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`.

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.

("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;

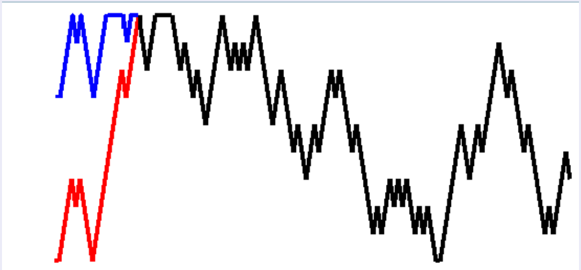
(e) Example with real data.

1. 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).

Classic CFTP for a simple random walk (I)

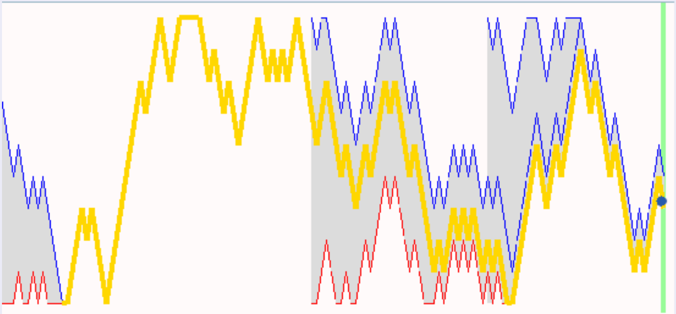
1. Consider a simple random walk on $0{:}9 = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$.
   - $\mathbb{P}\left[+1 \text{ jump}\right] = p \in (0, 1)$, while $\mathbb{P}\left[-1 \text{ jump}\right] = 1-p$, **except that**
   - at state 9 replace the $+1$ jump by "staying still", **and**
   - at state 0 replace 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 (I)

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!

A little 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;
   - 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.)

2. Perfect Epidemics: a challenge problem for CFTP

S-I-R deterministic epidemic:

based on susceptibles s, infectives i, removals r:

$$\begin{aligned} s' &= -\alpha\, s\, i\,, \\ i' &= (\alpha\, s - \beta\,)\; i\,, \\ r' &= \beta\, i\,. \end{aligned}$$

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

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

Infection:	$S \to S - 1\,,$	$I \to I + 1$	at rate	$\alpha\, S\, I\,,$
Removal:	$I \to I - 1\,,$	$R \to R + 1$	at rate	$\beta\, I\,.$

Both make an unrealistic assumption: homogeneous mixing.

In contrast, Fraser *et al* (2021) use a UK model with 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 $\gg 1$ means 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?

An easier question

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.

From incidents to unconditioned epidemic trajectories (1/3)

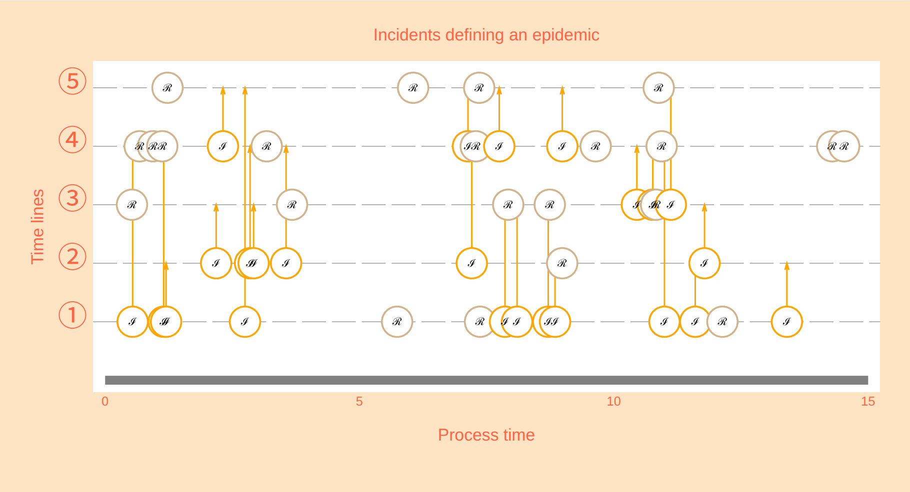


Figure 1: Light-orange circles denote potential infections (arrows point upwards to targets); light-brown circles denote potential removals.

