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.

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

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

1. A Visual Introduction to Perfect Simulation

- Propp & Wilson (1996) invented exact simulation / Coupling from the Past (CFTP) / perfect simulation;
- 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.
- 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)

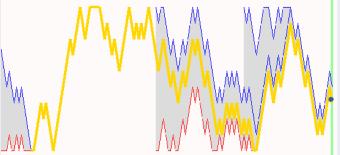
- Consider a simple random walk on $0:9 = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$.
 - ${\Bbb P}\left[+1\ {
 m jump}\
 ight]=p\in(0,1),$ while ${\Bbb P}\left[-1\ {
 m jump}\
 ight]=1-p,$ except that
 - at state 9 replace the +1 jump by "staying still", and
 - at state 0 replace the -1 jump by "staying still".
- Onventional 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;
- Generally not true that location at coupling is a draw from equilibrium.

Classic CFTP for a simple random walk (II)

• 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!
- May need to iterate back-off doubling several times.
- When coupled, top and bottom yield a common value at time 0.
- The common value (golden thread) is an exact draw from equilibrium!

Some more CFTP theory

- 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).
- 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).
- Dominated CFTP delivers perfect simulation for stable point processes (WSK & Møller, 2000);
- 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: differential equation system for (s, i, r)

Susceptible: $s' = -\alpha s i$,

Infected: $i' = (\alpha s - \beta) i$,

Removed: $r' = \beta i$.

Constant total population s + i + r = n.

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

Infection: $S \to S - 1$, $I \to I + 1$ at rate αSI ,

Removal: $I \rightarrow I-1$, $R \rightarrow R+1$ at rate βI .

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:

- Modelling is tough. Either massive assumptions (homogeneous mixing)
 or very many parameters;
- Inference is really tough: hard to get information about infection times;
- 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);
- Markov chain Monte Carlo (MCMC) can be used (see next slide) but what about burn-in?
- Can we use perfect simulation?

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.

- 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.
- Opinion point processes of appropriate rates yield an S-I-R epidemic.
- First step: evolve whole S-I-R trajectory in *algorithmic time* (alter potential infections and removals using immigration-death in discrete algorithmic time).
- Sesult: *trajectory-valued chain*, unconditioned S-I-R as equilibrium.

From incidents to unconditioned epidemic trajectories (1/3)

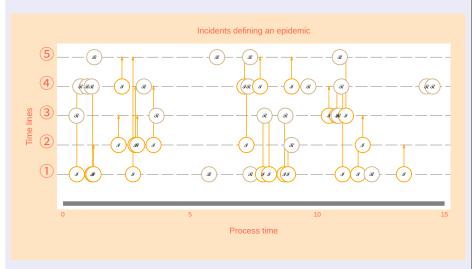


Figure 1: Light-orange circles denote potential infections (arrows point upwards to targets); light-brown circles denote potential removals.

From incidents to unconditioned epidemic trajectories (2/3)

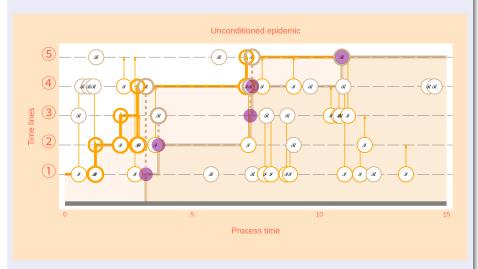


Figure 2: (a) *Infections* activate if on infected timeline and pointing to lowest uninfected timeline; (b) *Removals* activate if on infected timeline; remove lowest infected (purple disk).

From incidents to unconditioned epidemic trajectories (3/3)

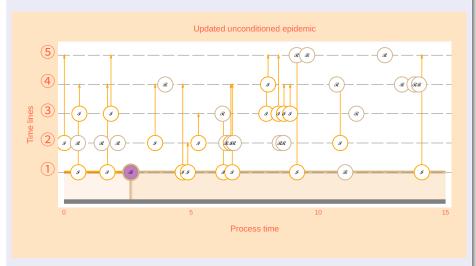
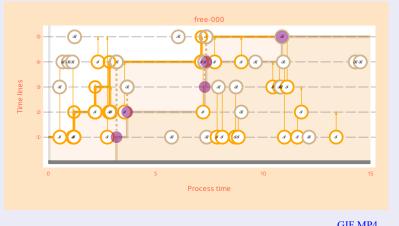


Figure 3: A step in algorithmic time for the unconditioned epidemic simply involves replacing all original incidents by an entirely new set of incidents.

