

A Short History of Markov Chain Monte Carlo: Subjective Recollections from Incomplete Data¹

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This paper is dedicated to the memory of our friend Julian Besag, a giant in the field of MCMC.

Abstract. We attempt to trace the history and development of Markov chain Monte Carlo (MCMC) from its early inception in the late 1940s through its use today. We see how the earlier stages of Monte Carlo (MC, not MCMC) research have led to the algorithms currently in use. More importantly, we see how the development of this methodology has not only changed our solutions to problems, but has changed the way we think about problems.

Key words and phrases: Gibbs sampling, Metropolis–Hasting algorithm, hierarchical models, Bayesian methods.

1. INTRODUCTION

Markov chain Monte Carlo (MCMC) methods have been around for almost as long as Monte Carlo techniques, even though their impact on Statistics has not been truly felt until the very early 1990s, except in the specialized fields of Spatial Statistics and Image Analysis, where those methods appeared earlier. The emergence of Markov based techniques in Physics is a story that remains untold within this survey (see Landau and Binder, 2005). Also, we will not enter into a description of MCMC techniques. A comprehensive treatment of MCMC techniques, with further references, can be found in Robert and Casella (2004).

We will distinguish between the introduction of Metropolis–Hastings based algorithms and those related to Gibbs sampling, since they each stem from radically different origins, even though their mathematical justification via Markov chain theory is the same. Tracing the development of Monte Carlo methods, we will also briefly mention what we might call the “second-generation MCMC revolution.” Starting in the mid-to-late 1990s, this includes the development of particle filters, reversible jump and perfect sampling, and concludes with more current work on population or sequential Monte Carlo and regeneration and the computing of “honest” standard errors.

As mentioned above, the realization that Markov chains could be used in a wide variety of situations only came (to mainstream statisticians) with Gelfand and Smith (1990), despite earlier publications in the statistical literature like Hastings (1970), Geman and Geman (1984) and Tanner and Wong (1987). Several reasons can be advanced: lack of computing machinery (think of the computers of 1970!), or background on Markov chains, or hesitation to trust in the practicality of the method. It thus required visionary researchers like Gelfand and Smith to convince the community, supported by papers that demonstrated, through a series of applications, that the method was easy to un-

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derstand, easy to implement and practical (Gelfand et al., 1990; Gelfand, Smith and Lee, 1992; Smith and Gelfand, 1992; Wakefield et al., 1994). The rapid emergence of the dedicated BUGS (Bayesian inference Using Gibbs Sampling) software as early as 1991, when a paper on BUGS was presented at the Valencia meeting, was another compelling argument for adopting, at large, MCMC algorithms.²

2. BEFORE THE REVOLUTION

Monte Carlo methods were born in Los Alamos, New Mexico during World War II, eventually resulting in the Metropolis algorithm in the early 1950s. While Monte Carlo methods were in use by that time, MCMC was brought closer to statistical practicality by the work of Hastings in the 1970s.

What can be reasonably seen as the first MCMC algorithm is what we now call the Metropolis algorithm, published by Metropolis et al. (1953). It emanates from the same group of scientists who produced the Monte Carlo method, namely, the research scientists of Los Alamos, mostly physicists working on mathematical physics and the atomic bomb.

MCMC algorithms therefore date back to the same time as the development of regular (MC only) Monte Carlo methods, which are usually traced to Ulam and von Neumann in the late 1940s. Stanislaw Ulam associates the original idea with an intractable combinatorial computation he attempted in 1946 (calculating the probability of winning at the card game “solitaire”). This idea was enthusiastically adopted by John von Neumann for implementation with direct applications to neutron diffusion, the name “Monte Carlo” being suggested by Nicholas Metropolis. (Eckhardt, 1987, describes these early Monte Carlo developments, and Hitchcock, 2003, gives a brief history of the Metropolis algorithm.)

These occurrences very closely coincide with the appearance of the very first computer, the ENIAC, which came to life in February 1946, after three years of construction. The Monte Carlo method was set up by von Neumann, who was using it on thermonuclear and fission problems as early as 1947. At the same time, that is, 1947, Ulam and von Neumann invented inversion and accept-reject techniques (also recounted in

²Historically speaking, the development of BUGS initiated from Geman and Geman (1984) and Pearl (1987), in accord with the developments in the artificial intelligence community, and it predates Gelfand and Smith (1990).

Eckhardt, 1987) to simulate from nonuniform distributions. Without computers, a rudimentary version invented by Fermi in the 1930s did not get any recognition (Metropolis, 1987). Note also that, as early as 1949, a symposium on Monte Carlo was supported by Rand, NBS and the Oak Ridge laboratory and that Metropolis and Ulam (1949) published the very first paper about the Monte Carlo method.

2.1 The Metropolis et al. (1953) Paper

The first MCMC algorithm is associated with a second computer, called MANIAC, built³ in Los Alamos under the direction of Metropolis in early 1952. Both a physicist and a mathematician, Nicolas Metropolis, who died in Los Alamos in 1999, came to this place in April 1943. The other members of the team also came to Los Alamos during those years, including the controversial Teller. As early as 1942, he became obsessed with the hydrogen (H) bomb, which he eventually managed to design with Stanislaw Ulam, using the better computer facilities in the early 1950s.