From incidents to unconditioned epidemic trajectories (2/3)

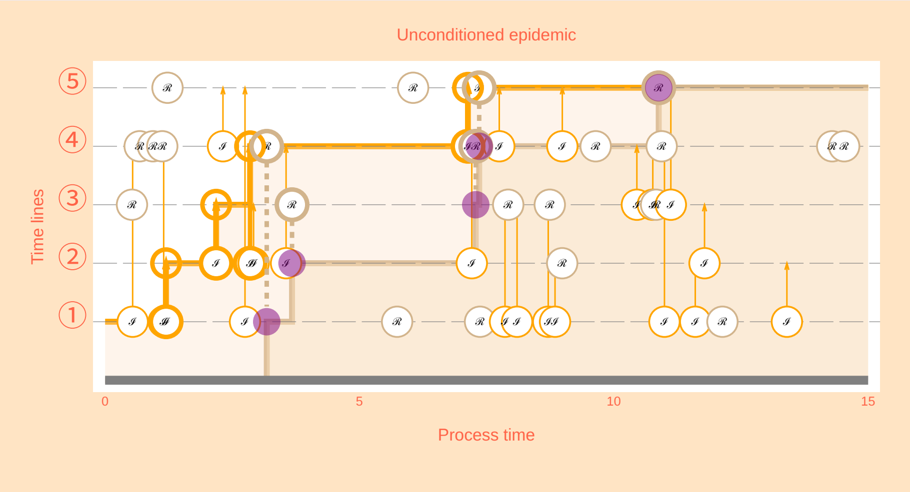


Figure 2: (a) *Infection* activates if target lies on the lowest uninfected timeline; and (b) *removal* activates if on infected timeline; remove lowest infected (purple disk).

From incidents to unconditioned epidemic trajectories (3/3)

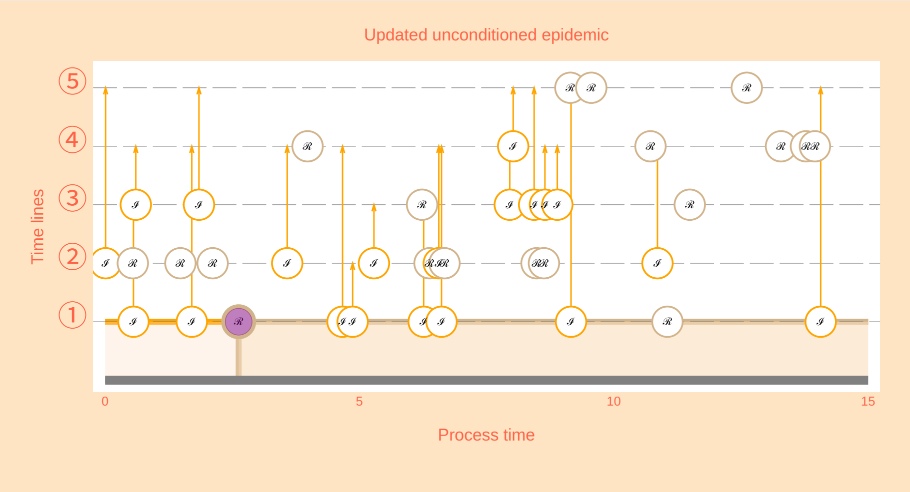
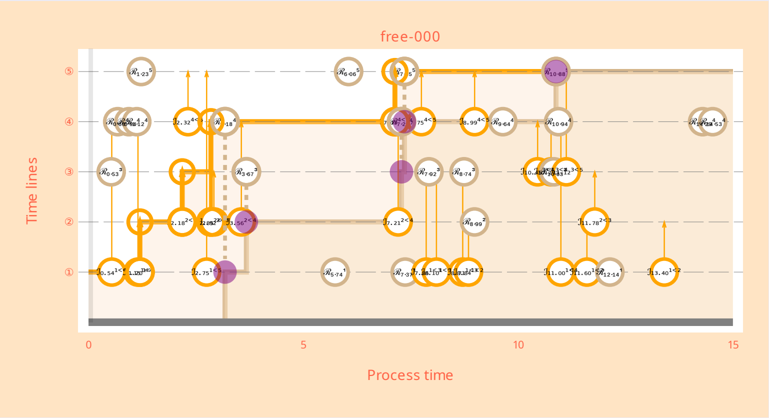


Figure 3: A step in algorithmic time for the unconditioned epidemic simply involves replacing all original incidents by an entirely new set of incidents.

Crucial technical point

- Updates in algorithmic time τ are then (algorithmic-)*time-reversible*: so restriction to a subset S of state-space (the *activated / conditioned* removals to 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.)

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).

