# Computing Bayes: Bayesian Computation from 1763 to the 21st Century[*]

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## Abstract

The Bayesian statistical paradigm uses the language of probability to express uncertainty about the phenomena that generate observed data. Probability distributions thus characterize Bayesian inference, with the rules of probability used to transform *prior* probability distributions for all unknowns - models, parameters, latent variables - into *posterior* distributions, subsequent to the observation of data. Conducting Bayesian inference requires the evaluation of integrals in which these probability distributions appear. Bayesian *computation* is all about evaluating such integrals in the typical case where no analytical solution exists. This paper takes the reader on a chronological tour of Bayesian computation over the past two and a half centuries. Beginning with the one-dimensional integral first confronted by Bayes in 1763, through to recent problems in which the unknowns number in the millions, we place all computational problems into a common framework, and describe all computational methods using a common notation. The aim is to help new researchers in particular - and more generally those interested in adopting a Bayesian approach to empirical work - make sense of the plethora of computational techniques that are now on offer; understand when and why different methods are useful; and see the links that do exist, between them all.

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# 1 The Beginning

*December 23 1763: London.* Richard Price reads to the Royal Society a paper penned by a past Fellow, the late Thomas Bayes:

'*An Essay Towards Solving a Problem in the Doctrine of Chances.*'

With that reading, the concept of 'inverse probability' - *Bayesian inference* as we know it now - has its first public airing.

To our modern eyes, the problem tackled by Bayes in his essay is a simple one: If one performs $n$ independent Bernoulli trials, with a probability, $\theta$, of success on each trial, what is the probability - given $n$ outcomes - of $\theta$ lying between two values, $a$ and $b$? The answer Bayes offered is equally simple to re-cast in modern terminology. Define $Y_i \sim i.i.d.\ Bernoulli(\theta)$, $i = 1, 2, ..., n$; record the observed sequence of successes ($Y_i = 1$) and failures ($Y_i = 0$) as $\mathbf{y} = (y_1, y_2, ..., y_n)'$; denote by $L(\theta|\mathbf{y}) \propto p(\mathbf{y}|\boldsymbol{\theta})$ the likelihood function for $\theta$; and invoke a uniform prior, $p(\theta)$, on the interval $(0, 1)$. Bayes sought:

$$P(a < \theta < b|\mathbf{y}) = \int_a^b p(\theta|\mathbf{y})d\theta, \tag{1}$$

where $p(\theta|\mathbf{y})$ denotes the posterior probability density function (pdf) for $\theta$,

$$p(\theta|\mathbf{y}) = \frac{L(\theta|\mathbf{y})p(\theta)}{p(\mathbf{y})}, \tag{2}$$

$p(\mathbf{y}) = \int_0^1 L(\theta|\mathbf{y})p(\theta)d\theta$ defines the marginal likelihood, and the scale factor $[p(\mathbf{y})]^{-1}$ in (2) ensures that $p(\theta|\mathbf{y})$ integrates to one. Given the Bernoulli assumption for $Y$, the uniform prior on $\theta$, and defining $x = \Sigma_{i=1}^n y_i$, $p(\theta|\mathbf{y})$ has a closed-form representation as the beta pdf,

$$p(\theta|\mathbf{y}) = [B(x + 1, n - x + 1)]^{-1} \theta^x(1 - \theta)^{n-x}, \tag{3}$$

where $B(x + 1, n - x + 1) = \Gamma(x + 1)\Gamma(n - x + 1)/\Gamma(n + 2) = \int_0^1 \theta^x(1 - \theta)^{n-x}d\theta$ is the beta function, and $\Gamma(x)$ is the gamma function. *Bayesian inference* - namely, quantification of uncertainty about an unknown $\theta$, conditioned on known data, $\mathbf{y}$ - thus first emerges as the analytical solution to a particular inverse probability problem.[1]

Bayes, however, did not seek the pdf in (3) *per se.* Rather, he sought to evaluate the probability in (1) which, for either $a \neq 0$ or $b \neq 1$, involved evaluation of the *incomplete* beta function. Except for the case when either $x$ or $(n - x)$ were small, a closed-form solution to (1) eluded Bayes. Hence, along with the elegance of (2) - *Bayes' theorem* as it is now known - and the availability of the analytical expression in (3), came the need to approximate, or *compute*, the quantity of interest in (1). The quest for a computational solution to a Bayesian problem was thus born.

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[1] Bayes expressed this problem in terms of its equivalent representation as one of deriving the probability of $a < \theta < b$ conditional on the value of $x$, where $X \sim Bin(n, \theta)$. We have chosen to denote the conditioning values explicitly as a *sample* of n (Bernoulli) observations, $\mathbf{y}$, in order to establish the notation $p(\theta|\mathbf{y})$ from the outset. Due to the sufficiency of $x$, $p(\theta|x)$ is of course equivalent to $p(\theta|\mathbf{y})$. Bayes also cast this problem in physical terms: as one in which balls were rolled across a square table, or plane. Over time his pictorial representation of the problem has come to be viewed as a 'billiard table', despite Bayes making no overt reference to such an item in his essay. For this, and other historical anecdotes, see Stigler (1986a) and Fienberg (2006).

# 2 Bayesian Computation in a Nutshell

## 2.1 Statement of the General Bayesian Computational Problem

Bayes' probability of interest in (1) can be re-expressed as a posterior expectation, $E(\mathcal{I}_{(a<\theta<b)}|\mathbf{y}) = \int_\Theta \mathcal{I}_{(a<\theta<b)}p(\theta|\mathbf{y})d\theta$, where $\mathcal{I}_{(a<\theta<b)}$ equals 1 if $a < \theta < b$, and equals 0 otherwise. This representation is insightful, as it reminds us that any integral evaluated with respect to a probability measure, like $dP = p(\theta|\mathbf{y})d\theta$, can be viewed as the expectation of a particular function of $\theta$; $\mathcal{I}_{(a<\theta<b)}$ in this case. Generalizing at this point to any problem with unknown $\boldsymbol{\theta} = (\theta_1, \theta_2, ..., \theta_p)' \in \Theta$ and joint posterior pdf $p(\boldsymbol{\theta}|\mathbf{y})$, virtually all Bayesian quantities of interest can be similarly expressed as posterior expectations, some familiar examples being: $E(\boldsymbol{\theta}|\mathbf{y}) = \int_\Theta \boldsymbol{\theta}p(\boldsymbol{\theta}|\mathbf{y})d\boldsymbol{\theta}$, $Var(\boldsymbol{\theta}|\mathbf{y}) = \int_\Theta [\boldsymbol{\theta} - E(\boldsymbol{\theta}|\mathbf{y})][\boldsymbol{\theta} - E(\boldsymbol{\theta}|\mathbf{y})]'p(\boldsymbol{\theta}|\mathbf{y})d\boldsymbol{\theta}$, $p(\theta_1^*|\mathbf{y}) = \int_\Theta p(\theta_1^*|\theta_2, ..., \theta_p, \mathbf{y})p(\boldsymbol{\theta}|\mathbf{y})d\boldsymbol{\theta}$ (at some point $\theta_1^*$ in the support of $p(\theta_1|\mathbf{y})$), and $p(y_{n+1}^*|\mathbf{y}) = \int_\Theta p(y_{n+1}^*|\boldsymbol{\theta}, \mathbf{y})p(\boldsymbol{\theta}|\mathbf{y})d\boldsymbol{\theta}$ (with $y_{n+1}^*$ a point in the support of the 'out-of-sample' random variable, $y_{n+1}$). This leads us to make the following statement:

*The general Bayesian computational problem is that of computing an expectation of the form*

$$E(g(\boldsymbol{\theta})|\mathbf{y}) = \int_\Theta g(\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{y})d\boldsymbol{\theta}, \tag{4}$$

*for some $g(\boldsymbol{\theta})$, in the typical case where the expectation has no closed-form solution.*

Even in cases where the quantity of interest is not immediately of this form, typically *underpinning* the computation of such quantities is the numerical evaluation of some form of posterior expectation. Hence, we are justified in viewing any computational method as a means of providing a numerical solution to (4), whether this solution is the final goal of the investigation, or not.[2]

## 2.2 The Scope of this Review

The need for numerical computation arises simply because analytical solutions to (4) are rare. Indeed, Bayes' original problem highlights that such solutions can elude us even when the posterior pdf itself has a closed form. Typically, the move from the generative problem (the specification of $p(\mathbf{y}|\boldsymbol{\theta})$) to the inverse problem (the production of $p(\boldsymbol{\theta}|\mathbf{y})$), yields a posterior pdf for $\boldsymbol{\theta}$ that is known *only* up to a constant of proportionality, as

$$p(\boldsymbol{\theta}|\mathbf{y}) \propto L(\boldsymbol{\theta}|\mathbf{y})p(\boldsymbol{\theta}). \tag{5}$$

Exceptions to this rule include the case where $p(\mathbf{y}|\boldsymbol{\theta})$ is from the exponential family, and either a natural conjugate, or convenient noninformative, prior is adopted (as was the case for Bayes' problem, for example). The availability of $p(\boldsymbol{\theta}|\mathbf{y})$ only up to the integrating constant immediately precludes the analytical solution of (4), for any $g(\boldsymbol{\theta})$. Situations where $p(\mathbf{y}|\boldsymbol{\theta})$, itself, is unavailable in closed form render the analytical solution of (4) an even more distant dream. Hence the need for *computational* solutions.

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[2]For example, Bayesian decision theory (Berger, 1985) involves the optimization of a utility or loss function to produce an optimal procedure; but this most often involves a quantity represented as a posterior expectation.

Despite their large number, it is useful to think about all Bayesian computational techniques falling into one or more of three broad categories:

1) *Deterministic integration methods*

2) *Simulation methods*

3) *Approximation (including asymptotic) methods*

In brief, the methods in *1)* define $L$ grid-points, $\boldsymbol{\theta}_1$, $\boldsymbol{\theta}_2, ..., \boldsymbol{\theta}_L$, to span the support of $\boldsymbol{\theta}$, compute $g(\boldsymbol{\theta}_l)p(\boldsymbol{\theta}_l|\mathbf{y})$, for $l = 1, 2, ..., L$, and estimate (4) as a weighted sum of these $L$ values of the integrand. Different deterministic numerical integration (or quadrature) rules are based on different choices for $\boldsymbol{\theta}_l$, $l = 1, 2, ..., L$, and different formulae for the weights. The methods in *2)* use simulation to produce $M$ posterior draws of $g(\boldsymbol{\theta})$, $g(\boldsymbol{\theta}^{(i)})$, $i = 1, 2, ..., M$, a (weighted) mean of which is used to estimate (4). Different simulation methods are distinguished by the way in which the draws are produced and weighted. Finally, the methods in *3)* involve replacing the integrand in (4) with an approximation of some sort, and evaluating the resultant integral. Different approximation methods are defined by the choice of replacement for the integrand, with the nature of this replacement determining the way in which the final integral is computed. In particular, certain approximate methods use simulation to evaluate the resultant integral. *Asymptotic* approximation methods replace the integrand with an expansion that is accurate for large $n$, and yield an estimate of (4) (via analytical means) that is accurate asymptotically.

