

# 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/>.

# 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 said that] Teller was the only monomaniac he knew who had several manias: see 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  $a \rightarrow b$  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!

## Sketch of MCMC (III)

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

- ❶ **Independence sampler**: draw from a fixed probability distribution, apply Metropolis-Hastings;
- ❷ **Random walk Metropolis** or **RWM**: propose move using a random walk, apply Metropolis-Hastings;
- ❸ **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:

- Ⓐ **Burn-in**: *How long* till approximate equilibrium?
- Ⓑ **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.

# 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?

# Perfect Simulation

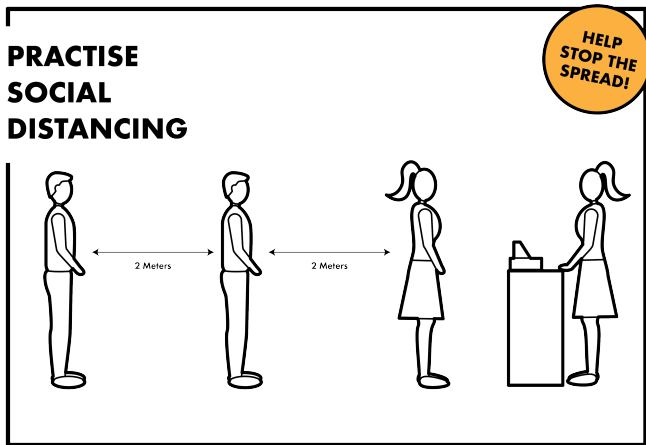
- The idea of exact simulation / Coupling from the Past (CFTP) / perfect simulation Propp & Wilson (1996) (Persi Diaconis: “Like seeing the landscape of Mars for the first time”);
- Ideas (of “*classic CFTP*”):
  - ▶ extending simulation *backwards* through time,
  - ▶ exploit monotonicity by coupling 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 :-).

## An example and some theory

- An intensely visual example, which helps many people see intuitively what is going on here, is *DeadLeaves-CFTP* (WSK & Thönnies, 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.



# Applications to Queues and Epidemics



<https://covidposters.github.io/>

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

# Perfect Queues

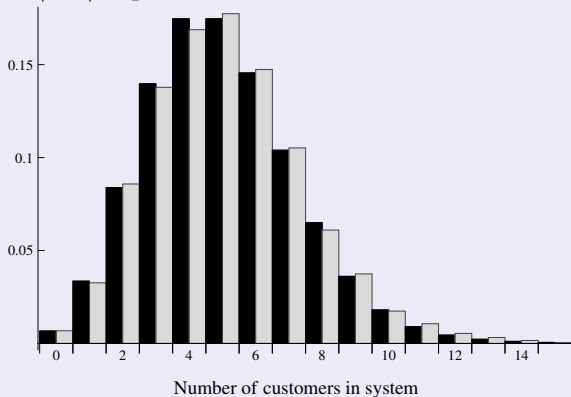
The simplest queuing model (Poisson arrivals, exponential service times, single server) can be analyzed very thoroughly;

- Poisson arrivals are not unreasonable, but exponential service times are ludicrous. The  $M/G/1$  case of general service time *for just one server* can use the “embedded chain” (sample at instants of 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.

- Connor & WSK (2015) show how to extend Sigman (2011), showing how Dominated CFTP can be applied to simulate (sub-critical!) queues perfectly (and this has now been generalized by others to the case of non-Poissonian inter-arrival times). (Technical point: pathwise domination requires service times to be assigned in order of commencement of service!)
  - ▶ dominate  $M/G/cFCFS$  (FCFS means first come first served) by  $M/G/cRA = [M/G/1RA]^c$  (RA means assign to individual servers on arrival);
  - ▶ use fact that *workload* of  $M/G/1FCFS$  is same as  $M/G/1PS$  which can be run backwards in time in equilibrium; (PS means arrivals Share Processor.)
  - ▶ so  $[M/G/1PS]^c$  can be used to provide Dominated CFTP.
- Connor & WSK (2015) also compare
  - Ⓐ CFTP coupling when dominating process empties,
  - Ⓑ a faster CFTP coupling using upper and lower processes starting respectively at dominating process and at empty state.

