Markov chain Monte Carlo and Perfect Simulation

Lecture at Aristotle University of Thessaloniki

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Introduction

Figure 1: Αριστοτέλης 384–322 BCE

Aristotle:

- "Pleasure in the job puts perfection in the work."
- "The more you know, the more you know you don't know."

Handout available on the web: either use the QR-code

or visit https://wilfridskendall.github.io/talks/Thessaloniki-2024/.

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Sketch of MCMC (I)

Figure 2: Edward Teller (1908-2003)

The original Markov chain Monte Carlo method (MCMC) was introduced by Metropolis *et al.* (1953). The senior author was Edward Teller ("father of the H-bomb").

[Fermi once remarked that] Teller was the only monomaniac he knew who had *several* manias (Brown & May, 2004).

Sketch of MCMC (II)

- Markov chain basics:
  - Transition probabilities $p(a, b)$ (or transition rates in continuous time: unified view using exponential distribution);
  - Equilibrium probabilities $\pi(a)$, balance,
    detailed balance $\pi(a)p(a, b) = \pi(b)p(b, a)$, reversibility;
  - Aperiodicity, recurrence (and uniform and geometric recurrence);
  - under detailed balance we can condition by forbidding transitions;
- We can modify any chain, transition probabilities $p(a, b)$, to leave a specified target distribution $\pi(a)$ invariant, by censoring each possible transition $a \to b$ with probability $\alpha(a, b) \in [0, 1]$ such that
  $\alpha(a, b)\pi(a)p(a, b) = \alpha(b, a)\pi(b)p(b, a)$;
- Common choice: Metropolis-Hastings
  $\alpha(a, b) = \min\{1, (\pi(b)p(b, a))/(\pi(a)p(a, b))\}$.
- If result still irreducible aperiodic, then $\pi(a)$ is its long-term equilibrium.
- This is MCMC, now of intense interest to statisticians.
- But, physicists always remind us, physicists got there fifty years earlier!

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Sketch of MCMC (III)

Given the $\pi(a)$, how to design a Markov chain to have this as equilibrium?

(i) Independence sampler: draw from a fixed probability distribution, apply Metropolis-Hastings;
(ii) Random walk Metropolis or RWM: propose move using a random walk, apply Metropolis-Hastings;
(iii) Metropolis-adjusted Langevin or MALA: make a Gaussian jump shifted using gradient of $\log \pi$, apply Metropolis-Hastings.

Can mix-and-match! RWM is often favourite: flexible, not too complicated.

Issues:

(A) Burn-in: *How long* till approximate equilibrium?
(B) Scaling: *How big* should be the RWM jump?

Question (B) is about how to get fast mixing. There is a beautiful and useful theory, but that is for another day.

Question (A) is what this lecture is all about.

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Sketch of MCMC (IV)

- MCMC practicalities: Burn-in: what to do about it?
  - Theory tends to be much too pessimistic. Example: Zanella (2015a, 2015b) developed statistical methods for Anglo-Saxon history: a *simplified* model appeared to converge approximately in 10^5 steps (about 1 week on compute cluster), *versus* 10^9 steps in theory (around 2 centuries);
  - Is (a) one long run better or (b) many short runs? (Option (b) requires starts of short runs spread "evenly" over the sample space — almost as hard in high dimensions as the original problem!)
  - Diagnostics? (Meta-theorem: for any diagnostic technique there is a chain for which the technique is deceptive!)
  - Conclusion: effective MCMC requires very careful thought about appropriate length of run — think deeply about the problem!
- Can there ever be a better way?

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Perfect Simulation

- The Propp & Wilson (1996) idea of exact simulation / Coupling from the Past (CFTP) / perfect simulation (Persi Diaconis: "Like seeing the landscape of Mars for the first time");
- Ideas (of "*classic CFTP*"):
  - extending simulation *backwards* through time,
  - exploit monotonicity by coupling maximal and minimal processes,
  - seek coalescence;
- Details for *random-walk-CFTP*, which can be boosted as above to provide simple image reconstruction of an image using Ising model, Propp & Wilson (1996) show how to vary a clever algorithm to get exact samples for critical Ising model (this is what impressed Diaconis);
- "Perfect simulation" (WSK, 1998): because everyone knows it isn't going to be perfect, whereas people might imagine "exact simulation" would somehow miraculously defeat numerical approximation error :-).