Conditional on unlimited computing power (i.e. the ability to allow $L$ and $M$ to be arbitrarily large) the methods in *1)* and *2)* yield estimates of (4) that are essentially *exact*. The accuracy of the methods in *3)* is determined by the accuracy of the approximation of the integrand and, for the asymptotic versions, the size of $n$. For instance, a simulation method such as Markov chain Monte Carlo (MCMC) is an example of *2)* and viewed as 'exact' in the sense described here, whilst variational Bayes methods are examples of *3)* and are viewed as inherently approximate.

In the sections that follow we make reference, where helpful, to the category (or categories) into which a particular computational method falls. However, the over-arching structure that we adopt is primarily one of chronology, as understanding *when* a computational method has appeared aids in the appreciation of *why*. Statistics is an inherently practical science and, hence, the nature of the empirical imperatives, the accessibility of data, and the state of technology all determine both what is desired, and what is possible, in a statistical method. All such things change over time; hence the need to place the evolution of computational methods in some sort of historical context. Importantly, we give particular focus to computational developments that have ultimately been linked to the need to solve Bayesian problems. Hence, whilst deterministic numerical integration remains an important tool in the Bayesian arsenal, and despite the recent explosion of probabilistic numerics creating new connections between Bayesian concepts and numerical integration (Briol *et al.*, 2019), we make scant reference to developments in *1)*.[3] Instead, our focus is primarily on the techniques in categories *2) and 3)* that have either had their genesis within, or been transformational for, Bayesian inference.

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[3]We refer to Davis and Rabinowitz (1975) for a review of deterministic integration techniques; to Naylor and Smith (1982) for application of such techniques to Bayesian problems; and to Vanslette et al. (2019) for a recent comparison of quadrature- and simulation-based methods of integration.

To render the scope of the paper manageable, we state (4), and all computational solutions to it, in terms of a *finite* set of unknowns in a *parametric* model, $p(\boldsymbol{y}|\boldsymbol{\theta})$, and do not attempt to review Bayesian computation in nonparametric settings.[4] With a similar motivation, we do not cover the large and important literature on *sequential Monte Carlo (SMC)* methods, other than making brief references to it, most notably when discussing pseudo-marginal MCMC techniques.[5] Nor do we discuss either the Bayesian bootstrap (Rubin, 1981) or Bayesian optimization (Gutmann and Corander, 2016; Frazier, 2018).

Finally, we note that framing the general Bayesian computational problem in terms of calculating a quantity like (4) is standard practice, and reviews that focus on *specific* ways of completing this task abound (and will indeed be referenced herein). What we do here, instead, is to bring together in one place, and using a common notation, a wide array of techniques for computing (4) that have evolved since the reading (and subsequent publication) of Bayes' paper. In so doing we aim to impose some coherence on an expanding and increasingly fragmented literature; and to do so in a way that makes clear the rationale for - and relationship between - distinct methods; all within a broad historical context. Excessive formalism, and extensive technical detail, is avoided in order to make the paper as accessible as possible, in particular to new researchers whose knowledge of Bayesian inference and computation is not comprehensive. Whilst our referencing is reasonably thorough, to keep the size of the paper within bounds we have still been selective; directing readers to key review papers, handbook chapters and other texts, for a more complete coverage of published work. We also defer to these other resources - in particular recent review papers - for a complete coverage of the dedicated software that is available for implementing specific computational methods.[6]

## 2.3 The Structure of this Review

We begin, in Section 3, by returning to Bayes' integral in (1), and briefly discussing the nature of the computational problem. We then use this as a springboard for pinpointing *four* particular points in time during the two centuries (or so) subsequent to 1763: 1774, 1953, 1964 and 1970. These time points correspond, in turn, to *four* publications - by Laplace, Metropolis *et al.,* Hammersley and Handscomb, and Hastings, respectively - in which computational methods that produce estimates of integrals like that of Bayes, were proposed. Whilst only the method of Laplace was set within the explicit context of 'inverse probability' (or Bayesian inference), all four methods of computing integrals can be viewed as harbingers of what was to come in Bayesian computation *per se*.

In Section 4, we look at Bayesian computation in the last three decades of the 20th century. As will be seen, all three categories of technique delineated above - deterministic integration, simulation, and (asymptotic) approximation - featured in these three decades. However, the inexorable rise in the speed, and accessibility, of computers led to *simulation* methods, most notably *importance sampling* and

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[4]See Ghosal and Van der Vaart (2017) for a thorough coverage of computation in that sphere.

[5]We direct the reader to Naesseth et al. (2019) for a comprehensive review of SMC methods, in which all seminal work is cited and discussed.

[6]We draw the attention of readers at this point to Green et al. (2015), whose review of computational methods is also quite broad. Our paper, however, in addition to differing in style and scope from that of Green et al., has different goals. It is deliberately designed: both as an entry point into the field for researchers who are not expert in Bayesian techniques, and as an accessible historical overview of Bayesian computation for all who may be interested.

*MCMC sampling*, becoming increasing dominant. This set the stage for what we (as have others before us!) refer to as the first computational *revolution*. Whilst significant advances were made in econometrics (Kloek and van Dijk, 1978; Bauwens and Richard, 1985, Geweke, 1989a) and signal processing (Gordon et al., 1993), using the principles of importance sampling, the 'revolution' was driven primarily by MCMC algorithms. As many treatments of Bayesian computation have covered this late part of the 20th century, we keep our coverage of this period very brief, deferring certain details to more specialized reviews and seminal articles. Our main aim in Section 4 is to alert the reader to (or to remind them of) the key principles underpinning the techniques developed over this period, and the features of the data generating process (DGP) that are required in order to actually *implement* these techniques. This then provides a context for subsequent computational developments.

The coverage in Section 5 - of what may be viewed as a *second computational revolution* - is more extensive, given that we attempt to bring together in one place, and using a common framework and notation, the large variety of computational methods that have evolved during the 21st century. We begin with *pseudo-marginal* methods, including particle MCMC, before covering the main *approximate* methods: approximate Bayesian computation (ABC), Bayesian synthetic likelihood (BSL), variational Bayes (VB) and integrated nested Laplace (INLA). Our primary goal here is to link the development of these new computational techniques, in particular those that aim only for an approximate solution to the Bayesian problem, to the increased complexity - and size - of the empirical problems being analyzed. Section 5 is completed by a brief review of important modifications and refinements of MCMC that have occurred since its initial appearance, including Hamiltonian up-dates, adaptive sampling, and coupling; developments that are, again, motivated by the challenges presented by modern problems, most notably, the need to process huge data sets and/or to infer high-dimensional unknowns. We round off the review in Section 6 by switching focus from parameter inference to model choice and prediction, and to the role of computation therein. We then end the paper with Section 7, bravely entitled: 'The Future', in which the key computational challenges that remain, and the directions in which solutions to those challenges are being sought, are articulated.[7]

## 3 The First 200-Odd Years of Bayesian Computation: 1763 to 1970

### 3.1 Bayes' Integral

Bayes' desire was to evaluate the probability in (1). As noted above, for either $a \neq 0$ or $b \neq 1$, this required evaluation of the incomplete beta function. For either $x$ or $(n - x)$ small, Bayes proposed a binomial expansion and term-by-term integration to give an exact solution (his 'Rule 1'). However, for $x$ and $(n-x)$ both large, this approach was infeasible: prompting Bayes (and, subsequently, Price himself)[8] to resort to producing upper and lower bounds for (1) using quadrature. Indeed, Stigler (1986a, p. 130) speculates that the inability to produce an approximation to (1) that was sufficiently accurate may

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[7]We acknowledge a degree of arbitrariness in how we have chosen to signal key developments in computation between 1763 and the present: the particular historical publications we have chosen to highlight, and the moments in time we identify as sparking 'computational revolutions'. However, any historical narrative requires chronological signposts! We have selected ones we believe to be broadly sensible and, hopefully, not too controversial.

[8]Price (1764).

explain Bayes' reluctance to publish his work and, perhaps, the lack of attention it received subsequent to its (posthumous) presentation by Price and publication in Bayes (1764).[9]

Whilst the integral that Bayes wished to compute was a very particular one, it was representative of the general hurdle that needed to be overcome if the principle of inverse probability were to be a useful practical tool. In brief, inference about $\theta$ was expressed in probabilistic terms and, hence, required either the direct computation of probability intervals, or the computation of distributional moments of some sort. Ironically, the choice of the Bernoulli model, possibly the simplest process for generating data 'forward' (conditional on $\theta$) that Bayes could have assumed, exacerbated this problem, given that the 'inversion' problem does not possess the simplicity of the generative problem. What was required was a solution that was, in large measure, workable no matter what the nature of the generative model, and the first solution came via the 1774 *'Mémoire sur la probabilité des causes par les événemens'* by Pierre Laplace.

## 3.2 1774: The Asymptotic Approximation Method of Laplace

The remarkable contributions of Laplace to the fields of probability and statistics - including his first statement of the central limit theorem - have been documented (e.g. Stigler, 1975, 1986a). We focus here on only two of those contributions: *i)* his independent discovery of the concept of inverse probability, and *ii)* his proposed normal asymptotic approximation to a posterior distribution. Both contributions first appeared in Laplace (1774) and, somewhat ironically, given his apparent lack of knowledge of Bayes' prior work, were articulated in the context of the binomial problem.[10]

Laplace envisaged an experiment in which $n$ tickets were drawn with replacement from an urn containing a given proportion of white and black tickets. Recasting his analysis in our notation, $\theta$ is the probability of drawing a white ticket, $\mathbf{y} = (y_1, y_2, ..., y_n)'$ denotes the sequence of white tickets ($Y_i = 1$) and black tickets ($Y_i = 0$) in the $n$ independent draws of $Y$, and $x = \Sigma_{i=1}^n y_i$ is the number of white tickets drawn. Laplace's aim was to show that, for arbitrary $w$: $P(\left|\frac{x}{n} - \theta\right| < w|\mathbf{y}) = P(\frac{x}{n} - w < \theta < \frac{x}{n} + w|\mathbf{y}) \to 1$ as $n \to \infty$. That is, Laplace wished to demonstrate *posterior consistency*: concentration of the posterior onto the true proportion of white tickets in the urn, $\theta_0 = \lim_{n \to \infty} \frac{x}{n}$. Along the way, however, he stumbled upon the same problem as had Bayes: computing the following probability of a beta random variable,

$$P(a < \theta < b|\mathbf{y}) = [B(x+1, n-x+1)]^{-1} \int_a^b \theta^x (1-\theta)^{n-x} d\theta, \tag{6}$$

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[9]On November 10, 1763, Price sent an edited and annotated version of Bayes' essay to the Secretary of the Royal Society, with his own Appendix added. Price read the essay to the Society on December 23, as noted earlier. The essay and appendix were subsequently published in 1764, in the *Philosophical Transactions of the Royal Society of London*. The front matter of the issue appears here: https://royalsocietypublishing.org/cms/asset/f005dd95-c0f8-45b2-8347-0296a93c4272/front.pdf. The publication has been reprinted since, including in Barnard and Bayes (1958), with a biographical note by G.A. Barnard. Further historical detail on the important role played by Price in the dissemination of Bayes' ideas can be found in Hooper (2013) and Stigler (2018).

