

# Markov chain Monte Carlo and Perfect simulation

Lecture at Aristotle University of Thessaloniki

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Handout available on the web:



# Introduction



Aristotle: “The more you know, the more you know you don’t know.”

Figure 1: Αριστοτέλης 384–322 BCE

# Sketch of MCMC (I)



Figure 2: Edward Teller (1908-2003)

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

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- But, physicists always remind us, physicists got there fifty years earlier!

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

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- Can there ever be a better way?

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- “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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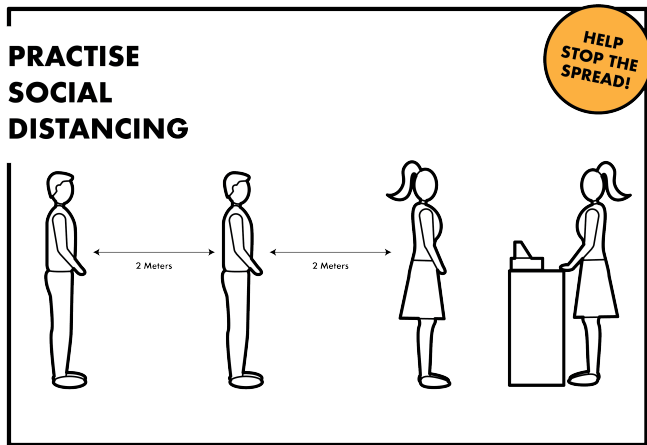
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- Detailed expositions are given by WSK (2005), Huber (2015). WSK (2015) shows how to implement CFTP in R.



# 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;

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- 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!)

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- (indicate how the perfect simulation algorithm can be used as a high-dimensional integration device to enable simulation-based Bayesian inference!).

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- 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.

# References I

- Brown, H. & May, M. (2004) Edward Teller in the Public Arena. *Physics Today*, **57**, 51–53.
- Connor, S.B. & WSK (2007) Perfect simulation for a class of positive recurrent Markov chains. *Annals of Applied Probability*, **17**, 781–808.
- Connor, S.B. & WSK (2015) Perfect simulation of M/G/c queues. *Advances in Applied Probability*, **47**, 1039–1063.
- Foss, S.G. & Tweedie, R.L. (1998) Perfect simulation and backward coupling. *Stochastic Models*, **14**, 187–203.
- Huber, M.L. (2015) *Perfect Simulation*. Boca Raton: Chapman; Hall/CRC.
- Kiefer, J. & Wolfowitz, J. (1955) On the Theory of Queues With Many Servers. *Transactions of the American Mathematical Society*, **78**, 1.
- Metropolis, N., Rosenbluth, A.W., Rosenbluth, M.N., Teller, A.H., & Teller, E. (1953) Equation of State Calculations by Fast Computing Machines. *The Journal of Chemical Physics*, **21**, 1087.
- 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.
- R Development Core Team (2010) *R: A Language and Environment for Statistical Computing*.
- Sigman, K. (2011) Exact simulation of the stationary distribution of the FIFO M/G/c queue. *Journal of Applied Probability*, **48**, 209–213.

# References II

- 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.
- WSK & Thönnies, E. (1999) Perfect simulation in stochastic geometry. *Pattern Recognition*, **32**, 1569–1586.
- Zanella, G. (2015a) Random partition models and complementary clustering of Anglo-Saxon place-names. *Annals of Applied Statistics*, **9**, 1792–1822.
- Zanella, G. (2015b) Bayesian Complementary Clustering, MCMC, and Anglo-Saxon Placenames (PhD Thesis).



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