# **Perfect Epidemics**

### Applied Probability Seminar Department of Statistics, University of Warwick

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Warwick, York

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#### Introduction

"Maybe the only significant difference between a really smart simulation and a human being was the noise they made when you punched them."

(The Long Earth, Pratchett & Baxter, 2012)





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

This is initial work on using perfect simulation (CFTP) for epidemics. WSK acknowledges the support of UK EPSRC grant EP/R022100.

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- Simplest possible example: *random-walk-CFTP* (can boost to use Ising model to do simple image reconstruction).

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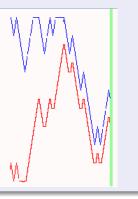
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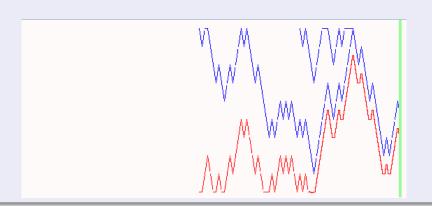
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- Generally not true that location at coupling is a draw from equilibrium.



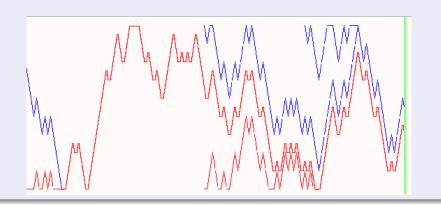
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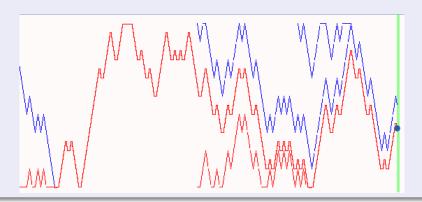
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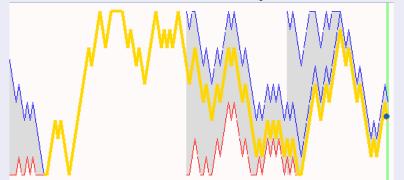
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- The common value is an exact draw from equilibrium!



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- Detailed expositions: WSK (2005), Huber (2015).
   (Want to implement CFTP in R? see WSK, 2015.)

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Many important inferential questions (Cori & Kucharski, 2024).

Simplest models (versus UK model with 10<sup>6</sup> agents!, Fraser & Others, 2023):

**S-I-R deterministic epidemic:** susceptibles s, infectives i, removals r (constant total population s+i+r=n):

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

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*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.



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

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- Can we use perfect simulation?

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An important step on the way: generating an unconditioned epidemic.

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- Sesult: *trajectory-valued chain*, unconditioned S-I-R as equilibrium.

#### From incidents to unconditioned epidemic trajectories (1/3)

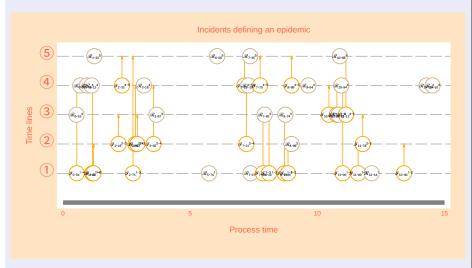


Figure 1: Light-orange circles denote potential infections (arrows point upwards to targets); light-brown circles denote potential removals.

#### From incidents to unconditioned epidemic trajectories (2/3)

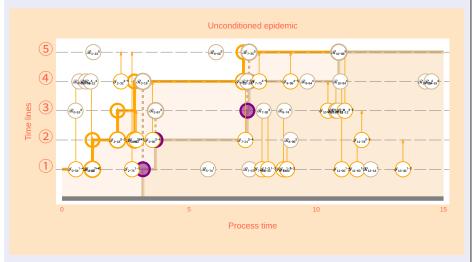


Figure 2: Activate (a) *infection* if target on lowest uninfected timeline; (b) *removal* if in infected region, then remove lowest infected (purple disk if different timeline).

#### From incidents to unconditioned epidemic trajectories (3/3)

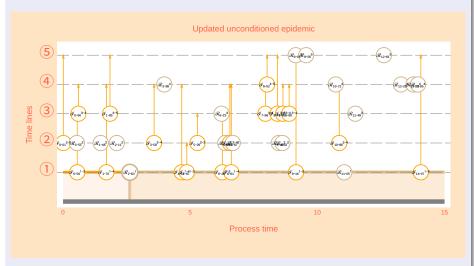


Figure 3: A step in algorithmic time for the unconditioned epidemic simply involves replacing the original incidents by a new set of incidents.

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  - $\textbf{ § For } (2n+1)T < \tau < (2n+2)T, \text{ update old } I\text{s in } ((2n+2)T-\tau,T).$
- Thus the original update is expressible as a (continuous) composition of updates, each of which satisfies detailed balance in equilibrium.
- The connection "restriction=conditioning" is thereby preserved.