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:
 - 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].
 - $\bullet \ \, \text{For}\, 2nT < \tau < (2n+1)T \text{, update old}\,\, \mathcal{R}\text{s with times in}\,\, (0,\tau-2nT);$
 - ② For $\tau = (2n+1)T$, resample timelines (not times) of \Re s;
 - $\textbf{ § For } (2n+1)T < \tau < (2n+2)T, \text{ update old } \mathcal{I}\text{s in } ((2n+2)T \tau, T).$
- 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

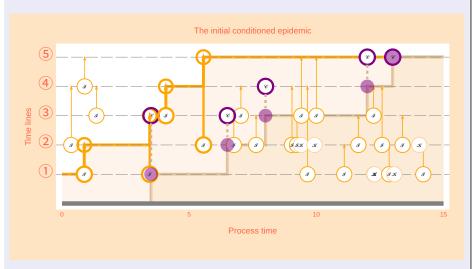


Figure 4: Initial conditioned epidemic, with conditioned removals indicated using purple circles (and purple disks when non-target timelines are infected).

Conditional epidemic update

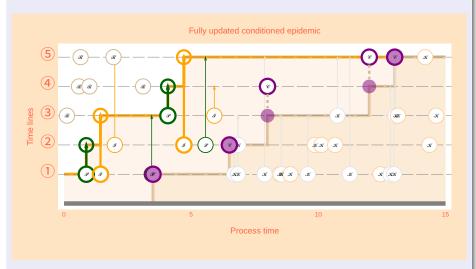


Figure 5: Epidemic updated under restriction: all conditioned removals remain activated, no new removals are activated. Green infections have been "perpetuated".

Laziest feasible epidemic (LFE)

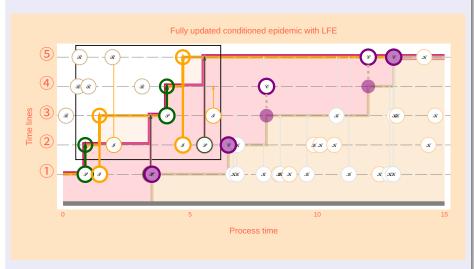


Figure 6: LFE computed recursively working right-to-left: slowest sequence of infections (and perpetuated infections) generating all conditioned removals. Can be used to identify perpetuated infections.

LFE: construction details



• Recursive definition of LFE: working over [0, T),

$$\begin{array}{lll} s_N & = & T \\ & s_i & \leq & \min \left\{ s_{i+1} \, , \inf \{ s \, : \, \text{there is a } \mathcal{C}^i_s \} \right\} \, . \end{array}$$

- **②** Intrinsic definition of LFE: Slowest/lowest epidemic activating all re-marked Cs, amongst epidemics 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).
- Omparisons based on intrinsic definition show monotonic dependence of LFE on old epidemic history.

No-fly zone (NFZ)

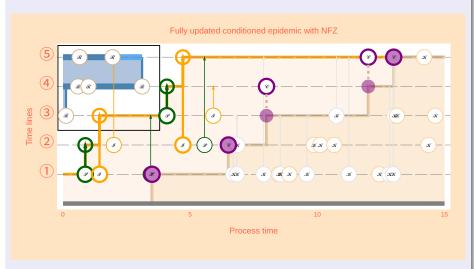
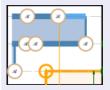


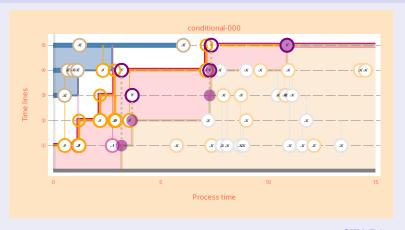
Figure 7: NFZ computed recursively working right-to-left: it traces a region of timelines such that unobserved removals are not activated if region not infected.

NFZ: construction details



- 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}^i_t and following potential \mathcal{I} s down by one step per \mathcal{I} that does *not* have a target in the infected or removed regions.
- On then show monotonic dependence of NFZ on old epidemic history.

Conditioned evolution evolving in continuous algorithmic time



GIF MP4

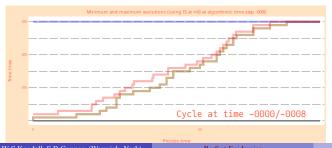
If a new $\mathcal{I}_t^{i < j}$ has i, j in infected zone then LFE is relevant; if i in infected zone and j in susceptible zone then NFZ is relevant. New epidemic is monotonic in LFE, NFZ!

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 α n/β 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?



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

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:	0.2.2.726 (2025-10-09-Dublin-preparation)
Author:	Wilfrid Kendall <w.s.kendall@warwick.ac.uk></w.s.kendall@warwick.ac.uk>
Date:	Wed Oct 15 17:35:41 2025 +0100

Comment:

Near-final preparation for Dublin October 2025 talk. Detailed edits, and a few indicative notes towards monotonicity proofs.