Published in June 1953 in the *Journal of Chemical Physics*, the primary focus of Metropolis et al. (1953) is the computation of integrals of the form

$$\mathfrak{J} = \frac{\int F(\theta) \exp\{-E(\theta)/kT\} d\theta}{\int \exp\{-E(\theta)/kT\} d\theta},$$

on \mathbb{R}^{2N} , θ denoting a set of N particles on \mathbb{R}^2 , with the energy E being defined as

$$E(\theta) = \frac{1}{2} \sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N V(d_{ij}),$$

where V is a potential function and d_{ij} the Euclidean distance between particles i and j in θ . The Boltzmann distribution $\exp\{-E(\theta)/kT\}$ is parameterized by the temperature T , k being the Boltzmann constant, with a normalization factor

$$Z(T) = \int \exp\{-E(\theta)/kT\} d\theta,$$

that is not available in closed form, except in trivial cases. Since θ is a $2N$ -dimensional vector, numerical integration is impossible. Given the large dimension of the problem, even standard Monte Carlo techniques fail to correctly approximate \mathfrak{J} , since $\exp\{-E(\theta)/kT\}$

³MANIAC stands for *Mathematical Analyzer, Numerical Integrator and Computer*.

is very small for most realizations of the random configurations of the particle system (uniformly in the $2N$ square). In order to improve the efficiency of the Monte Carlo method, Metropolis et al. (1953) propose a random walk modification of the N particles. That is, for each particle i ($1 \leq i \leq N$), values

$$x'_i = x_i + \sigma \xi_{1i} \quad \text{and} \quad y'_i = y_i + \sigma \xi_{2i}$$

are proposed, where both ξ_{1i} and ξ_{2i} are uniform $\mathcal{U}(-1, 1)$. The energy difference ΔE between the new configuration and the previous one is then computed and the new configuration is accepted with probability

$$(1) \quad \min\{1, \exp(-\Delta E/kT)\},$$

and otherwise the previous configuration is replicated, in the sense that its counter is increased by one in the final average of the $F(\theta_t)$'s over the τ moves of the random walk, $1 \leq t \leq \tau$. Note that Metropolis et al. (1953) move one particle at a time, rather than moving all of them together, which makes the initial algorithm appear as a primitive kind of Gibbs sampler!

The authors of Metropolis et al. (1953) demonstrate the validity of the algorithm by first establishing irreducibility, which they call *ergodicity*, and second proving ergodicity, that is, convergence to the stationary distribution. The second part is obtained via a discretization of the space: They first note that the proposal move is reversible, then establish that $\exp\{-E/kT\}$ is invariant. The result is therefore proven in its full generality, minus the discretization. The number of iterations of the Metropolis algorithm used in the paper seems to be limited: 16 steps for burn-in and 48 to 64 subsequent iterations, which required four to five hours on the Los Alamos computer.

An interesting variation is the *Simulated Annealing* algorithm, developed by Kirkpatrick, Gelatt and Vecchi (1983), who connected optimization with *annealing*, the cooling of a metal. Their variation is to allow the temperature T in (1) to change as the algorithm runs, according to a “cooling schedule,” and the Simulated Annealing algorithm can be shown to find the global maximum with probability 1, although the analysis is quite complex due to the fact that, with varying T , the algorithm is no longer a time-homogeneous Markov chain.

2.2 The Hastings (1970) Paper

The Metropolis algorithm was later generalized by Hastings (1970) and his student Peskun (1973, 1981) as a statistical simulation tool that could overcome the curse of dimensionality met by regular Monte Carlo

methods, a point already emphasized in Metropolis et al. (1953).⁴

In his *Biometrika* paper,⁵ Hastings (1970) also defines his methodology for finite and reversible Markov chains, treating the continuous case by using a discretization analogy. The generic probability of acceptance for a move from state i to state j is

$$\alpha_{ij} = \frac{s_{ij}}{1 + (\pi_i/\pi_j)(q_{ij}/q_{ji})},$$

where $s_{ij} = s_{ji}$, π_i denotes the target and q_{ij} the proposal. This generic form of probability encompasses the forms of both Metropolis et al. (1953) and Barker (1965). At this stage, Hastings mentions that *little is known about the relative merits of those two choices* (even though) *Metropolis's method may be preferable*. He also warns against *high rejection rates as indicative of a poor choice of transition matrix*, but does not mention the opposite pitfall of low rejection rates, associated with a slow exploration of the target.

The examples given in the paper are a Poisson target with a ± 1 random walk proposal, a normal target with a uniform random walk proposal mixed with its reflection, that is, a uniform proposal centered at $-\theta_t$ rather than at the current value θ_t of the Markov chain, and then a multivariate target where Hastings introduces a Gibbs sampling strategy, updating one component at a time and defining the composed transition as satisfying the stationary condition because each component does leave the target invariant. Hastings (1970) actually refers to Ehrman, Fosdick and Handscomb (1960) as a preliminary, if specific, instance of this sampler. More precisely, this is Metropolis-within-Gibbs except for the name. This first introduction of the Gibbs sampler has thus been completely overlooked, even though the proof of convergence is completely general, based on a composition argument as in Tierney (1994), discussed in Section 4.1. The remainder of the paper deals with (a) an importance sampling version of MCMC, (b) general remarks about assessment of the error, and (c) an application to random orthogonal matrices, with another example of Gibbs sampling.

Three years later, Peskun (1973) published a comparison of Metropolis' and Barker's forms of acceptance probabilities and shows in a discrete setup that

⁴In fact, Hastings starts by mentioning a decomposition of the target distribution into a *product of one-dimensional conditional distributions*, but this falls short of an early Gibbs sampler.

⁵Hastings (1970) is one of the ten *Biometrika* papers reproduced in Titterton and Cox (2001).

1 the optimal choice is that of Metropolis, where op- 52
 2 timality is to be understood in terms of the asymp- 53
 3 totic variance of any empirical average. The proof is 54
 4 a direct consequence of a result by Kemeny and Snell 55
 5 (1960) on the asymptotic variance. Peskun also estab- 56
 6 lishes that this asymptotic variance can improve upon 57
 7 the i.i.d. case if and only if the eigenvalues of $\mathbf{P} - \mathbf{A}$ 58
 8 are all negative, when \mathbf{A} is the transition matrix corre- 59
 9 sponding to i.i.d. simulation and \mathbf{P} the transition matrix 60
 10 corresponding to the Metropolis algorithm, but he con- 61
 11 cludes that the trace of $\mathbf{P} - \mathbf{A}$ is always positive. 62
 12