[10]See Stigler (1975), Stigler (1986a), Stigler (1986b) and Fienberg (2006) on this matter of attribution. The first recorded reference to Bayes' prior claim to inverse probability is in the preface, written by Condorcet, to Laplace's later 1781 publication: *'Mémoire sur la probabilité'*. Stigler (1975, Section 2) states that he has found no documentary evidence that Laplace's ideas on inverse probability, as presented in the 1774 publication, including his own statement of 'Bayes' theorem' in (2), were informed by Bayes' earlier ideas. See Stigler (1986a, Chapter 3) for discussion of Laplace's later extensions of Bayes' theorem to the case of a nonuniform prior.

with $a = \frac{x}{n} - w \neq 0$ and $b = \frac{x}{n} + w \neq 1$. Laplace's genius (allied with the power of asymptotics!) was to recognize that the exponential of the integrand in (6) has the bulk of its mass in the region of its mode, as $n$ gets large, and that the integral can be computed in closed form in this case. This enabled him to prove (in modern notation) that $P(|\theta_0 - \theta| > w|\mathbf{y}) = o_p(1)$, where $p$ denotes the probability law for $\mathbf{y}$.

The route he took to this proof, however, involved approximating the beta posterior with a normal distribution, which (under regularity) is an approach that can be used to provide a large sample approximation of virtually *any* posterior probability. Specifically, express an *arbitrary posterior probability* as

$$P(a < \theta < b|\mathbf{y}) = \int_a^b p(\theta|\mathbf{y})d\theta = \int_a^b \exp\{nf(\theta)\}\,d\theta, \tag{7}$$

where $f(\theta) = \log\left[p(\theta|\mathbf{y})\right]/n$, and assume appropriate regularity for $L(\theta|\mathbf{y})$ and $p(\theta)$. What is now referred to as the *Laplace asymptotic approximation* involves first taking a second-order Taylor series approximation of $f(\theta)$ around its mode, $\widehat{\theta}$: $f(\theta) \approx f(\widehat{\theta}) + \frac{1}{2}f''(\widehat{\theta})(\theta - \widehat{\theta})^2$.[11] Defining $\sigma^2 = -[nf''(\widehat{\theta})]^{-1}$, and substituting the expansion into (7) then yields

$$\begin{aligned} P(a < \theta < b|\mathbf{y}) &\approx \exp\left\{nf(\widehat{\theta})\right\} \int_a^b \exp\left\{-\frac{1}{2\sigma^2}(\theta - \widehat{\theta})^2\right\}d\theta \\ &= \exp\left\{nf(\widehat{\theta})\right\}\sqrt{2\pi\sigma^2} \times \{\Phi[\tfrac{b-\widehat{\theta}}{\sigma}] - \Phi[\tfrac{a-\widehat{\theta}}{\sigma}]\}, \end{aligned} \tag{8}$$

where $\Phi(.)$ denotes the standard normal cumulative distribution function (cdf).[12]

Laplace had thus devised a general way of implementing inverse probability: probabilistic statements about an unknown parameter, $\theta$, conditional on data generated from any (regular) model, could now be made, at least up to an error of approximation. Whilst his focus was solely on the computation of a specific posterior probability, and in a single parameter setting, his method was eventually used to approximate general posterior expectations of the form in (4) (Lindley, 1980; Tierney and Kadane, 1986; Tierney et al., 1989) and, indeed, applied as an integral approximation method in its own right (De Bruijn, 1961). The approach also underpins the modern INLA technique to be discussed in Section 5.3.4 (Rue et al., 2009).

Meanwhile, it would take 170-odd years for the *next* major advance in the computation of probability integrals to occur; an advance that would eventually transform the way in which problems in inverse probability could be tackled. This development was based on a new form of thinking and, critically, required a platform on which such thinking could operate: namely, machines that could *simulate* repeated random draws of $\boldsymbol{\theta}$ from $p(\boldsymbol{\theta}|\mathbf{y})$, or from some representation thereof. Given a sufficient number of such draws, and the correct use of them, an estimate of (4) could be produced that - unlike the Laplace approximation - would be accurate for any sample size, $n$, and would require less analytical input. This potential to accurately estimate (4) for essentially any problem, and any given sample size, was the

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[11]Where we have assumed that $f'(\widehat{\theta}) = 0$.

[12]Of course, buried within the symbol $\approx$ above is a rate of convergence that is a particular order of $n$, and is probabilistic if randomness in $\mathbf{y}$ is acknowledged. We refer to reader to Tierney and Kadane (1986) and Robert and Casella (2004) for demonstrations of the error in the approximation in (8). We refer to Ghosal et al. (1995) and van der Vaart (1998) for more formal demonstrations of the conditions under which a posterior distribution converges in probability to a normal distribution, and the so-called Bernstein-von Mises theorem - the modern day version of Laplace's 1774 approximation - holds.

catalyst for a flourishing of Bayesian inference in the late 20th century and beyond. The 1953 publication in the *Journal of Chemical Physics* by Metropolis, Rosenbluth, Rosenbluth, Teller and Teller: *'Equation of State Calculations by Fast Computing Machines'*, was the first major step in this journey.[13]

## 3.3  1953: Monte Carlo Simulation and the Metropolis Algorithm

The convergence of: the idea of simulating random draws from a probability distribution, and the production of such draws by computing machines, occurred in the scientific hothouse of the Los Alamos Laboratory, New Mexico, in the 1940s and 1950s; the primary impetus being the need to simulate physical processes, including neutrons in the fissile material in atomic bombs. We refer the reader to Liu (2001), Hitchcock (2003) and Robert and Casella (2011) for reviews of this period, including details of the various personalities who played a role therein.[14] Our focus here is simply on the nature of the problem that was at the heart of Metropolis et al. (1953), the solution proposed, and the ultimate importance of that solution to Bayesian computation.

In short, the authors wished to compute an expectation of the form,

$$E(g(\mathbf{x})) = \int_{\mathcal{X}} g(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}, \tag{9}$$

where $p(\mathbf{x})$ denotes the so-called Boltzmann distribution of a set, $\mathbf{x}$, of $N$ particles on $\mathbb{R}^2$. (See Robert and Casella, 2011, Section 2.1, for all details.) Two particular characteristics of (9) are relevant to us here: *i)* the integral is of very high dimension, $2N$, with $N$ large; and *ii)* $p(\mathbf{x})$ is generally known only up to its integrating constant. The implication of *i)* is that a basic rectangular integration method, based on $L$ grid-points in each of the $2N$ directions, is infeasible, having a computational burden of $L^{2N}$ or, equivalently, an approximation error of $O(L^{-1/2N})$.[15] The implication of *ii)* is that a Monte Carlo (MC) estimate of (9), based on $M$ *i.i.d.* direct draws from $p(\mathbf{x})$, $\mathbf{x}^{(i)}$, $i = 1, 2, ..., M$:

$$\widehat{E}_{MC}(g(\mathbf{x})) = \frac{1}{M} \sum_{i=1}^{M} g(\mathbf{x}^{(i)}),$$

with approximation error of $O(M^{-1/2})$ independent of dimension, is not available.[16]

Features *i)* and *ii)* - either individually or in tandem - broadly characterize the posterior expectations in (4) that are the focus of this review. Hence, the relevance to Bayesian computation of the solution offered by Metropolis et al. (1953) to the non-Bayesian problem in (9); and we describe their solution with direct reference to (4) and the notation used therein.

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[13]With reference to the mechanical simulation of a random variable, we acknowledge the earlier 1870s' invention of the *quincunx* by Francis Galton. This machine used the random dispersion of metal shot to illustrate (amongst other things) draws from a hierarchical normal model and regression to the mean. Its use can thus be viewed as the first illustration of the conjugation of a normal likelihood and a normal prior. See Stigler (1986a) for more details, including Galton's graphical illustration of his machine in a letter to his cousin (and Charles Darwin's son), George Darwin.

[14]For instance, the respective contributions of the five authors of the 1953 paper (who included two married couples) are the source of some controversy.

[15]See Kloek and van Dijk (1978) for further discussion.

[16]The authors actually make mention of a *naive* Monte Carlo method, based on *uniform* sampling over the $2N$ dimensional space, followed by a reweighting of the uniform draws by a kernel of $p(\mathbf{x})$. The idea is dismissed, however, as 'not practical'. In modern parlance, whilst this method would yield an $O(M^{-1/2})$ approximation error, the constant term within the order would be large, since the uniform distribution used to produce draws of $\mathbf{x}$ differs substantially from the *actual* distribution of $\mathbf{x}$, $p(\mathbf{x})$.

Specifically, the authors advocate computing an integral such as (4) via the *simulation* of a *Markov chain:* $\boldsymbol{\theta}^{(i)}$, $i = 1, 2, ..., M$, with *invariant distribution* $p(\boldsymbol{\theta}|\mathbf{y})$. The draw at iteration $i+1$ in the chain is created by taking the value at the *ith* iteration, $\boldsymbol{\theta}^{(i)}$, and perturbing it according to a random walk: $\boldsymbol{\theta}^c = \boldsymbol{\theta}^{(i)} + \delta\boldsymbol{\varepsilon}$, where each element of $\boldsymbol{\varepsilon}$ is drawn independently from $U(-1, 1)$, and $\delta$ 'tunes' the algorithm.[17] The 'candidate' draw $\boldsymbol{\theta}^c$ is accepted as draw $\boldsymbol{\theta}^{(i+1)}$ with probability:

$$\alpha = \min\{p^*(\boldsymbol{\theta}^c|\mathbf{y})/p^*(\boldsymbol{\theta}^{(i)}|\mathbf{y}), 1\}, \tag{10}$$

where $p^*$ is a kernel of $p$. Subject to convergence to $p(\boldsymbol{\theta}|\mathbf{y})$ (conditions for which were verified by the authors for their particular problem) the dependent sequence of draws in this *Markov chain* can be used to estimate (4) as the sample mean,

$$\overline{g(\boldsymbol{\theta})} = \frac{1}{M}\sum_{i=1}^{M} g(\boldsymbol{\theta}^{(i)}), \tag{11}$$

and an appropriate weak law of large numbers (WLLN) and central limit theorem (CLT) invoked to prove $\sqrt{M}$-consistency of the estimator. (See Geyer, 2011b, for details.)

