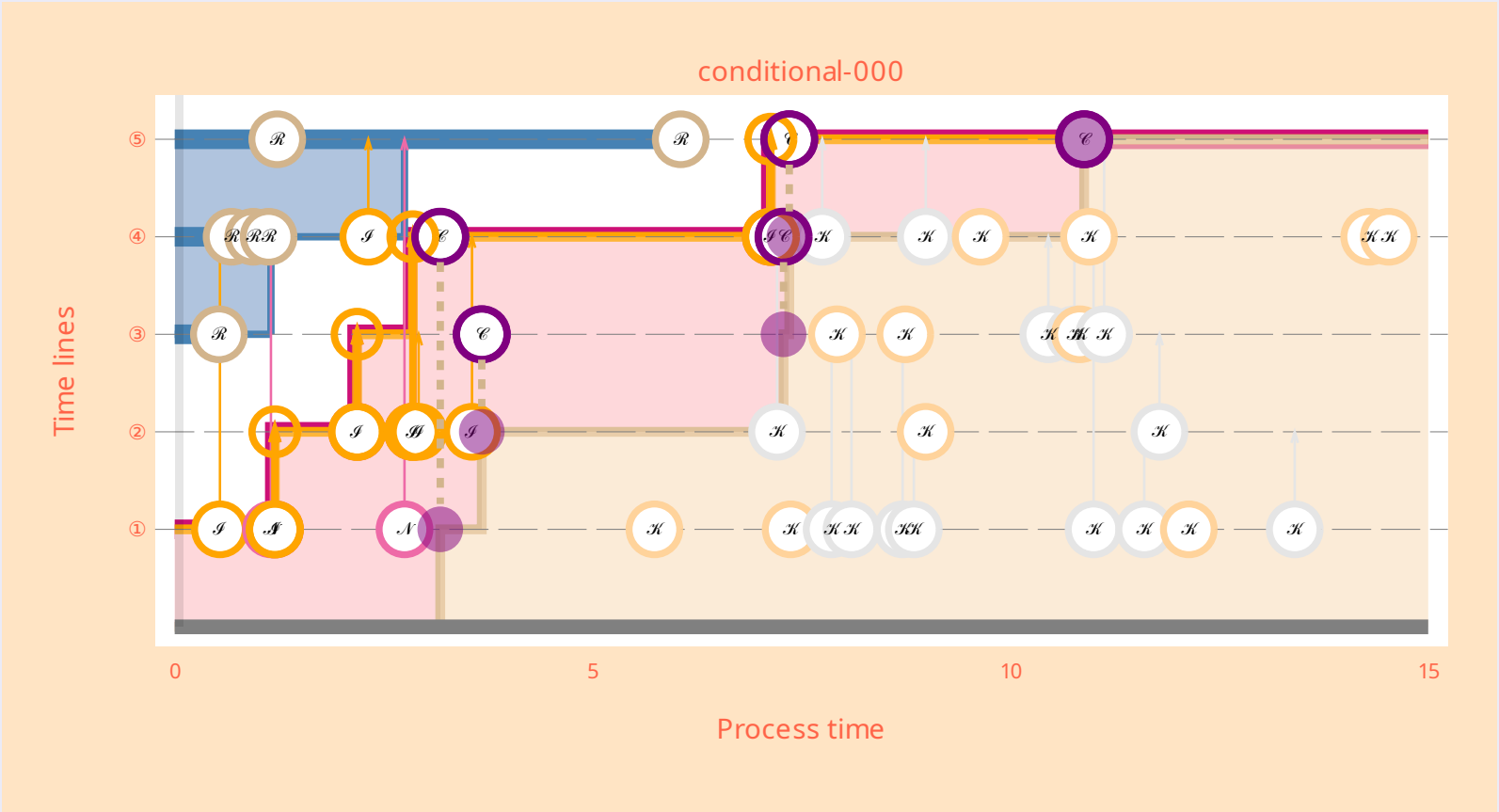


1. NFZ is union of timeline intervals $[0, u_i] \times \{i\}$, expressible as union of regions (for each new *inactivated* $\mathcal{R}_t^i$) each with right-boundary
   - (r, t) for $r = i, \ldots, N$,
   - working backwards in time from $\mathcal{R}_t^i$ and following potential $\mathcal{I}$s down by one step per $\mathcal{I}$ with target *not* in the removed region and infectee at current bottom of NFZ, unless NFZ and infected region touch at that time.
2. Can then show monotonic dependence of NFZ on old epidemic history.

CFTP monotonicity

Full monotonicity (hence CFTP) follows by showing new epidemic history depends monotonically on LFE and NFZ.