13 **3. SEEDS OF THE REVOLUTION** 64

14 A number of earlier pioneers had brought forward 65
 15 the seeds of Gibbs sampling; in particular, Ham- 66
 16 mersley and Clifford had produced a constructive argu- 67
 17 ment in 1970 to recover a joint distribution from its 68
 18 conditionals, a result later called the *Hammersley–* 69
 19 *Clifford* theorem by Besag (1974, 1986). Besides Hast- 70
 20 ings (1970) and Geman and Geman (1984), already 71
 21 mentioned, other papers that contained the seeds of 72
 22 Gibbs sampling are Besag and Clifford (1989), Bro- 73
 23 niatowski, Celeux and Diebolt (1984), Qian and Titter- 74
 24 ington (1990) and Tanner and Wong (1987). 75
 25

26 **3.1 Besag’s Early Work and the Fundamental** 76
 27 **(Missing) Theorem** 77
 28

29 In the early 1970’s, Hammersley, Clifford and Besag 80
 30 were working on the specification of joint distributions 81
 31 from conditional distributions and on necessary and 82
 32 sufficient conditions for the conditional distributions to 83
 33 be compatible with a joint distribution. What is now 84
 34 known as the *Hammersley–Clifford* theorem states that 85
 35 a joint distribution for a vector associated with a depen- 86
 36 dence graph (edge meaning dependence and absence of 87
 37 edge conditional independence) must be represented as 88
 38 a product of functions over the *cliques* of the graphs, 89
 39 that is, of functions depending only on the components 90
 40 indexed by the labels in the clique.⁶ 91

41 From a historical point of view, Hammersley (1974) 92
 42 explains why the Hammersley–Clifford theorem was 93
 43 never published as such, but only through Besag 94
 44 (1974). The reason is that Clifford and Hammersley 95
 45 were dissatisfied with the positivity constraint: The 96
 46 joint density could be recovered from the full condi- 97
 47 tionals only when the support of the joint was made 98
 48

49 ⁶A clique is a maximal subset of the nodes of a graphs such 100
 50 that every pair of nodes within the clique is connected by an edge 101
 51 (Cressie, 1993). 102

of the product of the supports of the full conditionals. 52
 While they strived *to make the theorem independent* 53
of any positivity condition, their graduate student pub- 54
 lished a counter-example that put a full stop to their 55
 endeavors (Moussouris, 1974). 56

While Besag (1974) can certainly be credited to 57
 some extent of the (re-)discovery of the Gibbs sampler, 58
 Besag (1975) expressed doubt about the practicality of 59
 his method, noting that “the technique is unlikely to 60
 be particularly helpful in many other than binary sit- 61
 uations and the Markov chain itself has no practical 62
 interpretation,” clearly understating the importance of 63
 his own work. 64

A more optimistic sentiment was expressed earlier 65
 by Hammersley and Handscomb (1964) in their text- 66
 book on Monte Carlo methods. There they cover such 67
 topics as “Crude Monte Carlo,” importance sampling, 68
 control variates and “Conditional Monte Carlo,” which 69
 looks surprisingly like a missing-data completion ap- 70
 proach. Of course, they do not cover the Hammersley– 71
 Clifford theorem, but they state in the Preface: 72

73 We are convinced nevertheless that Monte 74
 75 Carlo methods will one day reach an im- 76
 77 pressive maturity. 78

Well said!

79 **3.2 EM and Its Simulated Versions as Precursors** 80

81 Because of its use for missing data problems, the 82
 EM algorithm (Dempster, Laird and Rubin, 1977) has 83
 early connections with Gibbs sampling. For instance, 84
 Broniatowski, Celeux and Diebolt (1984) and Celeux 85
 and Diebolt (1985) had tried to overcome the depen- 86
 dence of EM methods on the starting value by re- 87
 placing the E step with a *simulation* step, the missing 88
 data z being generated conditionally on the observa- 89
 tion x and on the current value of the parameter θ_m . 90
 The maximization in the M step is then done on the 91
 simulated complete-data log-likelihood, a predecessor 92
 to the Gibbs step of Diebolt and Robert (1994) for 93
 mixture estimation. Unfortunately, the theoretical con- 94
 vergence results for these methods are limited. Celeux 95
 and Diebolt (1990) have, however, solved the conver- 96
 gence problem of SEM by devising a hybrid version 97
 called SAEM (for *Simulated Annealing EM*), where 98
 the amount of randomness in the simulations decreases 99
 with the iterations, ending up with an EM algorithm.⁷ 100

⁷Other and more well-known connections between EM and 101
 MCMC algorithms can be found in the literature (Liu and Rubin, 102

1 **3.3 Gibbs and Beyond**

2 Although somewhat removed from statistical infer- 52
 3 ence in the classical sense and based on earlier tech- 53
 4 niques used in Statistical Physics, the landmark paper 54
 5 by Geman and Geman (1984) brought Gibbs sampling 55
 6 into the arena of statistical application. This paper is 56
 7 also responsible for the name *Gibbs sampling*, because 57
 8 it implemented this method for the Bayesian study of 58
 9 *Gibbs random fields* which, in turn, derive their name 59
 10 from the physicist Josiah Willard Gibbs (1839–1903). 60
 11 This original implementation of the Gibbs sampler was 61
 12 applied to a discrete image processing problem and did 62
 13 not involve completion. But this was one more spark 63
 14 that led to the explosion, as it had a clear influence on 64
 15 Green, Smith, Spiegelhalter and others. 65

16 The extent to which Gibbs sampling and Metropolis 66
 17 algorithms were in use within the image analysis and 67
 18 point process communities is actually quite large, as il- 68
 19 lustrated in Ripley (1987) where Section 4.7 is entitled 69
 20 “Metropolis’ method and random fields” and describes 70
 21 the implementation and the validation of the Metropo- 71
 22 lis algorithm in a finite setting with an application to 72
 23 Markov random fields and the corresponding issue of 73
 24 bypassing the normalizing constant. Besag, York and 74
 25 Mollié (1991) is another striking example of the activ- 75
 26 ity in the spatial statistics community at the end of the 76
 27 1980s. 77

28 **4. THE REVOLUTION**

29 The gap of more than 30 years between Metropolis 80
 30 et al. (1953) and Gelfand and Smith (1990) can still 81
 31 be partially attributed to the lack of appropriate com- 82
 32 puting power, as most of the examples now processed 83
 33 by MCMC algorithms could not have been treated 84
 34 previously, even though the hundreds of dimensions 85
 35 processed in Metropolis et al. (1953) were quite formi- 86
 36 dable. However, by the mid-1980s, the pieces were all 87
 37 in place. 88