Due to the (positive) autocorrelation in the Markov chain, the variance of the Metropolis estimator (as it would become known) is larger than that of the (infeasible) MC estimate, computed as in (11), but using $i.i.d$ draws from $p(\boldsymbol{\theta}|\mathbf{y})$, namely:

$$\sigma^2_{MC} = Var(g(\boldsymbol{\theta}))/M, \tag{12}$$

expressed here for the case of scalar $g(\boldsymbol{\theta})$. However, as is clear from (10), the Metropolis MCMC algorithm requires knowledge of $p(\boldsymbol{\theta}|\mathbf{y})$ only up to the normalizing constant, and does *not* require direct simulation from $p(\boldsymbol{\theta}|\mathbf{y})$ itself. It is this particular feature that would lend the technique its great power in the decades to come.[18]

### 3.4    1964: Importance Sampling: Hammersley and Handscomb

The obviation of the need to directly sample from $p(\boldsymbol{\theta}|\mathbf{y})$ also characterizes importance sampling, and underlies its eventual importance in solving difficult Bayesian computational problems. Nevertheless, Hammersley and Handscomb (1964) did not emphasize this feature but, rather, introduced the concept of importance sampling (IS) for the express purpose of variance reduction in simulation-based estimation of integrals.[19] Again, the focus was not on Bayesian integrals, but we describe the method in that setting.

In brief, given an 'importance' (or 'proposal') density, $q(\boldsymbol{\theta}|\mathbf{y})$, that preferably mimics $p(\boldsymbol{\theta}|\mathbf{y})$ well, and $M$ *i.i.d.* draws, $\boldsymbol{\theta}^{(i)}$, from $q(\boldsymbol{\theta}|\mathbf{y})$, an IS estimate of (4) is $\overline{g(\boldsymbol{\theta})}_{IS} = \frac{1}{M}\sum_{i=1}^{M} g(\boldsymbol{\theta}^{(i)})w(\boldsymbol{\theta}^{(i)})$, where $w(\boldsymbol{\theta}^{(i)}) = p(\boldsymbol{\theta}^{(i)}|\mathbf{y})/q(\boldsymbol{\theta}^{(i)}|\mathbf{y})$. In the typical case where $p(\boldsymbol{\theta}^{(i)}|\mathbf{y})$ is available only up to the integrating constant, and $w(\boldsymbol{\theta}^{(i)})$ cannot be evaluated as a consequence, the estimate is modified as

$$\overline{g(\boldsymbol{\theta})}_{IS} = \sum_{i=1}^{M} g(\boldsymbol{\theta}^{(i)})w(\boldsymbol{\theta}^{(i)})/\sum_{j=1}^{M} w(\boldsymbol{\theta}^{(i)}), \tag{13}$$

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[17]Metropolis et al. (1953) actually implemented their algorithm one element of $\boldsymbol{\theta}$ at a time, as a harbinger of the Gibbs sampler to come. See Robert and Casella (2011) for more details.

[18]Dongarra and Sullivan (2000) rank the Metropolis algorithm as one of the 10 algorithms "with the greatest influence on the development and practice of science and engineering in the 20th century".

[19]One could in fact argue that a similar aim motivated Metropolis and co-authors, given that they drew a sharp contrast (in effect) between the efficiency of their method and that of the naive Monte Carlo technique based on uniform sampling.

with the weights re-defined as $w(\boldsymbol{\theta}^{(j)}) = p^*(\boldsymbol{\theta}^{(i)}|\mathbf{y})/q^*(\boldsymbol{\theta}^{(i)}|\mathbf{y})$, for kernels, $p^*(\boldsymbol{\theta}^{(i)}|\mathbf{y})$ and $q^*(\boldsymbol{\theta}^{(i)}|\mathbf{y})$, of $p(\boldsymbol{\theta}|\mathbf{y})$ and $q(\boldsymbol{\theta}|\mathbf{y})$ respectively. Once again, and under regularity conditions pertaining to the *importance density* $q(\boldsymbol{\theta}|\mathbf{y})$, asymptotic theory can be invoked to prove that (13) is a $\sqrt{M}$-consistent estimator of $E(g(\boldsymbol{\theta})|\mathbf{y})$ (Geweke, 1989a). A judicious choice of $q(\boldsymbol{\theta}|\mathbf{y})$ is able to yield a sampling variance that is less than (12) in some cases, as befits the original motivation of IS as a variance reduction method. (See Geweke, 1989a, Robert and Casella, 2004, and Hoogerheide et al., 2009, for discussion and examples of more recent advances in IS.) Critically however, like the Metropolis method, (13) serves as a *feasible* estimate of $E(g(\boldsymbol{\theta})|\mathbf{y})$ when $p(\boldsymbol{\theta}|\mathbf{y})$ cannot be easily simulated; hence the significance of IS in Bayesian computation. Moreover, its maintenance of independent draws, allied with its re-weighting of draws from an approximating density, has led to the emergence of IS as a vehicle for implementing SMC algorithms, like particle filtering, to be referenced in Section 5.2 in the context of particle MCMC.

### 3.5  1970: A Generalization of the Metropolis Algorithm by Hastings

The final publication that we pinpoint during the 200-odd year period subsequent to 1763, is the 1970 *Biometrika* paper, '*Monte Carlo Sampling Methods Using Markov Chains and Their Applications'*, by Wilfred Keith Hastings. Whilst Metropolis et al. (1953) proposed the use of MCMC sampling to compute particular integrals in statistical mechanics, it was the Hastings paper that elevated the concept to a general one, and introduced it to the broader statistics community. Included in the paper is also the first mention of what would become known as the Metropolis-within-Gibbs sampler (Robert and Casella, 2011). Once again, the author's focus was *not* a Bayesian integral *per se*; however we describe the method in that context.

In contrast to Metropolis and co-authors, Hastings (1970) acknowledges up-front that the need to know $p(\boldsymbol{\theta}|\mathbf{y})$ only up to the integrating constant is a compelling feature of an MCMC-based estimate of (4). Hastings also generalizes the acceptance probability in (10) to one that accommodates a general 'candidate' distribution $q(\boldsymbol{\theta}|\mathbf{y})$ from which $\boldsymbol{\theta}^c$ is drawn, as:

$$\alpha = \min\left\{\left[p^*(\boldsymbol{\theta}^c|\mathbf{y})/q(\boldsymbol{\theta}^{(i)}|\boldsymbol{\theta}^c,\mathbf{y})\right] / \left[p^*(\boldsymbol{\theta}^{(i)}|\mathbf{y})/q(\boldsymbol{\theta}^c|\boldsymbol{\theta}^{(i)},\mathbf{y})\right], 1\right\}, \tag{14}$$

which clearly collapses to (10) when $q(\boldsymbol{\theta}|\mathbf{y})$ is symmetric (in $\boldsymbol{\theta}^c$ and $\boldsymbol{\theta}^{(i)}$), as in the original random walk proposal of Metropolis et al. (1953). Importantly, the more general algorithm allows for a targeted choice of $q(\boldsymbol{\theta}|\mathbf{y})$ that reduces the need for tuning and which can, potentially, reduce the degree of dependence in the chain and, hence, the variance of the estimate of $E(g(\boldsymbol{\theta})|\mathbf{y})$. Hastings formalizes the standard error of this estimate using time series theory, explicitly linking, for the first time, the autocorrelation in the Markov draws to the efficiency of the MCMC-based estimate of (4). Crucially, the author tackles the issue of dimension by advocating the treatment of one element (or several elements) of $\boldsymbol{\theta}$ at a time, conditional on all remaining elements.

In summary, all of the important ingredients from which the huge smorgasbord of future MCMC algorithms would eventually be constructed - for the *express* purpose of solving Bayesian problems - were now on the table, via this particular paper.

# 4 Bayesian Computation in the Late 20th Century

## 4.1 The 1970s: The State of Play in Bayesian Computation

By 1970, the key building blocks for Bayesian computation were thus in place: deterministic quadrature methods, (asymptotic) approximations, and techniques based on stochastic simulation. Let's now take a snapshot of the overall state of play at the beginning of the 1970s, posing the question: which, if any, of these computational tools did Bayesians *actually* exploit in practice? We answer this question, first through the lens of two monographs: *i)* Zellner, '*An Introduction to Bayesian Inference in Econometrics*' (Wiley, 1971); and *ii)* Lindley, '*Bayesian Statistics, A Review*' (Siam, 1971); and, secondly, via a glance at the broader published literature of the time.

A salient feature of Zellner (1971) is the liberal use of Gaussian (and associated) distributional assumptions and linear model structures, allied with standard non-informative and natural conjugate priors. That is, choices of both model and prior are made such that, analytical solutions to (4) - including marginal posterior distributions and moments, marginal likelihoods and predictive distributions - are usually available. In cases where closed-form solutions are not available, use is made of asymptotic approximations, and reference made to Fortran programs that implement low-dimensional deterministic integration. In other words, in terms of the taxonomy we have adopted in Section 2.2 for categorizing computational methods, any *computation* in the text is performed using either *1)* or *3)*. Not a single reference is made to *2)*! Whilst somewhat different in coverage and focus, Lindley (1971) similarly: works primarily with examples in which closed-form expressions for (4) are available, makes note of the role of asymptotic expansions, and makes not a single mention of simulation-based computation.

This same lack of focus on simulation techniques characterizes the Bayesian research literature of the time. In short, we are not aware of any paper published prior to the late 1970s in which the use of simulation to solve a Bayesian problem was proposed.[20] Fast forward to the *end* of the decade, and things do begin to change. Witness, for example, the first (explicitly) Bayesian application of importance sampling in Kloek and van Dijk, '*Bayesian Estimates of Equation System Parameters: An Application of Integration by Monte Carlo*' (*Econometrica*, 1978), with a simulation-based estimate of an integral of the form of (4) now front and centre. Even still, the authors adopt model structures and priors with a view to reducing the computational burden via analytical means, with the only integral requiring the application of simulation-based computation being of dimension three!

In brief, whilst the role that *could* be played by simulation in computation was known by the 1970s, the technology needed for that knowledge to be exploited lagged behind. At the beginning of the decade wide-spread access to computers was simply non-existent; and by the end of the decade, whilst computing *was* accessible, it was typically cumbersome and slow and, hence, limited the scope of what could be tackled by simulation.[21]

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[20]We note here that Hastings' student Peskun did contribute further to the understanding of the Metropolis algorithm in Peskun (1973); however the focus was still not on the computation of Bayesian integrals *per se.*

[21]Many readers may be too young to remember the punchcards! But there was a time when RAND's 1955 *A Million Random Digits with 100,000 Normal Deviates* was more than an entry for sarcastic Amazon comments, as producing this million digits took more than two months at the time.

## 4.2 The 1980s and 1990s: Gibbs Sampling and the MCMC Revolution

### 4.2.1 Overview

Over the next two decades, however, things changed. Indeed, *two* developments now went hand in hand to spawn a remarkable expansion in simulation-based Bayesian computation: *i)* the increased speed and availability of computers, including personal desktop computers, and *ii)* the collective recognition that MCMC draws from a joint posterior, $p(\boldsymbol{\theta}|\mathbf{y})$, could be produced via iterative sampling from lower dimensional, and often standard, *conditionals.* Evidence for, and historical details of *i)* are documented in, for example, Ceruzzi (2003). Just as significant, however, was *ii)* which, *when* allied with both the concept of *augmentation,* and an understanding of the theoretical properties of combinations of MCMC algorithms, would lead to *Gibbs sampling* (with or without Metropolis-Hastings (MH) subchains) becoming the work-horse of Bayesian computation in the 1990s.