- Updates in algorithmic time  $\tau$  are then (algorithmic-)time-reversible: so restriction to subset S of state-space (of activated removals occurring precisely at 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 (Rs);

  - 3 Replace infections (Is).
- Re-express using continuously varying  $\tau$ . Process time runs over [0, T].
  - For  $2nT < \tau < (2n+1)T$ , update old Rs with times in  $(0, \tau 2nT)$ ;
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- Thus the original update is expressible as a (continuous) composition of updates, each of which satisfies detailed balance in equilibrium.
- The connection "restriction=conditioning" is thereby preserved.
- Crucially, step 2 ensures composition action is irreducible over S! (So equilibrium under conditioning is unique.)

## Illustration of technical point (1/8)

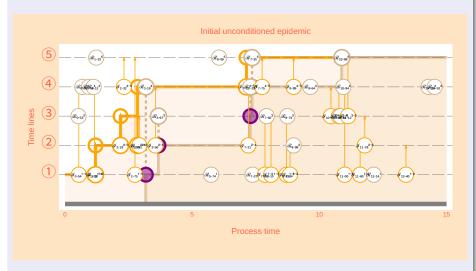


Figure 4: No change yet to removals or infections;

#### Illustration of technical point (2/8)

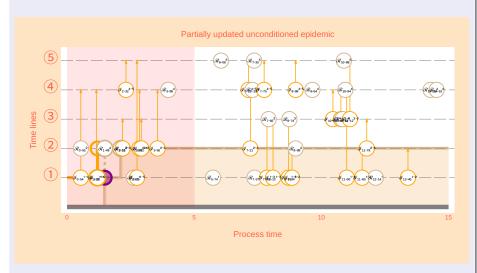


Figure 5: Replace first third of removals, infections unchanged;

#### Illustration of technical point (3/8)

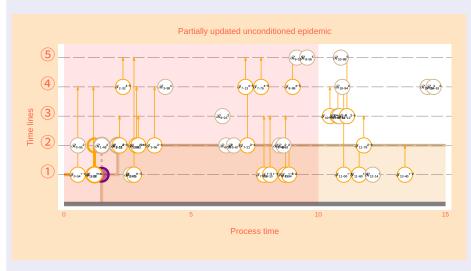


Figure 6: Replace first two-thirds of removals, infections unchanged;

#### Illustration of technical point (4/8)

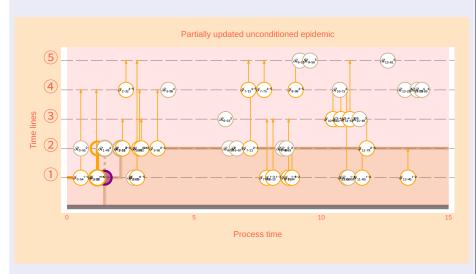


Figure 7: All removals resampled, infections as yet unchanged;

#### Illustration of technical point (5/8)

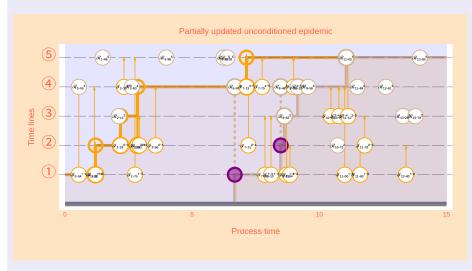


Figure 8: Re-sample all removal timelines, infections as yet unchanged;

## Illustration of technical point (6/8)

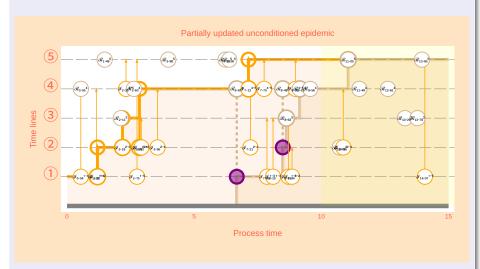


Figure 9: Re-sample last third of infections;

#### Illustration of technical point (7/8)

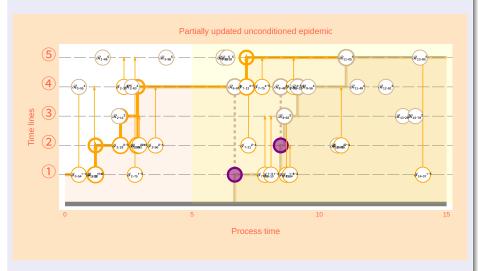


Figure 10: Re-sample last two-thirds of infections;

### Illustration of technical point (8/8)

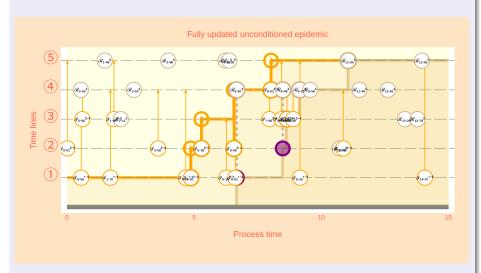


Figure 11: All infections now re-sampled.