38 After Peskun, MCMC in the statistical world was 89
 39 dormant for about 10 years, and then several papers 90
 40 appeared that highlighted its usefulness in specific set- 91
 41 tings like pattern recognition, image analysis or spa- 92
 42 tial statistics. In particular, Geman and Geman (1984) 93
 43 influenced Gelfand and Smith (1990) to write a paper 94
 44 that is the genuine starting point for an intensive use of 95

45 1994; Meng and Rubin, 1993; Wei and Tanner, 1990, but the con- 96
 46 nection with Gibbs sampling is more tenuous in that the simulation 97
 47 methods are used to approximate quantities in a Monte Carlo fash- 98
 48 ion. 99
 49
 50
 51

MCMC methods by the mainstream statistical commu- 52
 nity. It sparked new interest in Bayesian methods, sta- 53
 tistical computing, algorithms and stochastic processes 54
 through the use of computing algorithms such as the 55
 Gibbs sampler and the Metropolis–Hastings algorithm. 56
 (See Casella and George, 1992, for an elementary in- 57
 troduction to the Gibbs sampler.⁸) 58

59 Interestingly, the earlier paper by Tanner and Wong 59
 (1987) had essentially the same ingredients as Gelfand 60
 and Smith (1990), namely, the fact that simulating from 61
 the conditional distributions is sufficient to asymptot- 62
 ically simulate from the joint. This paper was con- 63
 sidered important enough to be a discussion paper in 64
 the *Journal of the American Statistical Association*, 65
 but its impact was somehow limited, compared with 66
 Gelfand and Smith (1990). There are several reasons 67
 for this; one being that the method seemed to only ap- 68
 ply to missing data problems, this impression being re- 69
 inforced by the name *data augmentation*, and another 70
 is that the authors were more focused on approximat- 71
 ing the posterior distribution. They suggested a MCMC 72
 approximation to the target $\pi(\theta|x)$ at each iteration of 73
 the sampler, based on 74

$$\frac{1}{m} \sum_{k=1}^m \pi(\theta|x, z^{t,k}),$$

$$z^{t,k} \sim \hat{\pi}_{t-1}(z|x), \quad k = 1, \dots, m,$$

75 that is, by replicating m times the simulations from the 75
 76 current approximation $\hat{\pi}_{t-1}(z|x)$ of the marginal poste- 76
 77 rior distribution of the missing data. This focus on esti- 77
 78 mation of the posterior distribution connected the origi- 78
 79 nal Data Augmentation algorithm to EM, as pointed 79
 80 out by Dempster in the discussion. Although the dis- 80
 81 cussion by Carl Morris gets very close to the two-stage 81
 82 Gibbs sampler for hierarchical models, he is still con- 82
 83 cerned about doing m iterations, and worries about how 83
 84 costly that would be. Tanner and Wong mention taking 84
 85 $m = 1$ at the end of the paper, referring to this as an 85
 86 “extreme case.” 86
 87

88 In a sense, Tanner and Wong (1987) were still too 88
 89 close to Rubin’s 1978 multiple imputation to start 89
 90 a new revolution. Yet another reason for this may be 90
 91

92 ⁸On a humorous note, the original Technical Report of this paper 92
 93 was called *Gibbs for Kids*, which was changed because a referee did 93
 94 not appreciate the humor. However, our colleague Dan Gianola, an 94
 95 Animal Breeder at Wisconsin, liked the title. In using Gibbs sam- 95
 96 pling in his work, he gave a presentation in 1993 at the 44th An- 96
 97 nual Meeting of the European Association for Animal Production, 97
 98 Aarhus, Denmark. The title: *Gibbs for Pigs*. 98
 99
 100
 101
 102

1 that the theoretical background was based on func- 52
 2 tional analysis rather than Markov chain theory, which 53
 3 needed, in particular, for the Markov kernel to be uni- 54
 4 formly bounded and equicontinuous. This may have 55
 5 discouraged potential users as requiring too much 56
 6 mathematics. 57

7 The authors of this review were fortunate enough 58
 8 to attend many focused conferences during this time, 59
 9 where we were able to witness the explosion of Gibbs 60
 10 sampling. In the summer of 1986 in Bowling Green, 61
 11 Ohio, Adrian Smith gave a series of ten lectures on hi- 62
 12 erarchical models. Although there was a lot of comput- 63
 13 ing mentioned, the Gibbs sampler was not fully devel- 64
 14 oped yet. In another lecture in June 1989 at a Bayesian 65
 15 workshop in Sherbrooke, Québec, he revealed for the 66
 16 first time the generic features of the Gibbs sampler, and 67
 17 we still remember vividly the shock induced on our- 68
 18 selves and on the whole audience by the sheer breadth 69
 19 of the method: This development of Gibbs sampling, 70
 20 MCMC, and the resulting seminal paper of Gelfand 71
 21 and Smith (1990) was an *epiphany* in the world of Sta- 72
 22 tistics. 73

23 DEFINITION (Epiphany n). A spiritual event in 74
 24 which the essence of a given object of manifestation 75
 25 appears to the subject, as in a sudden flash of recogni- 76
 26 tion. 77
 27

28 The explosion had begun, and just two years later, at 79
 29 an MCMC conference at Ohio State University orga- 80
 30 nized by Alan Gelfand, Prem Goel and Adrian Smith, 81
 31 there were three full days of talks. The presenters 82
 32 at the conference read like a Who’s Who of MCMC, 83
 33 and the level, intensity and impact of that conference, 84
 34 and the subsequent research, are immeasurable. Many 85
 35 of the talks were to become influential papers, in- 86
 36 cluding Albert and Chib (1993), Gelman and Rubin 87
 37 (1992), Geyer (1992), Gilks (1992), Liu, Wong and 88
 38 Kong (1994, 1995) and Tierney (1994). The program 89
 39 of the conference is reproduced in the [Appendix](#). 90