### 4.2.2 Gibbs sampling, data augmentation and combined MCMC chains

An MH algorithm 'works', in the sense of producing a Markov chain that converges to the required distribution, $p(\boldsymbol{\theta}|\mathbf{y})$, due to the form of the acceptance probability in (14) (or, the nested version in (10)). More formally, the algorithm, as based on candidate density $q(\boldsymbol{\theta}|\mathbf{y})$, and acceptance probability as defined in (14), defines a *transition kernel* with invariant distribution, $p(\boldsymbol{\theta}|\mathbf{y})$. The 'Gibbs sampler' similarly yields a Markov chain with invariant distribution, $p(\boldsymbol{\theta}|\mathbf{y})$, but via a transition kernel that is defined as the product of *full conditional posteriors* associated with the joint.

For the simplest case of a two-dimensional vector $\boldsymbol{\theta} = (\theta_1, \theta_2)'$, the steps of the Gibbs algorithm are as follows:

Step 1 Specify an initial value for $\theta_2$, $\theta_2^{(0)}$.

Step 2 For $i = 1, 2, ..., M$, cycle iteratively through the two conditional distributions, drawing respectively:

 a. $\theta_1^{(i)}$ from $p_1(\theta_1^{(i)}|\theta_2^{(i-1)}, \mathbf{y})$; and b. $\theta_2^{(i)}$ from $p_2(\theta_2^{(i)}|\theta_1^{(i)}, \mathbf{y})$

Given the satisfaction of the required convergence conditions (which essentially place sufficient regularity on the conditionals), the draws $\boldsymbol{\theta}^{(i)} = (\theta_1^{(i)}, \theta_2^{(i)})'$, $i = 1, 2, ..., M$, converge in distribution to the joint posterior distribution as $M \to \infty$, and can be used to produce a $\sqrt{M}$-consistent estimate of (4) in the form of (11). Extension to higher-dimensional problems is obvious, although decisions about how to 'block' the parameters, and thereby define the conditionals, now play a role (Roberts and Sahu, 1997).

Gibbs thus exploits the simplicity yielded by conditioning: whilst joint and marginal posterior distributions are usually complex in form, (full) conditional posteriors are often standard and, hence, able to be simulated from directly. While one may find hints in both Hastings (1970) and Besag (1974), this point was first made clearly by Geman and Geman (1984), who also coined the phrase 'Gibbs sampling' because their problem used Gibbs random fields in image restoration.[22] However, the later paper by Gelfand and Smith (1990) is generally credited with bringing this transformational idea to the attention of the broader statistical community, and illustrating its broad applicability.

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[22]Gibbs distributions, in turn, are named after the physicist, Josiah Willard Gibbs (1839–1903).

The idea of Gibbs sampling overlapped with a related proposal by Tanner and Wong (1987): that of 'augmenting' the set of unknowns ($\boldsymbol{\theta}$ in our notation) with latent data, $\mathbf{z} = (z_1, z_2, ..., z_n)'$, to yield conditionals - $p(\boldsymbol{\theta}|\mathbf{z}, \mathbf{y})$ and $p(\mathbf{z}|\boldsymbol{\theta}, \mathbf{y})$ - that facilitate the production of a simulation-based estimate of $p(\boldsymbol{\theta}|\mathbf{y})$; with $p(\boldsymbol{\theta}|\mathbf{z}, \mathbf{y})$, in particular, often being standard. The melding of these two ideas, i.e. sampling via conditionals *per se*, and yielding more tractable conditionals through the process of augmentation, enabled the analysis of complex models that had thus far eluded Bayesian treatment, due to their dependence on high-dimensional vectors of latent variables; selected examples being: Polson et al. (1992), Carter and Kohn (1994), Frühwirth-Schnatter (1994) and Jacquier et al. (1994). However, it also led to the realization that *artificial* latent variables could be judiciously introduced into a model for the sole purpose of producing tractable conditional posteriors over the augmented space, thereby opening up a whole range of additional models to a Gibbs-based solution (e.g. Diebolt and Robert, 1994; Kim et al., 1998; Damien et al., 1999).[23]

Of course, in most high-dimensional problems - and in particular those in which latent variables feature - *certain* of the conditionals will remain nonstandard, such that direct simulation from them is not possible. Critically though, the reduced dimension renders this a simpler sampling problem than sampling from the joint itself. For example, if the nonstandard conditional is inherently low-dimensional - that is, the argument of the distribution does not fall into a natural grouping with a large number of other parameters - it can be simulated via a deterministic approximation to the inverse cumulative distribution function (Devroye, 1986; referred to as 'Griddy Gibbs' by Ritter and Tanner, 1992). If, on the other hand, the nonstandard conditional is high-dimensional - and a grid-based procedure like Griddy Gibbs thus computationally infeasible - a convergent Markov chain can be produced by embedding an MH algorithm within the outer Gibbs loop (a so-called 'Metropolis-within-Gibbs' algorithm). Finding an MH candidate that is a good match for a target *conditional* is obviously easier than finding a suitable candidate for the higher-dimensional joint, with the efficiency of the chain, and the accuracy of the estimate of (4), potentially improved as a result.[24]

We complete this section by noting that towards the end of the 20th century, hope arose that MCMC could evolve into the '*perfect sampling*' machine: producing *independent* draws from the invariant distribution. Propp and Wilson (1996) explained how to achieve this goal by amalgamating the concept of coalescence with that of multiple coupled chains. In short, their proposal amounted - in effect - to beginning a chain in the infinite past (in algorithmic time), and producing at time 0 a draw from the invariant distribution that was independent of the starting value. Repeated application of this process yielded an independent sample from the invariant distribution; i.e. the 'ideal' or 'perfect' outcome. Whilst developments along these lines were to continue in the 21st century (see Casella et al., 2001, Craiu and Meng, 2011, and Huber, 2016 for reviews), the method has arguably not lived up to expecta-

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[23] The *slice sampler* (Roberts and Rosenthal, 1999; Neal, 2003) is a particularly notable, and generic, way of generating an MCMC algorithm via this principle of auxiliary variable augmentation.

[24] We refer the reader to: Besag and Green (1993), Smith and Roberts (1993) and Chib and Greenberg (1996) for early reviews of MCMC sampling; Casella and George (1992) and Chib and Greenberg (1995) for descriptions of the Gibbs and MH algorithms (respectively) that are useful for practitioners; Robert (2015), Betancourt (2018) and Dunson and Johndrow (2019) for more recent reviews; and Andrieu et al. (2004) and Robert and Casella (2011) for historical accounts of MCMC sampling. The two 2011 Handbooks: *Handbook of Markov Chain Monte Carlo* (Sisson et al., 2019) and *The Oxford Handbook of Bayesian Econometrics* (Geweke et al., 2011), also provide a broad sweep of applications of MCMC algorithms across a wide spectrum of fields.

tions, due to the large computational burden required to produce repeated instances of multiple chains. More recent approaches to producing unbiased MCMC (also to be referenced in Section 5.4) are, however, more promising in terms of delivering of an 'exact' Monte Carlo approximation with a finite number of draws. (Glynn and Rhee, 2014; Glynn, 2016; Jacob et al., 2020).

# 5 The 21st Century: A Second Computational Revolution

## 5.1 Why Did We Need a Second One?

The advent of accessible, fast computers in the last two decades of the 20th century, allied with the methodological and theoretical developments referenced above, led to an explosion in the use of simulation-based Bayesian computation, with variants of MCMC leading the charge. Despite their unquestioned power and versatility however, these existing simulation techniques did have certain limitations; with these limitations to become more marked as the empirical problems being tackled became more ambitious; and this despite a concurrent rise in computing power (parallel computing, access to GPUs etc.) over recent decades.

With reference to the posterior pdf in (5), two characteristics are worthy of note. First, as already highlighted, in all but the most stylized problems $p(\boldsymbol{\theta}|\mathbf{y})$ is available only up to its integrating constant, and is not of a standard form that can be directly simulated. Second, representation of $p(\boldsymbol{\theta}|\mathbf{y})$ only as a kernel, $p^*(\boldsymbol{\theta}|\mathbf{y}) \propto L(\boldsymbol{\theta}|\mathbf{y})p(\boldsymbol{\theta})$, still requires closed forms for $L(\boldsymbol{\theta}|\mathbf{y})$ and $p(\boldsymbol{\theta})$. With reference to $L(\boldsymbol{\theta}|\mathbf{y})$, this means that, for any $\boldsymbol{\theta}$, $p(\mathbf{y}|\boldsymbol{\theta})$ needs to be able to be evaluated at the observed $\mathbf{y}$. The MCMC and IS simulation methods obviate the first problem by drawing *indirectly* from $p(\boldsymbol{\theta}|\mathbf{y})$ via another distribution (or set of distributions) from which simulation is feasible. However, in so doing, these methods still make use of the second requirement. That is, all simulation algorithms discussed thus far explicitly require evaluation of $p(\mathbf{y}|\boldsymbol{\theta})$: in the computation of the importance weights in (13), in the computation of the acceptance probability in (10) or (14), and in the implementation of any Gibbs-based algorithm, in which the conditional posteriors are required either in full form or at least up to a scale factor.

The assumption that $p(\mathbf{y}|\boldsymbol{\theta})$ can be evaluated is a limitation for two reasons. First, some empirically relevant DGPs do not admit pdfs in closed form; examples being: probability distributions defined by quantile or generating functions (Devroye, 1986; Peters et al., 2012), continuous time models with unknown transition densities (Gallant and Tauchen, 1996), dynamic equilibrium models in economics (Calvet and Czellar, 2015), certain deep learning models in machine learning (Goodfellow et al., 2014); complex astrophysical models (Jennings and Madigan, 2017); and DGPs for which the normalizing constant is unavailable, such as Markov random fields (Rue and Held, 2005; Stoehr, 2017). Second, pointwise evaluation of $p(\mathbf{y}|\boldsymbol{\theta})$ (at any $\boldsymbol{\theta}$) (in the case where $p(\cdot|\boldsymbol{\theta})$ has a closed form) entails an $O(n)$ computational burden; meaning that the MCMC and IS methods described above are *not scalable* to so-called 'big (or tall) data' problems (Bardenet et al., 2017).

Just as important are the challenges that arise when the dimension of the unknowns themselves is very large (the so-called 'high-dimensional' problem); for instance, when a model contains a very large number of latent variables over which integration is required (e.g. Tavaré et al., 1997; Braun and McAuliffe, 2010; Beaumont, 2010; Lintusaari et al., 2017; Johndrow et al., 2019). In such cases, standard MCMC

methods - even if feasible in principle - may not (as highlighted further in Section 5.4) enable an accurate estimate of (4) to be produced in finite computing time; i.e. such methods are *not necessarily scalable* in the dimension of the unknowns.