## Results (I)

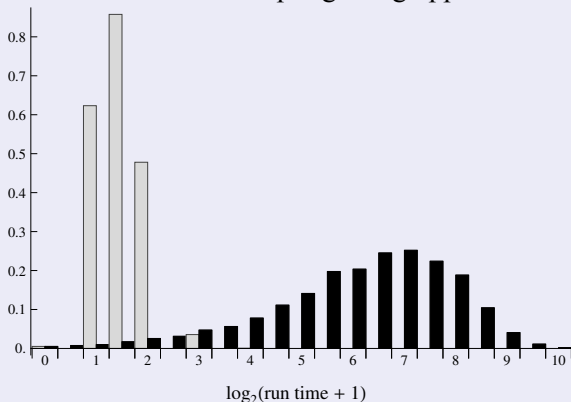
Histogram of customer numbers for  $M/M/c$  queue in equilibrium: arrival rate 10, service rate 2, and 10 servers, comparing theory (available for  $M/M/c$  queue) with results of Connor & WSK (2015) algorithm.



## Results (II)

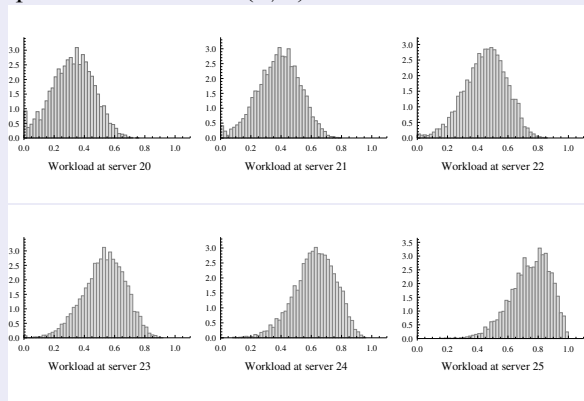
Comparison of log-run times for

- (a) CFTP coupling when dominating process empties (solid bars),
- (b) a faster CFTP coupling using upper and lower processes (grey bars).



## Results (III)

Workload distributions of six most heavily loaded servers in an  $M/G/c = 25$  queue with Uniform(0, 1) service time distribution and arrival rate 25.



# Perfect Epidemics

- Even the simple case of deterministic S-I-R permits only *partial* closed-form solution;
- Suppose **only** the “removal times” are observed? Can the infection times be simulated perfectly? (Given basic parameters.)
- **YES**: work in progress by Connor and Kendall. Here is a GIF illustrating this for a real-life small-pox epidemic;
- (be clear about assumptions!)
- (indicate how the perfect simulation algorithm can be used as a high-dimensional integration device to enable simulation-based Bayesian inference!).

# Conclusion

- You don't always have to put up with burn-in issues when doing MCMC;
- CFTP works even for significantly complex and relevant models of real-life phenomena;
- *Of course* really detailed models are still going to resist perfect simulation: but it will always be helpful to compare with a simpler model (using fewer parameters!).
- CFTP is clearly an important tool to be considered by the investigator seeking to do accurate and informative MCMC.



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# Image attributions

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Edward Teller	Lawrence Livermore National Laboratory restored by w>User:Greg L, Papa Lima Whiskey	<i>CC BY-SA 3.0</i> via Wikimedia Commons
Perfect Ising	Result of code written by WSK	
Dead leaves	Result of code written by WSK	
Queues	<a href="https://covidposters.github.io/">https://covidposters.github.io/</a>	<i>Open source</i>
Number of customers in $M/M/c$ queue	Result of code written by Stephen Connor	
Run-times for $M/M/c$ queues	Result of code written by Stephen Connor	
Epidemic	Result of code written by WSK	

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Still this early version.

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