40 Approximately one year later, in May of 1992, there 91
 41 was a meeting of the Royal Statistical Society on “The 92
 42 Gibbs sampler and other Markov chain Monte Carlo 93
 43 methods,” where four papers were presented followed 94
 44 by much discussion. The papers appear in the first vol- 95
 45 ume of *JRSSB* in 1993, together with 49(!) pages of 96
 46 discussion. The excitement is clearly evident in the 97
 47 writings, even though the theory and implementation 98
 48 were not always perfectly understood.⁹ 99

50 ⁹On another humorous note, Peter Clifford opened the discussion 100
 51 by noting “. . . we have had the opportunity to hear a large amount 101
 102

Looking at these meetings, we can see the paths that 52
 Gibbs sampling would lead us down. In the next two 53
 sections we will summarize some of the advances from 54
 the early to mid 1990s. 55

56 **4.1 Advances in MCMC Theory** 57

Perhaps the most influential MCMC theory paper of 58
 the 1990s is Tierney (1994), who carefully laid out 59
 all of the assumptions needed to analyze the Markov 60
 chains and then developed their properties, in par- 61
 ticular, convergence of ergodic averages and central 62
 limit theorems. In one of the discussions of that pa- 63
 per, Chan and Geyer (1994) were able to relax a con- 64
 dition on Tierney’s Central Limit Theorem, and this 65
 new condition plays an important role in research to- 66
 day (see Section 5.4). A pair of very influential, and 67
 innovative, papers is the work of Liu, Wong and Kong 68
 (1994, 1995), who very carefully analyzed the covari- 69
 ance structure of Gibbs sampling, and were able to for- 70
 mally establish the validity of Rao–Blackwellization in 71
 Gibbs sampling. Gelfand and Smith (1990) had used 72
 Rao–Blackwellization, but it was not justified at that 73
 time, as the original theorem was only applicable to 74
 i.i.d. sampling, which is not the case in MCMC. An- 75
 other significant entry is Rosenthal (1995), who ob- 76
 tained one of the earliest results on exact rates of con- 77
 vergence. 78

Another paper must be singled out, namely, Men- 79
 gersen and Tweedie (1996), for setting the tone for 80
 the study of the speed of convergence of MCMC al- 81
 gorithms to the target distribution. Subsequent works 82
 in this area by Richard Tweedie, Gareth Roberts, Jeff 83
 Rosenthal and co-authors are too numerous to be men- 84
 tioned here, even though the paper by Roberts, Gel- 85
 man and Gilks (1997) must be cited for setting ex- 86
 plicit targets on the acceptance rate of the random walk 87
 Metropolis–Hastings algorithm, as well as Roberts and 88
 Rosenthal (1999) for getting an upper bound on the 89
 number of iterations (523) needed to approximate the 90
 target up to 1% by a slice sampler. The untimely death 91
 of Richard Tweedie in 2001, alas, had a major impact 92
 on the book about MCMC convergence he was con- 93
 templating with Gareth Roberts. 94

95 about an important new area in statistics. It may well be remem- 96
 97 bered as the ‘afternoon of the 11 Bayesians.’ Bayesianism has ob- 97
 98 viously come a long way. It used to be that you could tell a Bayesian 98
 99 by his tendency to hold meetings in isolated parts of Spain and his 99
 100 obsession with coherence, self-interrogation and other manifesta- 100
 101 tions of paranoia. Things have changed, and there may be a general 101
 102 lesson here for statistics. Isolation is counter-productive.” 102

1 One pitfall arising from the widespread use of Gibbs
 2 sampling was the tendency to specify models only
 3 through their conditional distributions, almost always
 4 without referring to the positivity conditions in Sec-
 5 tion 3. Unfortunately, it is possible to specify a per-
 6 fectly legitimate-looking set of conditionals that do not
 7 correspond to any joint distribution, and the result-
 8 ing Gibbs chain cannot converge. Hobert and Casella
 9 (1996) were able to document the conditions needed
 10 for a convergent Gibbs chain, and alerted the Gibbs
 11 community to this problem, which only arises when
 12 improper priors are used, but this is a frequent occur-
 13 rence.

14 Much other work followed, and continues to grow
 15 today. Geyer and Thompson (1995) describe how to
 16 put a “ladder” of chains together to have both “hot”
 17 and “cold” exploration, followed by Neal’s 1996 in-
 18 troduction of tempering; Athreya, Doss and Sethura-
 19 man (1996) gave more easily verifiable conditions for
 20 convergence; Meng and van Dyk (1999) and Liu and
 21 Wu (1999) developed the theory of parameter expan-
 22 sion in the Data Augmentation algorithm, leading to
 23 construction of chains with faster convergence, and to
 24 the work of Hobert and Marchev (2008), who give pre-
 25 cise constructions and theorems to show how param-
 26 eter expansion can uniformly improve over the original
 27 chain.

28 **4.2 Advances in MCMC Applications**

29 The real reason for the explosion of MCMC meth-
 30 ods was the fact that an enormous number of problems
 31 that were deemed to be computational nightmares now
 32 cracked open like eggs. As an example, consider this
 33 very simple random effects model from Gelfand and
 34 Smith (1990). Observe

35 (2) $Y_{ij} = \theta_i + \varepsilon_{ij}, \quad i = 1, \dots, K, \quad j = 1, \dots, J,$

36 where

37 $\theta_i \sim N(\mu, \sigma_\theta^2),$
 38 $\varepsilon_{ij} \sim N(0, \sigma_\varepsilon^2), \quad \text{independent of } \theta_i.$

39 Estimation of the variance components can be difficult
 40 for a frequentist (REML is typically preferred), but it
 41 indeed was a nightmare for a Bayesian, as the inte-
 42 grals were intractable. However, with the usual priors
 43 on μ, σ_θ^2 and σ_ε^2 , the full conditionals are trivial to sam-
 44 ple from and the problem is easily solved via Gibbs
 45 sampling. Moreover, we can increase the number of
 46 variance components and the Gibbs solution remains
 47 easy to implement.
 48
 49
 50
 51