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An example and some theory

- An intensely visual example, which helps many people see intuitively what is going on here, is *DeadLeaves-CFTP* (WSK & Thönnes, 1999) (technically, *Occluded CFTP*);
- What about cases where monotonicity fails? or there isn't a sensible "maximal" process? 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);
- Theoretical limits: *in principle*
  - *Classical CFTP* equivalent to uniform ergodicity (Foss & Tweedie, 1998).
  - *Dominated CFTP* is achievable under geometric ergodicity (WSK, 2004).
  - It is even possible to carry out Dominated CFTP in some **non**-geometrically ergodicity cases [Connor & WSK (2007); *nb* corrigendum];
- We can use *Dominated CFTP* to carry out perfect simulation for stable point processes (WSK & Møller, 2000);
- Detailed expositions are given by WSK (2005), Huber (2015). WSK (2015) shows how to implement CFTP in R.

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Applications to Queues and Epidemics

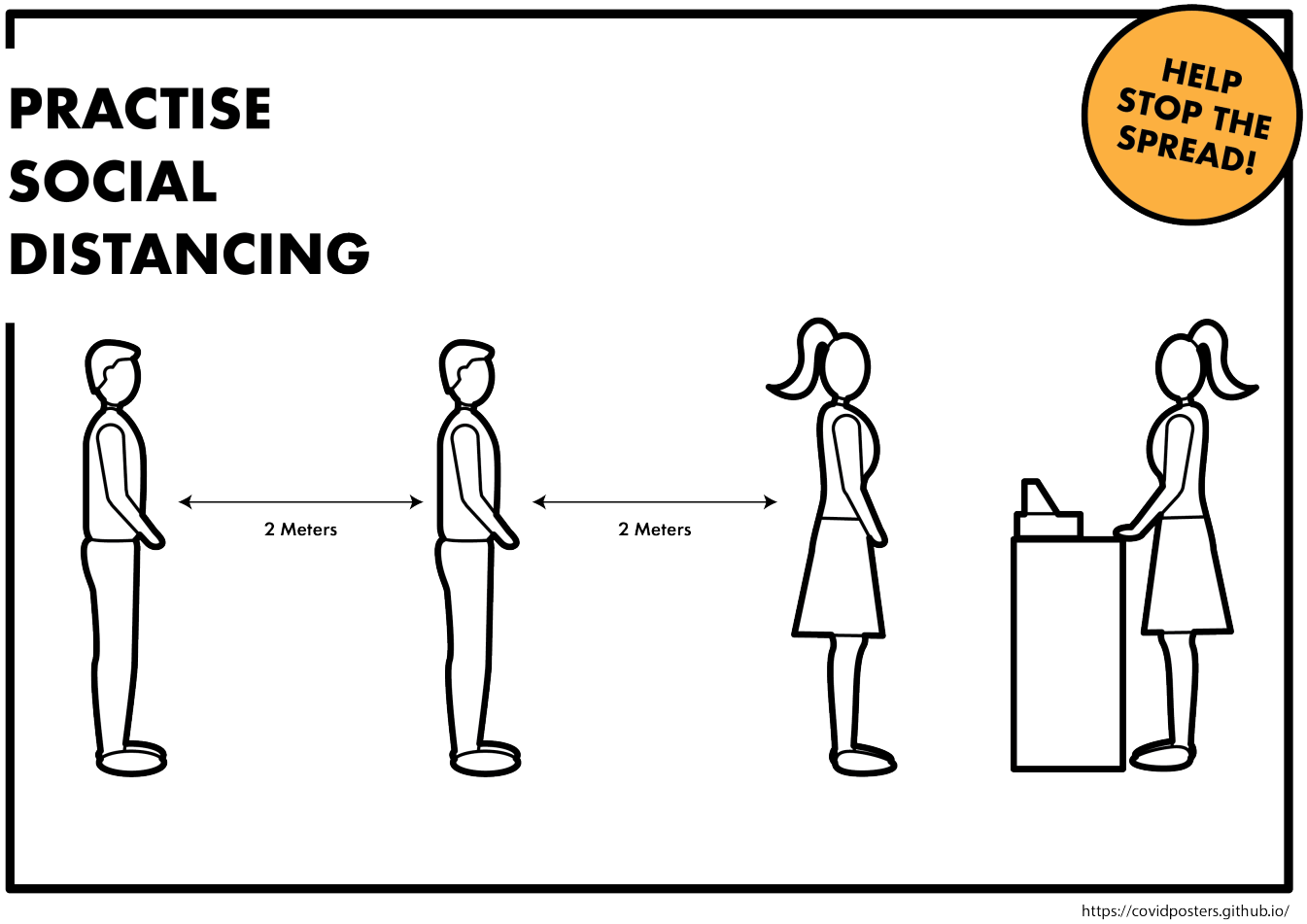

Figure 3: An illustration introducing *both* queues *and* epidemics!