Conditioned evolution evolving in continuous algorithmic time

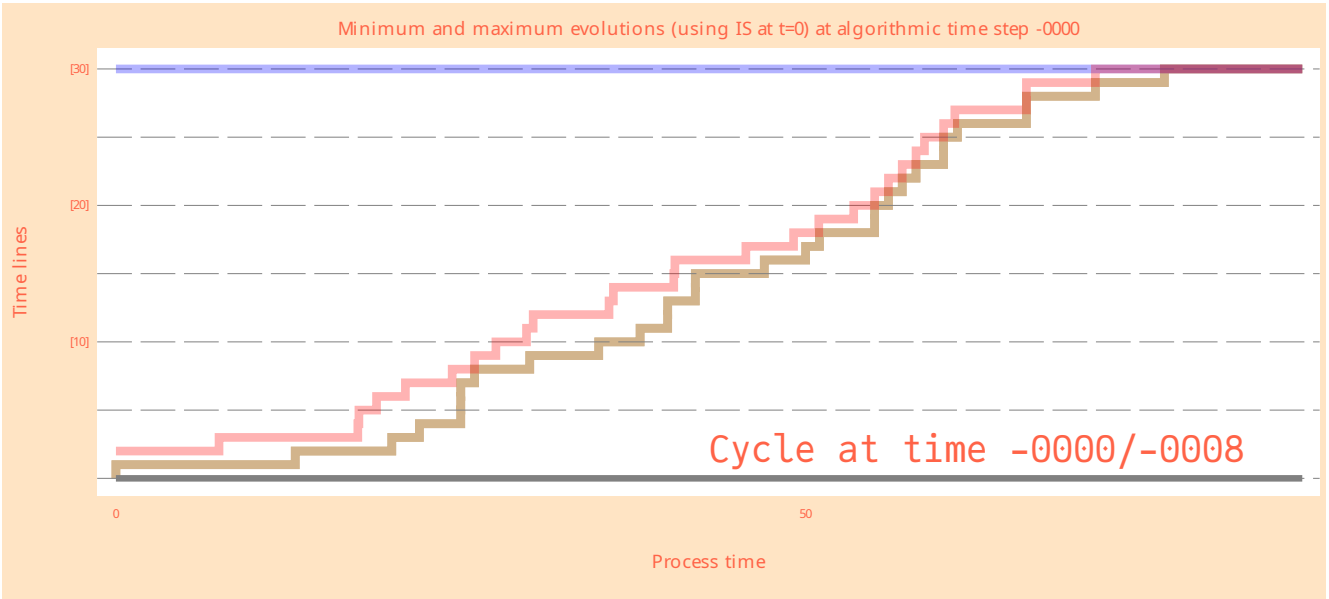


GIF MP4

If a new $\mathcal{J}_t^{i<j}$ has i, j in infected zone then LFE is relevant;
if i in infected zone and j in susceptible zone then NFZ is relevant.

4. Example

- Smallpox outbreak in a closed community of 120 individuals in Abakaliki, Nigeria (much studied! see page 125 of Bailey, 1975).
- **Assume**
  - first observed removal is also the first removal: under a plausible improper prior we can deduce the distribution of infectives I_{0-} at time 0;
  - *all* removals are recorded;
  - no further removals after last observed removal (makes life easier).
- Coding in *julia* (Bezanson *et al.*, 2017), animates (GIF or MP4) a perfect simulation of a draw from unobserved pattern of infections.



So what?

- What about accept-reject methods? (Simulations: CFTP is much better.)
- Why this emphasis on unobserved infections given fixed α and β, when we need inference on R-number $\alpha\, n/\beta$ for *unknown* α and β?
- Good question. But a re-weighting argument allows us to get (unbiased) estimates based on *different* α and β. The perfect simulation provides exact simulation-based computation to integrate out pattern of unobserved infections.
- So (**next steps after** SBC & WSK, 2025)
  - estimate likelihood test statistic for specified α and β;
  - Rao-Blackwell-ize: re-sample infection times given I at removals;
  - construct steepest ascent algorithm (in effect, variant of Robbins-Monro stochastic optimization) to find *maximum a posterior* estimates of α and β;
  - or even, with some computational effort, compute an approximation to the entire posterior joint density for α and β!
- **Finally:** generalize to other suitable compartment models?

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Conclusion

- If MCMC burn-in is a concern, try to build a perfect simulation!
- CFTP works even for significantly complex and relevant models of real-life phenomena.
- *Of course* detailed models resist perfect simulation (but it will be helpful to compare with a simpler model using fewer parameters).
- Experiments suggest CFTP out-competes non-naïve accept-reject.
- Still to be done: seek faster CFTP; statistical estimation of parameters, generalization to other compartment models.
- Thank you for your attention! **QUESTIONS?**

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Image information

Image	*Attribution*	
Book of Kells	Huber Gerhard	*CC BY 4.0*
Classic CFTP for a simple random walk	Result of code written by WSK	
Diamond Princess	Alpsdake	*CC BY-SA 4.0*
Epidemic CFTP images and animation	Result of code written by WSK	

Previous instances of this talk

Date	*Title*			*Location*
19/04/24	Perfect Epidemics	Short Research Talk	12mn	Warwick
15/05/24	McMC+Perfect Simulation	Graduate Seminar, Aristotle Univ.	50mn	Thessaloniki
17/01/25	Perfect Epidemics	Applied Probability Seminar	50mn	Warwick
27/06/25	Perfect Epidemics	UK Research Network Stochastics	45mn	Liverpool
20/10/25	Perfect Epidemics	Seminar		Dublin

Other technical information

Software used in computations

Software	*Version*	*Branch*	*Last commit*
`quarto`	`1.6.39`	—	
Running under `julia`	`1.12.0`	—	
`EpidemicsCFTP`	`2.2.532`	`develop`	`Tue Jul 8 17:13:42 2025 +0100`
`EpidemicsUtilities`	`0.1.2.177`	`main`	`Fri Sep 26 15:35:26 2025 +0100`
This `quarto` script	`0.2.2.725`	`2025-10-09-Dublin-preparation`	`Tue Oct 14 18:01:39 2025 +0100`

Project information

Version:	`0.2.2.729` (`2025-10-09-Dublin-preparation`)
Author:	Wilfrid Kendall <`W.S.Kendall@warwick.ac.uk`>
Date:	Fri Oct 17 15:23:14 2025 +0100

Comment:
Final version of Dublin talk 20 October 2025.

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