Each of the techniques discussed in Sections 5.2 and 5.3 relieves the investigator of one or more of these 'burdens'; although, as we shall see, the relief is not costless. In particular, the *approximation* methods covered in Section 5.3, whilst enabling some problems to be tackled that would be intractable for MCMC and IS, make the ultimate sacrifice. Such methods do not seek an estimate of (4) that is *exact* up to simulation error but, instead, accept as an outcome a representation of (4) that is only ever *approximate.*

Finally, we provide a very brief overview in Section 5.4 of further advances made in MCMC methods *per se* over the past decade or so; advances designed, in large measure, to improve the *accuracy* with which these dependent chains estimate posterior quantities of interest such as (4), most notably in large-scale problems.

## 5.2   Pseudo-Marginal Methods

### 5.2.1   The basic idea

Referencing the concept of data augmentation introduced in Section 4.2.2: given draws from the joint posterior of $\boldsymbol{\theta}$ and $\mathbf{z}$, $p(\boldsymbol{\theta}, \mathbf{z}|\mathbf{y})$, the draws of $\boldsymbol{\theta}$ can be used to produce an exact simulation-based estimate of $p(\boldsymbol{\theta}|\mathbf{y})$ or any associated quantity, for large enough $M$. Again, the latent states, $\mathbf{z}$, may be either intrinsic to the model, or introduced 'artificially' as a computational device, as highlighted therein. Initially, draws of $(\boldsymbol{\theta}, \mathbf{z})$ were produced via Gibbs-based MCMC schemes, with a variety of MH algorithms (based on alternative candidates) used to sample from $p(\mathbf{z}|\boldsymbol{\theta}, \mathbf{y})$, in the typical case where this conditional could not be simulated directly (see Fearnhead, 2011, and Giordani et al., 2011, for reviews). As highlighted in certain references cited in Section 5.1 however, depending on the problem, including the dimension of $\mathbf{z}$, such MH-within-Gibbs schemes can be slow to explore the joint space of $(\boldsymbol{\theta}, \mathbf{z})$ and, hence, to produce an *accurate* estimate of $p(\boldsymbol{\theta}|\mathbf{y})$.

The (combined) insight of Beaumont (2003) and Andrieu and Roberts (2009) was to recognize that draws of $\mathbf{z}$ could be used in a potentially more effective way to yield an estimate of the 'marginal' of interest: $p(\boldsymbol{\theta}|\mathbf{y})$ (and any associated integral of the form of (4)). Key to this insight is the following observation. Use $\mathbf{u} \in \mathcal{U}$ to denote all of the canonical (problem-specific) random variables that are used to generate $\mathbf{z}$. If $M$ draws of $\mathbf{u}$ can be used to produce an *unbiased* estimate of the likelihood function, $p(\mathbf{y}|\boldsymbol{\theta})$, then an MCMC scheme applied to the joint space $(\boldsymbol{\theta}, \mathbf{u})$, can target the required invariant distribution, $p(\boldsymbol{\theta}|\mathbf{y})$. An informal demonstration of this result is straightforward. Define $h(\mathbf{u})$ as the distribution of the random variables underpinning the generation of $\mathbf{z}$ (independently of the prior $p(\boldsymbol{\theta})$), and let $h(\mathbf{y}|\boldsymbol{\theta}, \mathbf{u})$ denote an estimate of the likelihood $p(\mathbf{y}|\boldsymbol{\theta})$, that is unbiased in the sense that $E_{\mathbf{u}}[h(\mathbf{y}|\boldsymbol{\theta}, \mathbf{u})] = p(\mathbf{y}|\boldsymbol{\theta})$. Then we have that

$$h(\boldsymbol{\theta}|\mathbf{y}) \propto \int_{\mathcal{U}} h(\boldsymbol{\theta}, \mathbf{u}|\mathbf{y})d\mathbf{u} = \int_{\mathcal{U}} h(\mathbf{y}|\boldsymbol{\theta}, \mathbf{u})p(\boldsymbol{\theta})h(\mathbf{u})d\mathbf{u} = p(\boldsymbol{\theta}) \int_{\mathcal{U}} h(\mathbf{y}|\boldsymbol{\theta}, \mathbf{u})h(\mathbf{u})d\mathbf{u},$$

from which the required result follows: $h(\boldsymbol{\theta}|\mathbf{y}) \propto p(\boldsymbol{\theta})p(\mathbf{y}|\boldsymbol{\theta}) \propto p(\boldsymbol{\theta}|\mathbf{y})$.

Use of $h(\mathbf{y}|\boldsymbol{\theta}, \mathbf{u})$ within an MH algorithm amounts to replacing the acceptance probability in (14) with

$$\alpha = \min\left\{\left[h(\mathbf{y}|\boldsymbol{\theta}^c, \mathbf{u}^c)p(\boldsymbol{\theta}^c)/q(\boldsymbol{\theta}^{(i)}|\boldsymbol{\theta}^c, \mathbf{y})\right] / \left[h(\mathbf{y}|\boldsymbol{\theta}^{(i)}, \mathbf{u}^{(i)})p(\boldsymbol{\theta}^{(i)})/q(\boldsymbol{\theta}^c|\boldsymbol{\theta}^{(i)}, \mathbf{y})\right], 1\right\}, \qquad (15)$$

where $\boldsymbol{\theta}^c$ is proposed from $q(\boldsymbol{\theta}^c|\boldsymbol{\theta}^{(i)}, \mathbf{y})$ and $\mathbf{u}^{(i)}$ and $\mathbf{u}^c$ are independent draws from $h(\mathbf{u})$. The use of an estimate of the likelihood in (15), prompted use of the term 'pseudo'-marginal MH (PMMH) by Andrieu and Roberts (2009) although, as noted, this replacement still yields a chain with an invariant distribution equal to the correct marginal, $p(\boldsymbol{\theta}|\mathbf{y})$, when the estimate is unbiased.

When a likelihood estimate is produced specifically via the use of *particle filtering* in a state space model (SSM), the term *particle* MCMC (PMCMC) has also been coined (Andrieu et al., 2011).[25] Whilst we omit details of the use of filtering to estimate a likelihood function (see reviews in Doucet et al., 2001, and Giordani et al., 2011), we do remark that particle filtering does involve the sequential application of IS, with independent, but differentially weighted draws of the latent states (from both 'filtered' and 'prediction' state distributions) being the outcome. As such, much of the early work on IS, including the impact of proposal choice on the efficiency of the sampler, has assumed a renewed importance in filtering-based settings, including PMCMC.[26]

Whilst unbiasedness of the likelihood estimate is required for a general PMMH algorithm to 'work', the variance of the estimate also affects the performance of the sampler and, hence, the simulation efficiency of any estimate of (4) that is produced. Pitt et al. (2012) demonstrate (in an SSM setting) that if the likelihood is estimated precisely, the mixing of the Markov chain will, essentially, be as rapid as if the true likelihood were used. However, improving the precision of the likelihood estimator $\widehat{p}(\mathbf{y}|\boldsymbol{\theta})$ by increasing the number of particles used in its production comes at a computational cost. Equivalently, if a computationally cheap estimate of $\widehat{p}(\mathbf{y}|\boldsymbol{\theta})$ is used this will typically slow the mixing of the chain, and the estimate of (4) will be less accurate, for any given number of Markov chain iterates. Pitt et al. (2012) suggest choosing the particle number that minimizes the so-called computing time: a measure that takes into account both the cost of obtaining $\widehat{p}(\mathbf{y}|\boldsymbol{\theta})$ and the speed of mixing of the chain. They show that the 'optimal' number of particles is that which yields a variance for the likelihood estimate that is approximately equal to one, at the true parameter vector. See Doucet et al. (2015) and Deligiannidis et al. (2018) for more recent advances on the optimal structuring and tuning of pseudo-marginal algorithms.

### 5.2.2 The benefits

The benefits of pseudo-marginal schemes are three-fold. First, in cases where the parameters and latent states are strongly correlated, use of a PMMH scheme rather than a Gibbs-based scheme (based on $p(\mathbf{z}|\boldsymbol{\theta}, \mathbf{y})$ and $p(\boldsymbol{\theta}|\mathbf{z}, \mathbf{y})$), may reap efficiency gains (conditional on appropriate 'tuning' choices, as flagged above). Linked to this, avoidance of the need to sample from $p(\mathbf{z}|\boldsymbol{\theta}, \mathbf{y})$ obviates the need to make choices regarding the blocking of $\mathbf{z}$ and the proposal densities for those blocks. Second, in cases where *only*

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[25]Whilst not a pseudo-marginal method, particle filtering has also been used to provide an estimate of $p(\mathbf{z}|\boldsymbol{\theta}, \mathbf{y})$ in a Gibbs scheme for an SSM - so-called 'particle Gibbs' (Andrieu et al., 2011).

[26]Indeed, this same point regarding the continued relevance of IS principles applies to the whole SMC literature; see Naesseth et al. (2019) for elaboration.

forward simulation of the latent process is possible, and point-wise evaluation of $p(\mathbf{y}, \mathbf{z}|\boldsymbol{\theta})$ is infeasible as a result, PMMH remains possible. For example, in an SSM an estimate of $p(\mathbf{y}|\boldsymbol{\theta})$ can be based on the bootstrap particle filter, for which only simulation from the transition density $p(z_t|z_{t-1}, \boldsymbol{\theta})$ (not evaluation thereof) is required. Third, in cases where the dimension of $\mathbf{y}$ is very large, an unbiased estimate of $p(\mathbf{y}|\boldsymbol{\theta})$ based on appropriately selected *subsamples* of data can be used to produce a valid PMMH scheme, at a *much* smaller computational cost than any scheme that requires full evaluation of $p(\mathbf{y}|\boldsymbol{\theta})$ (Bardenet et al., 2017; Quiroz et al., 2018b, and Quiroz et al., 2019).

## 5.3 Approximate Bayesian Inference

The goal of all simulation-based computational methods discussed thus far, including the pseudo-marginal techniques, has been to estimate the posterior expectation in (4) 'exactly', at least up to an order $O(M^{-1/2})$, where $M$ is the number of draws that defines the simulation scheme. The alternative methods do, of course, differ one from the other in terms of the constant term that quantifies the precise error of approximation. Hence, it may be the case that even for a very large $M$, a nominally 'exact' method (despite being 'tuned' optimally) has an approximation error that is non-negligible.[27] Nevertheless, the convention in the literature is to refer to all simulation methods outlined to this point as *exact*, typically without qualification.[28]

In contrast, when applying an *approximation* method (using the taxonomy from Section 2.2), investigators make no claim to exactness, other than citing the asymptotic (in $n$) accuracy of the Laplace methods (in Sections 3.2 and 5.3.4), or the asymptotic validity of certain other approximations (Fearnhead, 2018). That is, for finite $n$ at least, such methods are only ever acknowledged as providing an approximation to (4), with that approximation perhaps claimed to be as 'accurate' as possible, given the relevant choice variables that characterize the method; but no more.