Perfect Queues

The simplest queuing model ($M/M/1$: Poisson arrivals, exponential service times, single server) can be analyzed very thoroughly indeed! However:

- Poisson arrivals are not unreasonable, but exponential service times are ludicrous. The $M/G/1$ case (general service time *for just one server*) can be analyzed using the "embedded chain" (sample at each departure);
- Multi-server case: computation of *eg* waiting-time distribution is out of reach so use simulation (and insights from Kiefer & Wolfowitz, 1955);
- Sigman (2011) shows how to do CFTP in the "super-stable" case (traffic so low that it could have been handled by just one server), using Dominated CFTP and comparing to a "Processor-Sharing" discipline.

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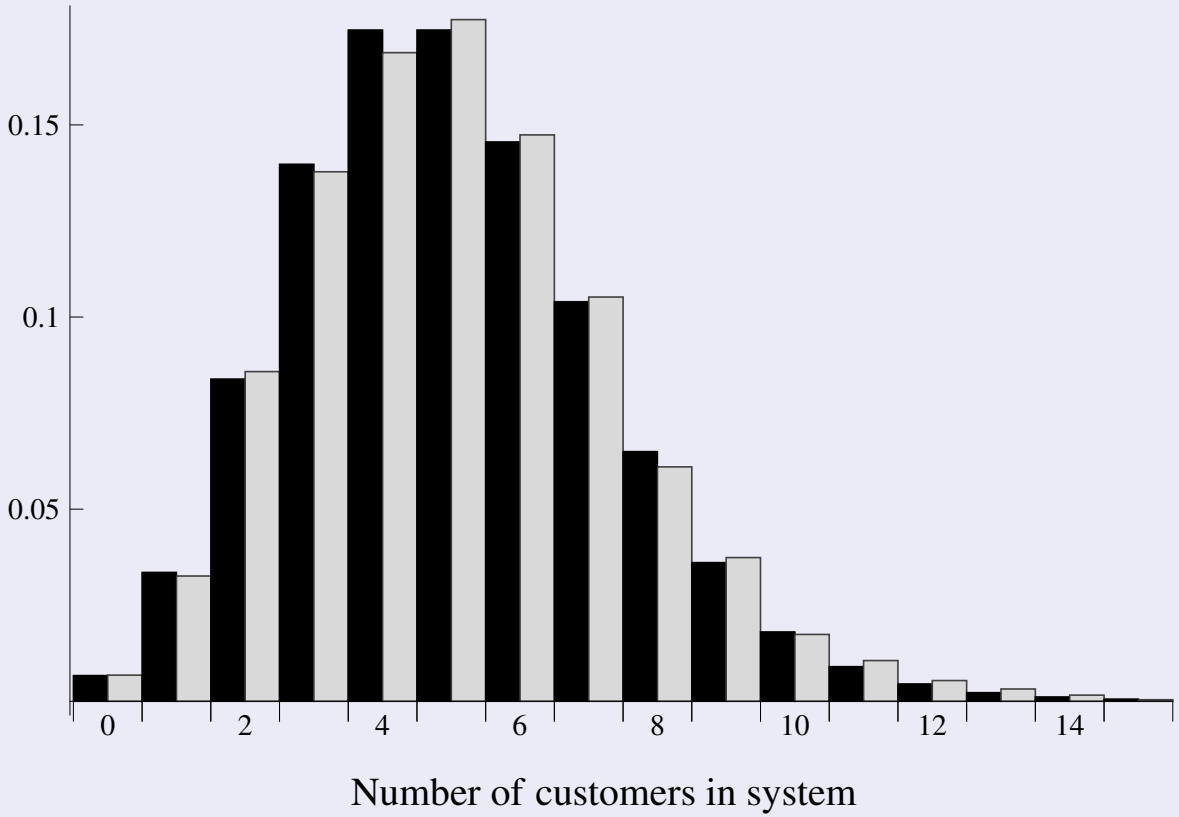
- Connor & WSK (2015) extend Sigman (2011), showing how to apply Dominated CFTP to simulate (sub-critical!) queues perfectly; now generalized by others to the case of non-Poissonian inter-arrival times. (Technical point: pathwise domination needs service times to be assigned in order of commencement of service!) The idea is
  - dominate $M/G/c$ FCFS (FCFS means first come first served) by $M/G/c$ RA $= [M/G/1 \text{ RA}]^c$ (RA means assign to individual servers on arrival);
  - use fact that $M/G/1$ FCFS and $M/G/1$ PS *workloads* agree (PS means Processor Sharing: pool servers to serve everyone simultaneously) and $M/G/1$ PS can be simulated backwards in time;
  - so $[M/G/1 \text{ PS}]^c$ can be used to provide Dominated CFTP.
- Connor & WSK (2015) describe
  (a) CFTP coupling when dominating process empties,
  (b) and a faster CFTP coupling using upper and lower processes starting respectively at dominating process and at empty state.