During the early 1990s, researchers found that Gibbs,
 or Metropolis–Hastings, algorithms would be able to
 give solutions to almost any problem that they looked
 at, and there was a veritable flood of papers apply-
 ing MCMC to previously intractable models, and get-
 ting good answers. For example, building on (2), it
 was quickly realized that Gibbs sampling was an easy
 route to getting estimates in the linear mixed models
 (Wang, Rutledge and Gianola, 1993, 1994), and even
 generalized linear mixed models (Zeger and Karim,
 1991). Building on the experience gained with the
 EM algorithm, similar arguments made it possible
 to analyze probit models using a latent variable ap-
 proach in a linear mixed model (Albert and Chib,
 1993), and in mixture models with Gibbs sampling
 (Diebolt and Robert, 1994). It progressively dawned
 on the community that latent variables could be arti-
 ficially introduced to run the Gibbs sampler in about
 every situation, as eventually published in Damien,
 Wakefield and Walker (1999), the main example be-
 ing the slice sampler (Neal, 2003). A very incomplete
 list of some other applications include changepoint
 analysis (Carlin, Gelfand and Smith, 1992; Stephens,
 1994), Genomics (Churchill, 1995; Lawrence et al.,
 1993; Stephens and Smith, 1993), capture–recapture
 (Dupuis, 1995; George and Robert, 1992), variable se-
 lection in regression (George and McCulloch, 1993),
 spatial statistics (Raftery and Banfield, 1991), and lon-
 gitudinal studies (Lange, Carlin and Gelfand, 1992).

Many of these applications were advanced though
 other developments such as the Adaptive Rejection
 Sampling of Gilks (1992); Gilks, Best and Tan (1995),
 and the simulated tempering approaches of Geyer and
 Thompson (1995) or Neal (1996).

5. AFTER THE REVOLUTION

After the revolution comes the “second” revolution,
 but now we have a more mature field. The revolution
 has slowed, and the problems are being solved in, per-
 haps, deeper and more sophisticated ways, even though
 Gibbs sampling also offers to the amateur the possibil-
 ity to handle Bayesian analysis in complex models at
 little cost, as exhibited by the widespread use of BUGS,
 which mostly focuses¹⁰ on this approach. But, as be-
 fore, the methodology continues to expand the set of
 problems for which statisticians can provide meaning-
 ful solutions, and thus continues to further the impact
 of Statistics.

¹⁰BUGS now uses both Gibbs sampling and Metropolis–Hastings algorithms.

5.1 A Brief Glimpse at Particle Systems

The realization of the possibilities of iterating importance sampling is not new: in fact, it is about as old as Monte Carlo methods themselves. It can be found in the molecular simulation literature of the 50s, as in Hammersley and Morton (1954), Rosenbluth and Rosenbluth (1955) and Marshall (1965). Hammersley and colleagues proposed such a method to simulate a self-avoiding random walk (see Madras and Slade, 1993) on a grid, due to huge inefficiencies in regular importance sampling and rejection techniques. Although this early implementation occurred in particle physics, the use of the term “particle” only dates back to Kitagawa (1996), while Carpenter, Clifford and Fernhead (1997) coined the term “particle filter.” In signal processing, early occurrences of a particle filter can be traced back to Handschin and Mayne (1969).

More in connection with our theme, the landmark paper of Gordon, Salmond and Smith (1993) introduced the bootstrap filter which, while formally connected with importance sampling, involves past simulations and possible MCMC steps (Gilks and Berzuini, 2001). As described in the volume edited by Doucet, de Freitas and Gordon (2001), particle filters are simulation methods adapted to sequential settings where data are collected progressively in time, as in radar detection, telecommunication correction or financial volatility estimation. Taking advantage of state-space representations of those dynamic models, particle filter methods produce Monte Carlo approximations to the posterior distributions by propagating simulated samples whose weights are actualized against the incoming observations. Since the importance weights have a tendency to degenerate, that is, all weights but one are close to zero, additional MCMC steps can be introduced at times to recover the variety and representativeness of the sample. Modern connections with MCMC in the construction of the proposal kernel are to be found, for instance, in Doucet, Godsill and Andrieu (2000) and in Del Moral, Doucet and Jasra (2006). At the same time, sequential imputation was developed in Kong, Liu and Wong (1994), while Liu and Chen (1995) first formally pointed out the importance of resampling in sequential Monte Carlo, a term coined by them.

The recent literature on the topic more closely bridges the gap between sequential Monte Carlo and MCMC methods by making adaptive MCMC a possibility (see, e.g., Andrieu et al., 2004, or Roberts and Rosenthal, 2007).

5.2 Perfect Sampling

Introduced in the seminal paper of Propp and Wilson (1996), perfect sampling, namely, the ability to use MCMC methods to produce an exact (or perfect) simulation from the target, maintains a unique place in the history of MCMC methods. Although this exciting discovery led to an outburst of papers, in particular, in the large body of work of Møller and coauthors, including the book by Møller and Waagepetersen (2003), as well as many reviews and introductory materials, like Casella, Lavine and Robert (2001), Fismen (1998) and Dimakos (2001), the excitement quickly dried out. The major reason for this ephemeral lifespan is that the construction of perfect samplers is most often close to impossible or impractical, despite some advances in the implementation (Fill, 1998a, 1998b).

There is, however, ongoing activity in the area of point processes and stochastic geometry, much from the work of Møller and Kendall. In particular, Kendall and Møller (2000) developed an alternative to the *Coupling From The Past* (CFPT) algorithm of Propp and Wilson (1996), called *horizontal CFTP*, which mainly applies to point processes and is based on continuous time birth-and-death processes. See also Fernández, Ferrari and Garcia (1999) for another horizontal CFTP algorithm for point processes. Berthelsen and Møller (2003) exhibited a use of these algorithms for nonparametric Bayesian inference on point processes.