Initial conditioned epidemic

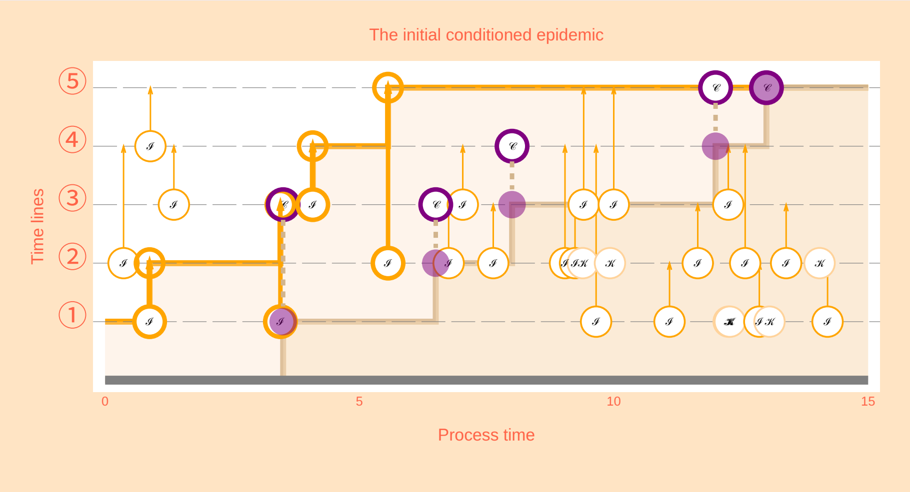


Figure 4: Initial conditioned epidemic, with conditioned removals indicated using purple circles (and purple disks when non-target timelines are infected).

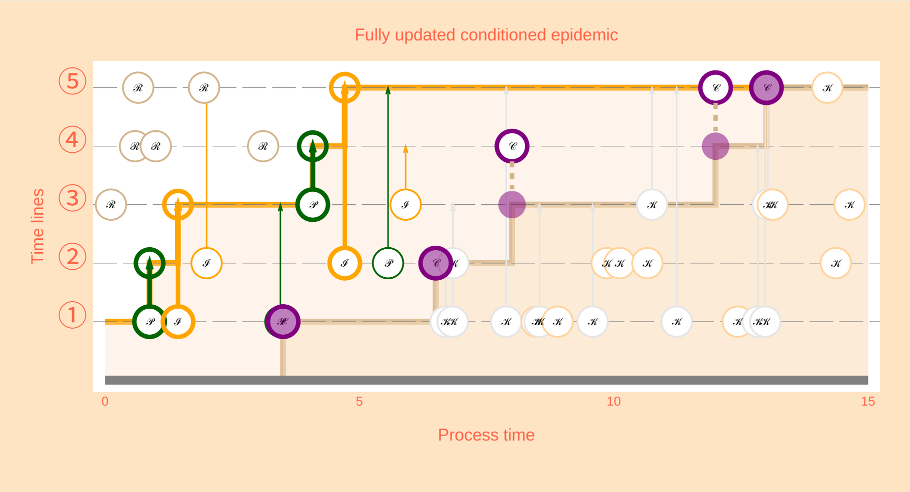


Figure 5: Epidemic updated under restriction: all conditioned removals remain activated, no new removals are activated. Green infections have been “perpetuated”.

Laziest feasible epidemic (LFE)

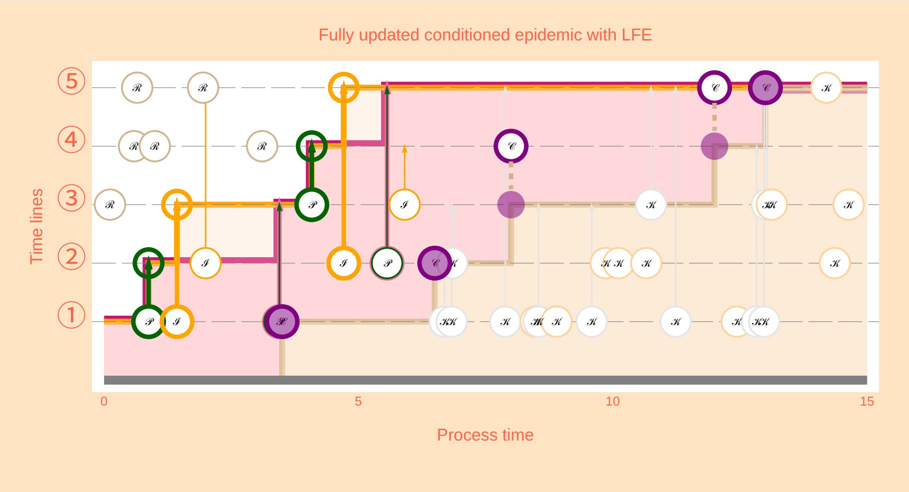


Figure 6: LFE computed recursively working right-to-left: slowest sequence of infections (including perpetuated infections) generating all observed removals in order.