Results (I)

Histogram of customer numbers for $M/M/c$ queue in equilibrium: arrival rate 10, service rate 2, and 10 servers, comparing theory (available for $M/M/c$ queue) with results of Connor & WSK (2015) algorithm.

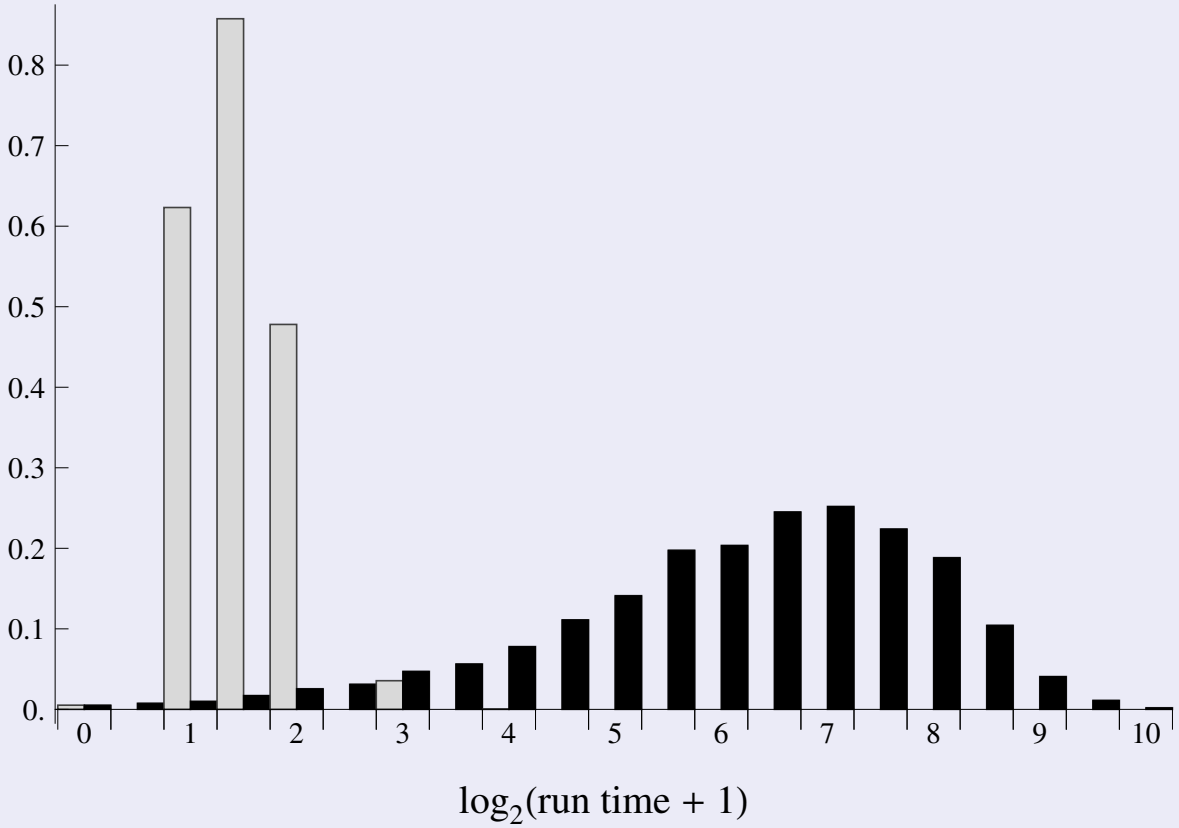


Results (II)

Comparison of log-run times for

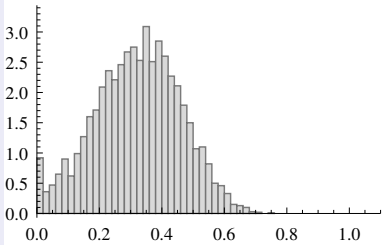
(a) CFTP coupling when dominating process empties (solid bars),

(b) a faster CFTP coupling using upper and lower processes (grey bars).