5.3 Reversible Jump and Variable Dimensions

From many viewpoints, the invention of the reversible jump algorithm in Green (1995) can be seen as the start of the second MCMC revolution: the formalization of a Markov chain that moves across models and parameter spaces allowed for the Bayesian processing of a wide variety of new models and contributed to the success of Bayesian model choice and subsequently to its adoption in other fields. There exist earlier alternative Monte Carlo solutions like Gelfand and Dey (1994) and Carlin and Chib (1995), the later being very close in spirit to reversible jump MCMC (as shown by the completion scheme of Brooks, Giudici and Roberts, 2003), but the definition of a proper balance condition on cross-model Markov kernels in Green (1995) gives a generic setup for exploring variable dimension spaces, even when the number of models under comparison is infinite. The impact of this new idea was clearly perceived when looking at the First European Conference on Highly Structured Stochastic Systems that took place in Rebild, Denmark,

1 the next year, organized by Stephen Lauritzen and Jes- 52
 2 per Møller: a large majority of the talks were aimed 53
 3 at direct implementations of RJMCMC to various in- 54
 4 ference problems. The application of RJMCMC to 55
 5 mixture order estimation in the discussion paper of 56
 6 Richardson and Green (1997) ensured further dissemi- 57
 7 nation of the technique. Continuing to develop RJM- 58
 8 CMct, Stephens (2000) proposed a continuous time 59
 9 version of RJMCMC, based on earlier ideas of Geyer 60
 10 and Møller (1994), but with similar properties (Cappé, 61
 11 Robert and Rydén, 2003), while Brooks, Giudici and 62
 12 Roberts (2003) made proposals for increasing the ef- 63
 13 ficiency of the moves. In retrospect, while reversible 64
 14 jump is somehow unavoidable in the processing of very 65
 15 large numbers of models under comparison, as, for in- 66
 16 stance, in variable selection (Marin and Robert, 2007), 67
 17 the implementation of a complex algorithm like RJM- 68
 18 CMc for the comparison of a few models is somewhat 69
 19 of an overkill since there may exist alternative solu- 70
 20 tions based on model specific MCMC chains, for ex- 71
 21 ample (Chen, Shao and Ibrahim, 2000). 72

22 **5.4 Regeneration and the CLT**

23
 24 While the Central Limit Theorem (CLT) is a central 75
 25 tool in Monte Carlo convergence assessment, its use in 76
 26 MCMC setups took longer to emerge, despite early sig- 77
 27 nals by Geyer (1992), and it is only recently that suf- 78
 28 ficiently clear conditions emerged. We recall that the 79
 29 Ergodic Theorem (see, e.g., Robert and Casella, 2004, 80
 30 Theorem 6.63) states that, if $(\theta_t)_t$ is a Markov chain 81
 31 with stationary distribution π , and $h(\cdot)$ is a function 82
 32 with finite variance, then under fairly mild conditions, 83

33
 34 (3)
$$\lim_{n \rightarrow \infty} \bar{h}_n = \int h(\theta)\pi(\theta) d\theta = E_\pi h(\theta),$$

35 almost everywhere, where $\bar{h}_n = (1/n) \sum_{i=1}^n h(\theta_i)$. For 85
 36 the CLT to be used to monitor this convergence, 86

37
 38 (4)
$$\frac{\sqrt{n}(\bar{h}_n - E_\pi h(\theta))}{\sqrt{\text{Var } h(\theta)}} \rightarrow N(0, 1),$$

39
 40 there are two roadblocks. First, convergence to normal- 87
 41 ity is strongly affected by the lack of independence. To 88
 42 get CLTs for Markov chains, we can use a result of 89
 43 Kipnis and Varadhan (1986), which requires the chain 90
 44 to be reversible, as is the case for holds for Metropolis- 91
 45 Hastings chains, or we must delve into mixing condi- 92
 46 tions (Billingsley, 1995, Section 27), which are typ- 93
 47 ically not easy to verify. However, Chan and Geyer 94
 48 (1994) showed how the condition of geometric er- 95
 49 godicity could be used to establish CLTs for Markov 96
 50 chains. But getting the convergence is only half of the 97
 51 98

problem. In order to use (4), we must be able to con- 52
 sistentlly estimate the variance, which turns out to be 53
 another difficult endeavor. The “naïve” estimate of the 54
 usual standard error is not consistent in the dependent 55
 case and the most promising paths for consistent vari- 56
 ance estimates seems to be through regeneration and 57
 batch means. 58

The theory of regeneration uses the concept of 59
 a split chain (Athreya and Ney, 1978), and allows us 60
 to independently restart the chain while preserving 61
 the stationary distribution. These independent “tours” 62
 then allow the calculation of consistent variance esti- 63
 mates and honest monitoring of convergence through 64
 (4). Early work on applying regeneration to MCMC 65
 chains was done by Mykland, Tierney and Yu (1995) 66
 and Robert (1995), who showed how to construct the 67
 chains and use them for variance calculations and di- 68
 agnostics (see also Guihenneuc-Jouyaux and Robert, 69
 1998), as well as deriving adaptive MCMC algorithms 70
 (Gilks, Roberts and Sahu, 1998). Rosenthal (1995) 71
 also showed how to construct and use regenerative 72
 chains, and much of this work is reviewed in Jones 73
 and Hobert (2001). The most interesting and practi- 74
 cal developments, however, are in Hobert et al. (2002) 75
 and Jones et al. (2006), where consistent estimators are 76
 constructed for $\text{Var } h(X)$, allowing valid monitoring 77
 of convergence in chains that satisfy the CLT. Inter- 78
 estingly, although Hobert et al. (2002) use regenera- 79
 tion, Jones et al. (2006) get their consistent estimators 80
 thorough another technique, that of cumulative batch 81
 means. 82

83
 84 **6. CONCLUSION**

85
 86 The impact of Gibbs sampling and MCMC was to 87
 change our entire method of thinking and attacking 88
 problems, representing a *paradigm shift* (Kuhn, 1996). 89
 Now, the collection of real problems that we could 90
 solve grew almost without bound. Markov chain Monte 91
 Carlo changed our emphasis from “closed form” so- 92
 lutions to algorithms, expanded our impact to solving 93
 “real” applied problems and to improving numerical al- 94
 gorithms using statistical ideas, and led us into a world 95
 where “exact” now means “simulated.” 96

This has truly been a quantum leap in the evolution 97
 of the field of statistics, and the evidence is that there 98
 are no signs of slowing down. Although the “explo- 99
 sion” is over, the current work is going deeper into the- 100
 ory and applications, and continues to expand our hori- 101
 zons and influence by increasing our ability to solve 102
 even bigger and more important problems. The size

1 of the data sets, and of the models, for example, in
 2 genomics or climatology, is something that could not
 3 have been conceived 60 years ago, when Ulam and von
 4 Neumann invented the Monte Carlo method. Now we
 5 continue to plod on, and hope that the advances that
 6 we make here will, in some way, help our colleagues
 7 60 years in the future solve the problems that we can-
 8 not yet conceive.

