Perfect Simulation



Mark L. Huber



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For my mother, who showed me Donald in Mathmagic Land and a great many other wonderful things.

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Preface

Suppose a new deck of cards is shuffled. Then as the number of shuffles grows, the distribution of the deck becomes closer and closer to uniform over the set of permutations of the cards. On the other hand, no matter how long you shuffle the deck, it will never be perfectly uniform over the set of permutations.

This technique—of making small changes to a state in order to move it closer to some target distribution—is known today as Markov chain Monte Carlo, or MCMC. Each step brings the chain closer to its target, but it never quite reaches it. With roots in The Manhattan Project, by the early 1990s this idea had become a cornerstone of simulation. For statistical physicists it was the only way to get approximately correct samples in a reasonable amount of time, especially for high dimensional examples such as the Ising model. For frequentist statisticians, it was the only way to calculate *p*-values for complex statistical models. For Bayesian statisticians, it allowed the use of a dizzying array of non-conjugate priors and models.

For almost half a century MCMC had been used, and still only a finite number of steps could be taken. No one realized that it might be possible to somehow jump to an infinite number of steps in a finite number of time. That changed when James Propp and David Wilson introduced coupling from the past (CFTP) in 1996. Their elegant idea allowed users for the first time to sample exactly from the stationary distribution of a Markov chain. That paper, "Exact sampling with coupled Markov chains and applications to statistical mechanics," gave the first exact sample from the Ising model at the critical temperature on an over 16 million dimensional problem.

The list of applications started to grow. Spatial statistics models, domino tilings, linear extensions, random spanning trees... the first few years after publication saw enormous growth in the field. Along the way *exact sampling* changed to *perfect simulation*. The term was introduced by Wilfred Kendall in 1998, and immediately caught on as a way to differentiate the CFTP protocol from other Monte Carlo algorithms that returned samples exactly from the distribution, but without using the peculiar ideas central to CFTP.

David Wilson created a website entitled, "Perfectly Random Sampling with Markov Chains" at http://dimacs.rutgers.edu/ dbwilson/exact/ to inform the nascent community about developments. As of July 2015 the site still exists; a snapshot of the early days of the field.

As time went on, variants of the CFTP method were developed. Read-once coupling from the past allowed samples to be taken using less memory, Fill's method and FMMR connected CFTP to the much older (and less widely applicable) method of acceptance/rejection.

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Then around 2000 something interesting happened. Protocols that were very different from CFTP, such as the Randomness Recycler, were developed. CFTP was now not the only way to draw from the stationary distribution of a Markov chain! New life was breathed into acceptance/rejection through the use of retrospective sampling and sequential acceptance/rejection, allowing for the first time perfect simulation from some diffusions and perfect matchings. Partially recursive acceptance/rejection even allowed for simulation from the classic problem of the Ising model.

CFTP was no longer unique, but fit within a larger framework of perfect simulation ideas. The connections between CFTP and acceptance/rejection became clearer, as each employs a recursive structure that could conceivably go on forever, but with probability 1 does not.

Today the set of perfect simulation algorithms continues to grow, albeit more slowly than in the early days. In researching and writing this text, I was astounded at the wide range of problems to which perfect simulation ideas had been applied. Coupling from the past was not just a protocol; it was the first to show that high dimensional simulation from interacting distributions was even possible, opening up areas of simulation that have yet to be fully explored.

Acknowledgments: My study of perfect simulation began with a special topics course taught by Persi Diaconis when I was a graduate student at Cornell. Persi later became my postdoc advisor as well, and his unflagging enthusiasm for new ideas was an inspiration to me.

I would also like to thank my Ph.D. advisor David Shmoys who took a chance in letting me change research directions in the middle of my graduate work to dive into this newly forming field.

Jim Fill introduced me to several intriguing problems in the area, and later became my first perfect simulation collaborator. Together we added the Randomness Recycler to the world of perfect simulation.

Thanks also to my many colleagues and collaborators who brought me up to speed on Bayesian statistics and patiently sat through the many talks I gave on perfect simulation while I was in the midst of figuring problems out. A great academic environment stimulates the mind in unexpected ways, and I have been privileged to belong to several.

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