So what benefits do such techniques offer, in return for sacrificing the goal of exact inference? With reference to the methods discussed below: ABC and BSL both *completely* obviate the need to evaluate $p(\mathbf{y}|\boldsymbol{\theta})$ and, in so doing, open up to Bayesian treatment a swathe of empirical problems - so-called *doubly-intractable* problems - that would otherwise not be amenable to Bayesian analysis. In computing (4), both methods replace the posterior in the integrand, $p(\boldsymbol{\theta}|\mathbf{y})$, with an approximation produced via simulation. A simulation-based estimate of the integral, $\overline{g(\boldsymbol{\theta})} = (1/M)\sum_{i=1}^{M} g(\boldsymbol{\theta}^{(i)})$, is then produced using draws, $\boldsymbol{\theta}^{(i)}$, from this approximate posterior.[29] In contrast, VB and INLA both require evaluation of $p(\mathbf{y}|\boldsymbol{\theta})$, but reap computational benefits in certain types of problems (in particular those of high-dimension) by replacing - at least in part - *simulation* with (in some cases closed-form) *optimization*.[30] In the case of VB, the posterior $p(\boldsymbol{\theta}|\mathbf{y})$ used to define (4) is replaced by an approximation produced via the calculus of variations. Depending on the nature of the problem, including the 'variational family' from which the 'optimal' approximation is produced, the integral is computed in either closed form or

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[27] A point that we revisit in Section 5.4.

[28] We note that we have omitted any mention herein of so-called 'quasi-Monte Carlo' integration schemes, which aim for exactness at a faster rate than $O(M^{-1/2})$. See Lemieux (2009) for a review of such methods and Gerber and Chopin (2015) for an entry on quasi-sequential Monte Carlo.

[29] It can also be argued that these are simulation methods for an exact, albeit different posterior, using either a degraded version of the observations or a projection of them via a nonsufficient statistic (Wilkinson, 2013).

[30] As noted below, modifications of VB to cater an intractable likelihood *have* been proposed.

via a simulation step. With INLA, the approximation of $p(\boldsymbol{\theta}|\mathbf{y})$ is chosen in such a way that (4) can be computed with the aid of low-dimensional deterministic integration.

### 5.3.1 Approximate Bayesian computation (ABC)

Whilst the initial popularity of ABC stemmed from its being a simple and intuitive practical tool for dealing with problems with intractable likelihoods (Tavaré et al., 1997; Pritchard et al., 1999), acceptance of the technique has grown to the extent that it is now part of the standard Bayesian toolbox in some areas.[31] As such, not only do several reviews of the area exist (Marin et al., 2011; Sisson and Fan, 2011), but the technique has recently reached 'handbook status', with the publication of Sisson et al. (2019); and it is to those resources that we refer the reader for extensive details on the method, application and theory of ABC. We provide only the essence of the approach here, including its connection to other computational methods.

The aim of ABC is to approximate $p(\boldsymbol{\theta}|\mathbf{y})$ in cases where - despite the complexity of the problem preventing the *evaluation* of $p(\mathbf{y}|\boldsymbol{\theta})$ - $p(\mathbf{y}|\boldsymbol{\theta})$ (and $p(\boldsymbol{\theta})$) can still be *simulated*. The simplest (accept/reject) form of the algorithm proceeds as follows: first, we simulate $\boldsymbol{\theta}^i$, $i = 1, 2, ..., M$, from $p(\boldsymbol{\theta})$, and artificial data $\mathbf{x}^i$ from $p(\cdot|\boldsymbol{\theta}^i)$; second, we use $\mathbf{x}^i$ to construct (a vector of) simulated summary statistics $\eta(\mathbf{x}^i)$, which we then then compare against the (vector of) *observed* statistics $\eta(\mathbf{y})$ using a distance $d\{\cdot, \cdot\}$; third, all values of $\boldsymbol{\theta}^i$ that yield simulated statistics, $\eta(\mathbf{x}^i)$, for which $d\{\eta(\mathbf{x}^i), \eta(\mathbf{y})\} \leq \varepsilon$, for some small tolerance $\varepsilon$, are retained.

ABC thus produces draws of $\boldsymbol{\theta}$ from a posterior that conditions not on the full data set $\mathbf{y}$, but on statistics $\eta(\mathbf{y})$ (with dimension less than $n$) that summarize the key characteristics of $\mathbf{y}$. Only if $\eta(\mathbf{y})$ are sufficient for conducting inference on $\boldsymbol{\theta}$, and for $\varepsilon \to 0$, does ABC provide draws from the exact posterior $p(\boldsymbol{\theta}|\mathbf{y})$. In practice, the complexity of the models to which ABC is applied implies - almost by definition - that a low-dimensional set of sufficient statistics is unavailable, and the implementation of the method (in finite computing time) requires a non-zero value for $\varepsilon$, and a given number of draws, $M$. As such, draws from the ABC algorithm provide (via kernel density methods) a simulation-based approximation of $p(\boldsymbol{\theta}|\eta(\mathbf{y}))$, which we denote by $\widehat{p}_\varepsilon(\boldsymbol{\theta}|\eta(\mathbf{y}))$.

The difference between $\widehat{p}_\varepsilon(\boldsymbol{\theta}|\eta(\mathbf{y}))$ and the unattainable $p(\boldsymbol{\theta}|\mathbf{y})$ has two components: the difference between the 'partial' posterior, $p(\boldsymbol{\theta}|\eta(\mathbf{y}))$, and $p(\boldsymbol{\theta}|\mathbf{y})$, and the difference between $\widehat{p}_\varepsilon(\boldsymbol{\theta}|\eta(\mathbf{y}))$ and $p(\boldsymbol{\theta}|\eta(\mathbf{y}))$. The first difference is the critical one, and depends on the informativeness, or otherwise, of the chosen summaries; loosely speaking, the 'closer' is $\eta(\mathbf{y})$ to being sufficient for $\boldsymbol{\theta}$, the 'closer' is $p(\boldsymbol{\theta}|\eta(\mathbf{y}))$ to $p(\boldsymbol{\theta}|\mathbf{y})$. Attention has been given to maximizing the information content of the summaries in some sense (e.g. Joyce and Marjoram, 2008; Blum, 2010; Fearnhead and Prangle, 2012). This includes the idea of defining $\eta(\mathbf{y})$ as (some function of) the maximum likelihood estimator (MLE) of the parameter vector of an approximating 'auxiliary' model; thereby producing summaries that are - via the properties of the MLE - close to being *asymptotically* sufficient, depending on the accuracy of the approximating model (Drovandi et al., 2011; Drovandi et al., 2015; Martin et al., 2019). This approach mimics, in the Bayesian setting, the frequentist methods of indirect inference (Gouriéroux et al., 1993) and efficient

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[31]The broad applicability, and ease of use, of ABC is highlighted by the fact it has garnered over 11,000 citations on Google Scholar since 2000.

method of moments (Gallant and Tauchen, 1996) using, as it does, an approximating model to produce feasible inference about an intractable true model. Whilst the price paid for the approximation in the frequentist case is reduced sampling efficiency, in the Bayesian case the cost is posterior inference that is conditioned on insufficient summaries, and is 'partial' inference as a consequence.

Regarding the second difference, at its simplest level: the smaller is $\varepsilon$ and the larger is $M$, the more accurate will $\widehat{p}_{\varepsilon}(\boldsymbol{\theta}|\eta(\mathbf{y}))$ be as a kernel density estimate of $p(\boldsymbol{\theta}|\eta(\mathbf{y}))$, for any given choice of $\eta(\mathbf{y})$, with the dimension of both $\eta(\mathbf{y})$ and $\boldsymbol{\theta}$ affecting accuracy (Blum et al., 2013; Frazier et al., 2018; Nott et al., 2018). For given $M$ (and, hence, a given computational burden), modifications of the basic accept/reject algorithm that improve the accuracy with which $p(\boldsymbol{\theta}|\eta(\mathbf{y}))$ is estimated by $\widehat{p}_{\varepsilon}(\boldsymbol{\theta}|\eta(\mathbf{y}))$ have been proposed which, variously, involve post-sampling corrections of the draws (Beaumont et al., 2002; Blum, 2010), the insertion of MCMC and/or SMC steps (Marjoram et al., 2003; Sisson et al., 2007; Beaumont et al., 2009), or the use of randomized quasi-Monte Carlo, rather than (standard) Monte Carlo in the simulation of $\boldsymbol{\theta}^{i}$, $i = 1, 2, ..., M$ (Buchholz and Chopin, 2019). Recent algorithms have also combined the principles of ABC and Gibbs sampling (Clarté et al., 2019; Rodrigues et al., 2019), once again with the primary aim of reducing the impact of dimension on the accuracy of ABC.

Finally, recent work has focused on the asymptotic (in $n$) behaviour of $\widehat{p}_{\varepsilon}(\boldsymbol{\theta}|\eta(\mathbf{y}))$, highlighting that - under certain conditions on $\eta(\mathbf{y})$, $\varepsilon$ and $M$ - $\widehat{p}_{\varepsilon}(\boldsymbol{\theta}|\eta(\mathbf{y}))$ concentrates onto the true vector $\boldsymbol{\theta}_0$ (i.e. is Bayesian consistent), satisfies a Bernstein-von Mises theorem (i.e. is asymptotically Gaussian) and yields an ABC posterior mean with an asymptotically Gaussian sampling distribution. (See Frazier et al., 2018, for this full suite of results; and Li and Fearnhead, 2018a, Li and Fearnhead, 2018b, and Frazier et al., 2020, for related work.) In this sense then, at least for large enough $n$, ABC can justly be viewed as a valid inferential method *per se*, rather than purely as a convenient computational tool.[32]

### 5.3.2   Bayesian synthetic likelihood (BSL)

ABC thus targets $p(\boldsymbol{\theta}|\eta(\mathbf{y})) \propto p(\eta(\mathbf{y})|\boldsymbol{\theta})p(\boldsymbol{\theta})$, with $p(\boldsymbol{\theta}|\eta(\mathbf{y}))$ itself, for nonsufficient $\eta(\mathbf{y})$, being an approximate representation of $p(\boldsymbol{\theta}|\mathbf{y})$. It is clear then that, embedded within the simplest accept/reject ABC algorithm, based on a tolerance $\varepsilon$, is a likelihood function of the form,

$$p_{\varepsilon}(\eta(\mathbf{y})|\boldsymbol{\theta}) = \int_{\mathcal{X}} p(\mathbf{x}|\boldsymbol{\theta}) \mathcal{I}\left(d\{\eta(\mathbf{y}), \eta(\mathbf{x})\} \leq \varepsilon\right) d\mathbf{x}. \tag{16}$$

For a given draw $\boldsymbol{\theta}^{i}$, and associated $\eta(\mathbf{x}^{i})$, (16) is approximated by its simulation counterpart, $\widehat{p}_{\varepsilon}(\eta(\mathbf{y})|\boldsymbol{\theta}^{i})$ $= \mathcal{I}\left(d\{\eta(\mathbf{y}), \eta(\mathbf{x}^{i})\} \leq \varepsilon\right),$ which can implicitly be viewed as a nonparametric estimator, based on a uniform kernel, for the quantity of interest $p_{\varepsilon}(\eta(\mathbf{y})|\boldsymbol{\theta})$. Following Andrieu and Roberts (2009), and as illustrated in detail by Bornn et al. (2017), $\widehat{p}_{\varepsilon}(\eta(\mathbf{y})|\boldsymbol{\theta}^{i})$ can serve as a likelihood estimate within a form of pseudo-marginal MCMC scheme (referred to as ABC-MCMC by the authors[33]) for sampling from $p_{\varepsilon}(\boldsymbol{\theta}|\eta(\mathbf{y})) \propto p_{\varepsilon}(\eta(\mathbf{y})|\boldsymbol{\theta})p(\boldsymbol{\theta})$, whereby in this context we take 'pseudo-marginal MCMC' to mean an

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[32]We note that in state space settings ABC principles have also been used to implement *particle filtering*, in particular in cases where the measurement density has no closed form and, hence, cannot be used to define the particle weights in the usual way. *ABC filtering* can be used to estimate the likelihood function, as either a basis for producing frequentist point estimates of $\boldsymbol{\theta}$ (Jasra et al., 2012; Calvet and Czellar, 2015) or as an input into a PMMH scheme (Dean et al., 2014; Jasra, 2015).