9
 10 **APPENDIX: WORKSHOP ON**
 11 **BAYESIAN COMPUTATION**

12 This section contains the program of the Workshop
 13 on *Bayesian Computation via Stochastic Simulation*,
 14 held at Ohio State University, February 15–17, 1991.
 15 The organizers, and their affiliations at the time, were
 16 Alan Gelfand, University of Connecticut, Prem Goel,
 17 Ohio State University, and Adrian Smith, Imperial Col-
 18 lege, London.

19 • *Friday, Feb. 15, 1991.*

20
 21 (a) Theoretical Aspect of Iterative Sampling, Chair:
 22 Adrian Smith.

23 (1) Martin Tanner, University of Rochester:
 24 *EM, MCEM, DA and PMDA.*

25 (2) Nick Polson, Carnegie Mellon University:
 26 *On the Convergence of the Gibbs Sampler and*
 27 *Its Rate.*

28 (3) Wing-Hung Wong, Augustin Kong and
 29 Jun Liu, University of Chicago: *Correlation*
 30 *Structure and Convergence of the Gibbs Sam-*
 31 *pler and Related Algorithms.*

32 (b) Applications—I, Chair: Prem Goel.

33 (1) Nick Lange, Brown University, Brad Car-
 34 lin, Carnegie Mellon University and Alan
 35 Gelfand, University of Connecticut: *Hierarchi-*
 36 *cal Bayes Models for Progression of HIV Infec-*
 37 *tion.*

38 (2) Cliff Litton, Nottingham University, Eng-
 39 land: *Archaeological Applications of Gibbs*
 40 *Sampling.*

41 (3) Jonas Mockus, Lithuanian Academy of
 42 Sciences, Vilnius: *Bayesian Approach to Global*
 43 *and Stochastic Optimization.*

44
 45 • *Saturday, Feb. 16, 1991.*

46 (a) Posterior Simulation and Markov Sampling,
 47 Chair: Alan Gelfand.

48 (1) Luke Tierney, University of Minnesota:
 49 *Exploring Posterior Distributions Using Markov*
 50 *Chains.*

(2) Peter Mueller, Purdue University: *A Ge-*
 51 *neric Approach to Posterior Integration and*
 52 *Bayesian Sampling.*

(3) Andrew Gelman, University of Califor-
 53 nia, Berkeley and Donald P. Rubin, Harvard
 54 University: *On the Routine Use of Markov*
 55 *Chains for Simulations.*

(4) Jon Wakefield, Imperial College, London:
 56 *Parameterization Issues in Gibbs Sampling.*

(5) Panickos Palettas, Virginia Polytechnic
 57 Institute: *Acceptance–Rejection Method in Pos-*
 58 *terior Computations.*

59 (b) Applications—II, Chair: Mark Berliner.

(1) David Stephens, Imperial College, Lon-
 60 don: *Gene Mapping via Gibbs Sampling.*

(2) Constantine Gatsonis, Harvard Univer-
 61 sity: *Random Efleeds Model for Ordinal Cate-*
 62 *gorica! Data with an Application to ROC Analy-*
 63 *sis.*

(3) Arnold Zellner, University of Chicago,
 64 Luc Bauwens and Herman Van Dijk: *Bayesian*
 65 *Specification Analysis and Estimation of Simul-*
 66 *taneous Equation Models Using Monte Carlo*
 67 *Methods.*

68 (c) Adaptive Sampling, Chair: Carl Morris.

(1) Mike Evans, University of Toronto and
 69 Carnegie Mellon University: *Some Uses of*
 70 *Adaptive Importance Sampling and Chaining.*

(2) Wally Gilks, Medical Research Council,
 71 Cambridge, England: *Adaptive Rejection Sam-*
 72 *pling.*

(3) Mike West, Duke University: *Mixture*
 73 *Model Approximations, Sequential Updating*
 74 *and Dynamic Models.*

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 90 • *Sunday, Feb. 17, 1991.*

(a) Generalized Linear and Nonlinear Models,
 91 Chair: Rob Kass.

(1) Ruey Tsay and Robert McCulloch, Uni-
 92 versity of Chicago: *Bayesian Analysis of Autore-*
 93 *gressive Time Series.*

(2) Christian Ritter, University of Wisconsin:
 94 *Sampling Based Inference in Non Linear Re-*
 95 *gression.*

(3) William DuMouchel, BBN Software, Bos-
 96 ton: *Application of the Gibbs Sampler to Vari-*
 97 *ance Component Modeling.*

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(4) James Albert, Bowling Green University and Sidhartha Chib, Washington University, St. Louis: *Bayesian Regression Analysis of Binary Data*.

(5) Edwin Green and William Strawderman, Rutgers University: *Bayes Estimates for the Linear Model with Unequal Variances*.

(b) Maximum Likelihood and Weighted Bootstrapping, Chair: George Casella.

(1) Adrian Raftery and Michael Newton, University of Washington: *Approximate Bayesian Inference by the Weighted Bootstrap*.

(2) Charles Geyer, University of Chicago: *Monte Carlo Maximum Likelihood via Gibbs Sampling*.

(3) Elizabeth Thompson, University of Washington: *Stochastic Simulation for Complex Genetic Analysis*.

(c) Panel Discussion—Future of Bayesian Inference Using Stochastic Simulation, Chair: Prem Gael.

- Panel—Jim Berger, Alan Gelfand and Adrian Smith.

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