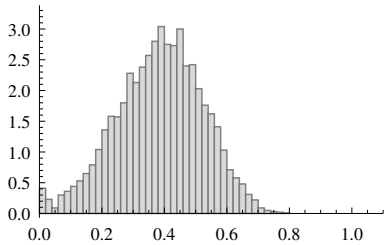


Results (III)

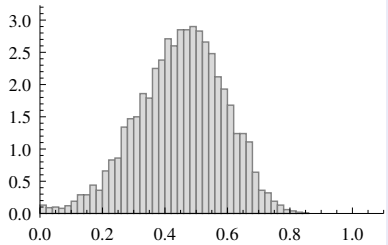
Marginal distributions of last six coordinates of the equilibrium Kiefer-Wolfowitz workload vector (anticipated work in system) for an $M/G/c = 25$ queue with Uniform$(0, 1)$ service times and arrival rate 25.



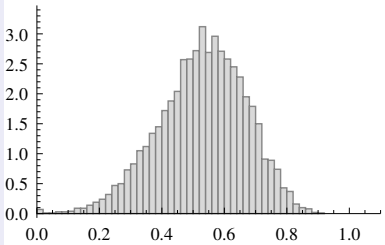
Workload at server 20



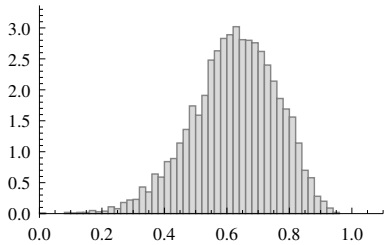
Workload at server 21



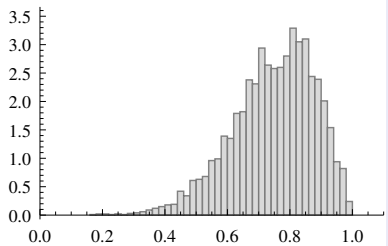
Workload at server 22



Workload at server 23



Workload at server 24



Workload at server 25

Perfect Epidemics

S-I-R deterministic epidemic: susceptibles s, infectives i, removals r:

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

(Total population $s + i + r = n$ is constant.)

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

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

Both models assume homogeneous mixing.

The first question asked about a new epidemic

"What is the R-number?"
The R-number is $\alpha\, n/\beta$: mean number of new infectives produced per infective at *start* of epidemic.
Whittle's threshold theorem: R-number $\gg 1$ means 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 $\alpha\, n/\beta \gg 1$ – 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. It's tough. *Either* massive assumptions (homogeneous mixing) or far too many parameters;
2. It's really tough. It's hard to get good information about infection times;
3. It's especially tough early on. You most need to know the answer when there is hardly any information available (I devised a simplified exercise for a Warwick second-year statistics module to show how tough this is);
4. Markov chain Monte Carlo (MCMC) can be used (O'Neill & Roberts, 1999) but what about burn-in?
5. Can we use perfect simulation?

An easier question

1. Suppose we know n, α, β, observe removals, but *don't* observe infections which must be inferred.
2. We need a new chain: namely, the whole S-I-R trajectory evolving in *algorithmic time* using varying pattern of potential infections and removals.
3. Visualize n time lines, along which are scattered incidents:
   - potential removals, activated if time line is infected;
   - potential infections, activated if time line is infected *and* if designated target time line is lowest uninfected time line.
4. Using Poisson point processes of appropriate rates to scatter these incidents, we obtain an S-I-R epidemic.
5. Now let the point patterns evolve *in algorithmic time*, adding and removing incidents according to spatial immigration-death processes.
6. Result is a trajectory-valued chain which has unconditioned S-I-R as equilibrium.

Conditioning on observed removals

- The trajectory-valued chain is *reversible*.
- So if we forbid the evolution to get rid of observed removals, and forbid it to introduce new activated removals, then the modified chain has invariant probability measure which conditions on observed pattern of removals. Implications:
  - conditioned removals can change time line (if still activated) but not time of occurrence;
  - removals can be introduced only if they don't activate;
  - sometimes infections cannot be removed (because that would result in losing a conditioned removal).
- More housekeeping details required to define algorithm precisely and make sure reversibility and mootonicity still work.
- Need to ensure irreducibility (or otherwise equilibrium will depend on starting point).
- Does this produce a feasible algorithm?