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- Does this produce a *feasible* and suitably monotonic algorithm?
- Housekeeping details required to establish that monotonicity still works. Key notions: *last feasible epidemic* (LFE) and *no-fly zone* (NFZ).

## Initial conditional epidemic

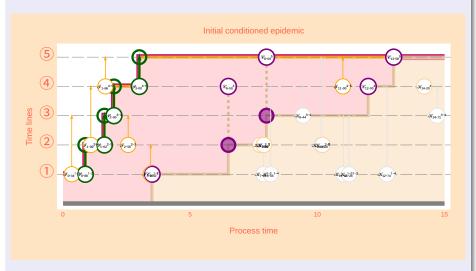


Figure 12: Initial epidemic with conditioned removals indicated using purple circles (and purple disks when different timelines are infected).

## Conditional epidemic update

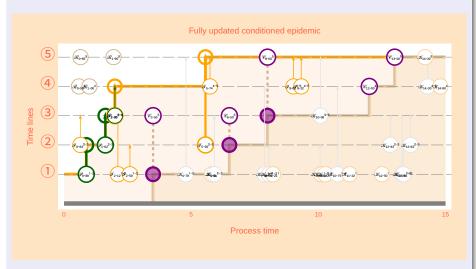


Figure 13: Epidemic updated under restriction: all conditioned removals remain activated, no new removals are activated. Green infections have been "perpetuated".

## Last feasible epidemic (LFE)

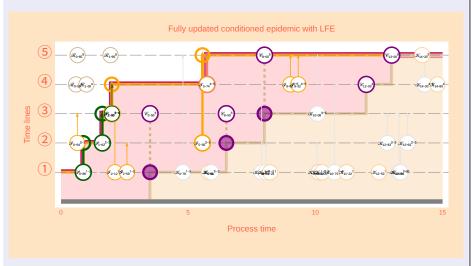


Figure 14: LFE computed recursively working right-to-left: the slowest sequence of infections deals with all infected timelines in order (includes perpetuated infections).

### No-fly zone (NFZ)

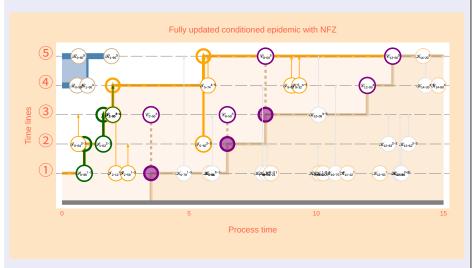


Figure 15: NFZ computed recursively working right-to-left: it traces the region of timelines that must not be infected if one is not to activate unobserved removals.

 Smallpox outbreak in a closed community of 120 individuals in Abakaliki, Nigeria (much studied! see page 125 of Bailey, 1975).



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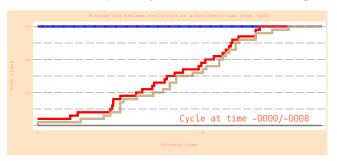
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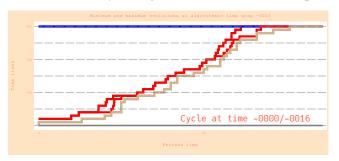
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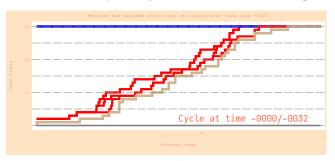
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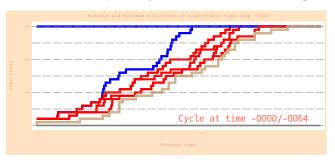
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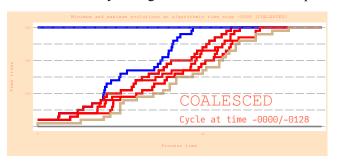
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  - or even, with some computational effort, compute the entire posterior joint density for  $\alpha$  and  $\beta$ !
- Finally: generalize to other suitable compartment models?