No-fly zone (NFZ)

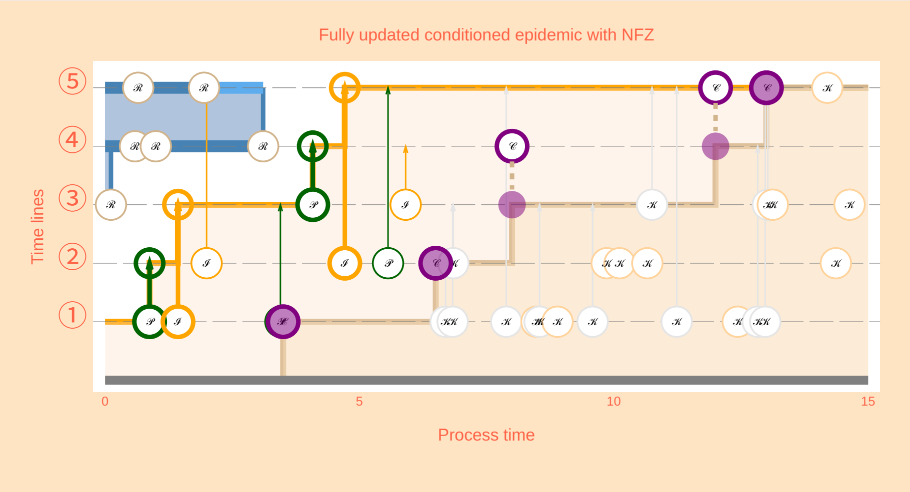
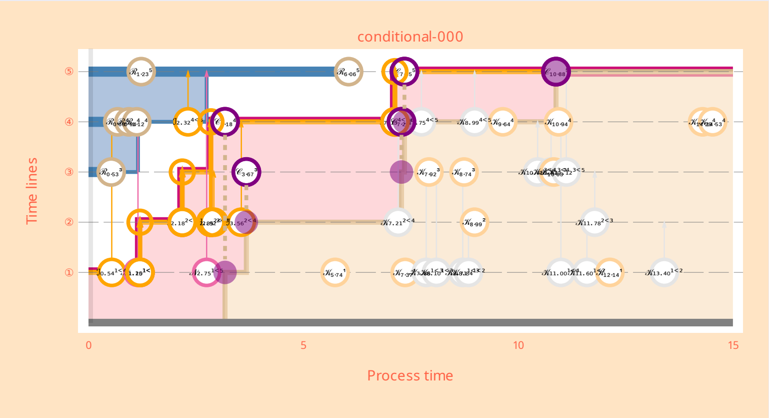


Figure 7: NFZ computed recursively working right-to-left: it traces the region of timelines that must not be infected if one is not to activate unobserved removals.

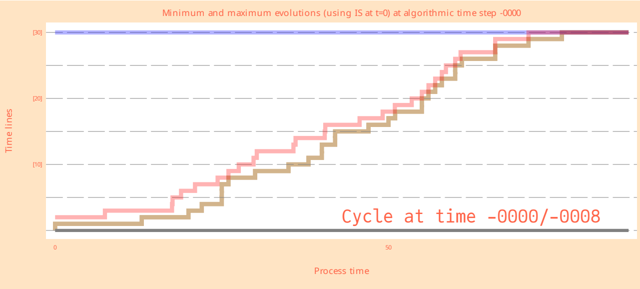
Conditioned evolution evolving in continuous algorithmic time



GIF MP4

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 then deduce what is 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?
- 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, 2024)
  - estimate likelihood test statistic for specified α and β;
  - 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 the entire posterior joint density for α and β!
- Finally: can we generalize to other suitable compartment models?

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?**

Warwick Statistics

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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

Other technical information

Software used in computations

Software	*Version*	*Branch*	*Last commit*
`quarto`	`1.6.39`	—	
Running under `julia`	`1.11.5`	—	
`EpidemicsCFTP`	`2.2.532`	`develop`	`Tue Jul 8 17:13:42 2025 +0100`
`EpidemicsUtilities`	`0.1.2.176`	`main`	`Fri Sep 26 15:11:24 2025 +0100`
This `quarto` script	`0.2.2.719`	`2025-10-09-Dublin-preparation`	`Thu Oct 9 10:38:07 2025 +0100`

Project information

Version:	`0.2.2.721` (`2025-10-09-Dublin-preparation`)
Author:	Wilfrid Kendall <`W.S.Kendall@warwick.ac.uk`>
Date:	Thu Oct 9 13:04:22 2025 +0100

Comment:
Fixed Fraser et al reference