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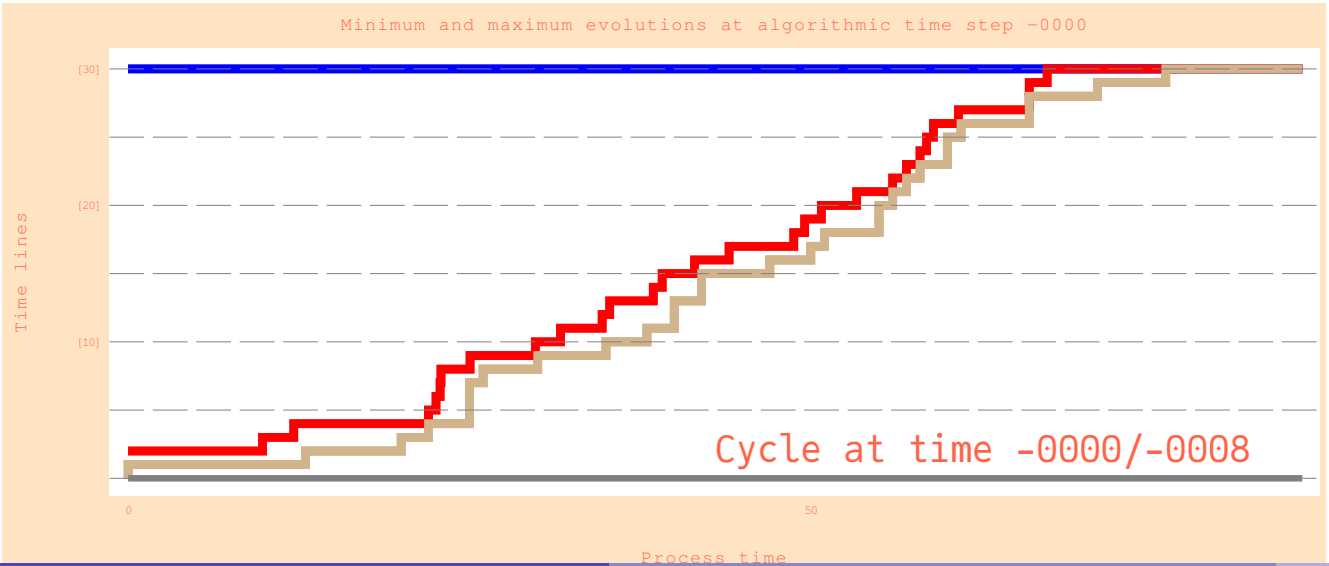
Example

- Smallpox outbreak in a closed community of 120 individuals in Abakaliki, Nigeria (Bailey, 1975; O'Neill & Roberts, 1999).
- **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;
  - there are no further removals after the last observed removal.
- Coding in *julia* (Bezanson *et al.*, 2017), we can construct a perfect simulation GIF resulting in a draw from the conditional distribution of pattern of infections.



So what?

- You may be wondering, why this emphasis on unobserved infections given fixed α and β, when what we really want is 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. Essentially the perfect simulation provides an exact simulation-based computation which permits us to integrate out the pattern of unobserved infections.
- This means we can (**work in progress**, Connor & WSK, 2024)
  - construct a steepest ascent algorithm (in effect, a variant on a Robbins-Monro stochastic optimization algorithm) 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!

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Conclusion

- Are you worried about burn-in issues when doing MCMC. Consider whether perfect simulation can be applied!
- CFTP works even for significantly complex and relevant models of real-life phenomena;
- *Of course* really detailed models will resist perfect simulation: but it can be helpful to compare with a simpler model (especially, using fewer parameters).
- CFTP is clearly an important tool to be considered by the investigator seeking to implement accurate and informative MCMC.
- Thank you for your attention! QUESTIONS?

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Dead leaves	Result of code written by WSK	
Queues	https://covidposters.github.io/	*Open source*
$M/M/c$ customers	Result of code written by Stephen Connor	
$M/M/c$ runtimes	Result of code written by Stephen Connor	
$M/M/c$ loads	Result of code written by Stephen Connor	
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Epidemic	Result of code written by WSK	

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Author: Wilfrid Kendall W.S.Kendall@warwick.ac.uk
Date: Wed May 8 20:15:40 2024 +0100
Summary: Remaining tasks:
Add visual summary for section 1: “Sketch of MCMC”
Fill in and add animations for section 2: “Perfect Simulation”
Correct animations for section 3.1: “Perfect Epidemics”

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