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- Still to be done: statistical estimation of parameters, generalization to other compartment models.
- Thank you for your attention! **QUESTIONS?**



### References I

- Bailey, N.T.J. (1975) The mathematical theory of infectious diseases and its applications, 2nd Ed. ed. Griffin.
- Bezanson, J., Edelman, A., Karpinski, S., & Shah, V.B. (2017) Julia: A Fresh Approach to Numerical Computing. *SIAM Review*, **59**, 65–98.
- Cori, A. & Kucharski, A. (2024) Inference of epidemic dynamics in the COVID-19 era and beyond. Epidemics, 48, 100784.
- Donnelly, P. & Kurtz, T.G. (1996) A countable representation of the Fleming-Viot measure-valued diffusion. The Annals of Probability, 24, 698–742.
- Foss, S.G. & Tweedie, R.L. (1998) Perfect simulation and backward coupling. Stochastic Models, 14, 187–203.
- Fraser, C. & Others (2023) OpenABM-Covid19: Agent-based model for modelling the Covid-19 and Contact-Tracing.
- Gibson, G.J. & Renshaw, E. (1998) Estimating parameters in stochastic compartmental models using Markov chain methods. *Mathematical and Medical Biology*, **15**, 19–40.
- Gibson, G.J. & Renshaw, E. (2001) Likelihood estimation for stochastic compartmental models using Markov chain methods. *Statistics and Computing*, 11, 347–358.
- Huber, M.L. (2015) Perfect Simulation. Boca Raton: Chapman; Hall/CRC.

### References II

- Liggett, T.M. (1985) Interacting Particle Systems, Grundlehren der mathematischen wissenschaften. Berlin, Heidelberg: Springer Berlin.
- O'Neill, P.D. & Roberts, G.O. (1999) Bayesian Inference for Partially Observed Stochastic Epidemics. Journal of the Royal Statistical Society Series A: Statistics in Society, 162, 121–129.
- Pratchett, T. & Baxter, S. (2012) The Long Earth. Doubleday.
- Propp, J.G. & Wilson, D.B. (1996) Exact sampling with coupled Markov chains and applications to statistical mechanics. *Random Structures and Algorithms*, 9, 223–252.
- SBC (2020) Omnithermal Perfect Simulation for Multi-server Queues. ACM Transactions on Modeling and Computer Simulation, 30, 1–15.
- SBC & WSK (2007a) Perfect simulation for a class of positive recurrent Markov chains. *Annals of Applied Probability*, **17**, 781–808.
- SBC & WSK (2007b) Perfect simulation for a class of positive recurrent Markov chains (corrigendum). *Annals of Applied Probability*, **17**, 1808–1810.
- SBC & WSK (2015) Perfect simulation of M/G/c queues. Advances in Applied Probability, 47, 1039–1063.
- SBC & WSK (2024) Perfect Epidemics.
- Whittle, P. (1955) The outcome of a stochastic epidemic—a note on Bailey's paper. *Biometrika*, **42**, 116–122.



### References III

- WSK (1998) Perfect Simulation for the Area-Interaction Point Process. *Probability towards 2000* (Accardi, L. & Heyde, C.C. eds). Springer-Verlag, pp. 218–234.
- WSK (2004) Geometric ergodicity and perfect simulation. *Electronic Communications in Probability*, **9**, 140–151.
- WSK (2005) Notes on Perfect Simulation. Singapore: World Scientific, pp. 93-146.
- WSK (2015) Introduction to CFTP using R. Stochastic geometry, spatial statistics and random fields, Lecture notes in mathematics. Springer, pp. 405–439.
- WSK & Møller, J. (2000) Perfect simulation using dominating processes on ordered spaces, with application to locally stable point processes. *Advances in Applied Probability*, **32**, 844–865.

## Image information

Image	Attribution	
Terry Pratchett Classic CFTP for a simple random walk	Luigi Novi Result of code written by WSK	CC BY 3.0
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 15/05/24	Perfect Epidemics McMC and Perfect Simulation	Short Research Talk (12min) Graduate Seminar, Aristotle Univ. (50min)	Warwick Thessaloniki
17/01/25	Perfect Epidemics	Applied Probability Seminar (50min)	Warwick



# A "near-maximal" configuration

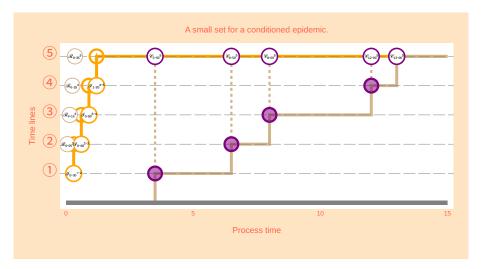


Figure 16: A conditional epidemic in which all activated infections occur before time 3.0, also before smallest observed removal time.

### Other technical information

#### Software versions

Software used in computations:

Software	Version	Branch	Date of last commit
Quarto	1.6.39	_	
Running under julia	1.11.2	_	
Module EpidemicsCFTP	2.2.488	main	Mon Jan 20 15:38:58 2025
Module EpidemicsUtilities	0.1.2.154	main	Wed Jan 15 13:23:36 2025
This Quarto script	2.2.598	Wilfrid	Wed Jan 22 18:01:24 2025

## Revision history

These notes were produced from PerfectEpidemics.qmd:

Author: Wilfrid Kendall W.S.Kendall@warwick.ac.uk

Date: Wed Jan 22 18:01:24 2025 +0000

Summary: Sorted out animation links

2.2.598