[33]See also Marjoram et al. (2003).

MCMC scheme that replaces the intractable likelihood, $p_\varepsilon(\eta(\mathbf{y})|\boldsymbol{\theta})$, within the MH ratio by an estimated quantity, $\widehat{p}_\varepsilon(\eta(\mathbf{y})|\boldsymbol{\theta}^i)$, that serves as an unbiased estimator for that intractable likelihood. However, in contrast with other results in the pseudo-marginal literature, Bornn et al. (2017) demonstrate that the efficiency of the MCMC chain so produced is not necessarily improved by using more than one draw of $\eta(\mathbf{x}^i)$ for a given draw $\boldsymbol{\theta}^i$.

Bayesian synthetic likelihood (BSL) (Price et al., 2018) also targets a posterior for $\boldsymbol{\theta}$ that conditions on $\eta(\mathbf{y})$, and requires only *simulation* from $p(\mathbf{y}|\boldsymbol{\theta})$ (not its evaluation) in so doing. However, in contrast to the nonparametric likelihood estimate that is implicit in ABC, BSL (building on Wood, 2010) adopts a Gaussian parametric approximation to $p(\eta(\mathbf{y})|\boldsymbol{\theta})$,

$$p_a(\eta(\mathbf{y})|\boldsymbol{\theta}) = \mathcal{N}\left[\eta(\mathbf{y}); \mu(\boldsymbol{\theta}), \Sigma(\boldsymbol{\theta})\right], \ \mu(\boldsymbol{\theta}) = \mathbb{E}[\eta(\mathbf{y})], \ \Sigma(\boldsymbol{\theta}) = Var\left[\eta(\mathbf{y})\right]. \tag{17}$$

Use of this parametric kernel leads to the *ideal* BSL posterior,

$$p_a(\boldsymbol{\theta}|\eta(\mathbf{y})) \propto p_a(\eta(\mathbf{y})|\boldsymbol{\theta})p(\boldsymbol{\theta}), \tag{18}$$

where the subscript 'a' highlights that (18) is still an approximation to $p(\boldsymbol{\theta}|\eta(\mathbf{y}))$, due to the Gaussian approximation, $p_a(\eta(\mathbf{y})|\boldsymbol{\theta})$, of $p(\eta(\mathbf{y})|\boldsymbol{\theta})$.

In general, however, the mean and variance-covariance matrix of $\eta(\mathbf{y})$ are unknown and must be estimated via simulation. Given $\mathbf{x}_j \sim i.i.d. \ p(\cdot|\boldsymbol{\theta})$, $j = 1, \ldots, m$, we can estimate $\mu(\boldsymbol{\theta})$ and $\Sigma(\boldsymbol{\theta})$ in (17) via their empirical Monte Carlo averages, $\mu_m(\boldsymbol{\theta}) = \frac{1}{m}\sum_{j=1}^m \eta(\mathbf{x}_j)$ and $\Sigma_m(\boldsymbol{\theta}) = \frac{1}{m-1}\sum_{j=1}^m (\eta(\mathbf{x}_j) - \mu_m(\boldsymbol{\theta}))(\eta(\mathbf{x}_j) - \mu_m(\boldsymbol{\theta}))'$, and thereby define

$$p_{a,m}(\eta(\mathbf{y})|\boldsymbol{\theta}) = \int_{\mathcal{X}} \mathcal{N}\left[\eta(\mathbf{y}); \mu_m(\boldsymbol{\theta}), \Sigma_m(\boldsymbol{\theta})\right] \prod_{j=1}^m p(\eta(\mathbf{x}_j)|\boldsymbol{\theta})d\mathbf{x}_1 \ldots d\mathbf{x}_m, \tag{19}$$

and the associated *target* BSL posterior,

$$p_{a,m}(\boldsymbol{\theta}|\eta(\mathbf{y})) \propto p_{a,m}(\eta(\mathbf{y})|\boldsymbol{\theta})p(\boldsymbol{\theta}). \tag{20}$$

Note that, even for a single draw $\eta(\mathbf{x}_j)$, $\mathbf{x}_j \sim p(\cdot|\boldsymbol{\theta})$, we have that $\mathcal{N}\left[\eta(\mathbf{y}); \mu_m(\boldsymbol{\theta}), \Sigma_m(\boldsymbol{\theta})\right]$ is an unbiased estimate of (19). Hence, with $p_{a,m}(\boldsymbol{\theta}|\eta(\mathbf{y}))$ then accessed via an MCMC algorithm, and with arguments in Drovandi et al. (2015) used to show that $p_{a,m} \to p_a$ as $m \to \infty$, BSL can yield a form of pseudo-marginal MCMC method. Due to the parametric nature of the approximation in (18), BSL can *sometimes* outperform ABC in cases where the summaries are high-dimensional (as befits problems where the unknowns themselves are high-dimensional), but only so long as they display features that tally with the Gaussian assumption adopted in (17); see Price et al. (2018) for details, and see Frazier and Drovandi (2019) and Frazier et al. (2019b) for theoretical results on the asymptotic behaviour of BSL.[34]

### 5.3.3 Variational Bayes (VB)

The two approximate methods discussed thus far, ABC and BSL, target an approximation of the posterior that is conditioned on a vector of low-dimensional summary statistics. As such, and most particularly

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[34]See also Dehideniya et al. (2019) for the production of an approximate posterior via the melding of BSL steps with a Laplace approximation.

when $\eta(\mathbf{y})$ is not sufficient for $\boldsymbol{\theta}$, these methods do not directly target the exact posterior $p(\boldsymbol{\theta}|\mathbf{y})$, nor any expectation, (4), defined with respect to it. In contrast, VB methods are a general class of algorithms that produce an approximation to the posterior $p(\boldsymbol{\theta}|\mathbf{y})$ - and hence (4) - *directly*, by replacing simulation with optimization.

The idea of VB is to search for the best approximation to the posterior $p(\boldsymbol{\theta}|\mathbf{y})$ over a class of densities $\mathcal{Q}$, referred to as the variational family, and where $q(\boldsymbol{\theta})$ indexes elements in $\mathcal{Q}$. The most common approach to VB is to find the best approximation to the exact posterior, in the class $\mathcal{Q}$, by minimizing the KL divergence between $q(\boldsymbol{\theta})$ and the posterior $p(\boldsymbol{\theta}|\mathbf{y})$, which defines such a density as the solution to the following optimal optimization problem,

$$q^*(\boldsymbol{\theta}) := \arg \min_{q(\boldsymbol{\theta})\in\mathcal{Q}} \mathrm{KL}\left[q(\boldsymbol{\theta})|p(\boldsymbol{\theta}|\mathbf{y})\right], \tag{21}$$

where

$$\mathrm{KL}\left[q(\boldsymbol{\theta})|p(\boldsymbol{\theta}|\mathbf{y})\right] = \int \log(q(\boldsymbol{\theta}))q(\boldsymbol{\theta})d\boldsymbol{\theta} - \int \log(p(\boldsymbol{\theta}|\mathbf{y}))q(\boldsymbol{\theta})d\boldsymbol{\theta} \equiv \mathbb{E}_q[\log(q(\boldsymbol{\theta}))] - \mathbb{E}_q[\log(p(\boldsymbol{\theta},\mathbf{y}))] + \log(p(\mathbf{y})). \tag{22}$$

Of course, the normalizing constant $p(\mathbf{y})$ is, in all but most simple problems (for which VB would not be required!), unknown; and the quantity in (22) inaccessible as a result. Rather, the approach adopted is to define the so-called evidence lower bound (ELBO),

$$\mathrm{ELBO}[q(\boldsymbol{\theta})] := \mathbb{E}_q[\log(p(\boldsymbol{\theta},\mathbf{y}))] - \mathbb{E}_q[\log(q(\boldsymbol{\theta}))], \tag{23}$$

where $\mathrm{KL}[q(\boldsymbol{\theta})|p(\boldsymbol{\theta}|\mathbf{y})]$ is equivalent to $-\mathrm{ELBO}[q(\boldsymbol{\theta})]$ up to the unknown constant, $\log(p(\mathbf{y}))$, with the latter not dependent on $q(\boldsymbol{\theta})$. Hence, we can obtain the variational density by solving an optimization problem that is equivalent to that in (21):

$$q^*(\boldsymbol{\theta}) := \arg \max_{q(\boldsymbol{\theta})\in\mathcal{Q}} \mathrm{ELBO}[q(\boldsymbol{\theta})]. \tag{24}$$

The beauty of VB is that, for *certain* choices of the class $\mathcal{Q}$, the optimization problem in (24) can either yield a closed-form solution, or be solved relatively quickly with various numerical algorithms; (see Ormerod and Wand, 2010, Blei et al., 2017, and Zhang et al., 2018, for reviews). Most importantly, given that - by design - the variation family is defined in terms of standard forms of distributions, replacement of $p(\boldsymbol{\theta}|\boldsymbol{y})$ by $q(\boldsymbol{\theta})^*$ in (4) yields an expectation that is either available in closed form, or amenable to a relatively simple simulation-based solution.

VB *truly* shines in cases where $\boldsymbol{\theta}$ is high-dimensional, and an efficient MCMC algorithm may well be simply out of reach. Indeed, in such cases, the family $\mathcal{Q}$ can be chosen in such a way that the resulting posterior approximations remain tractable even when the dimension of $\boldsymbol{\theta}$ is in the thousands, or the tens of thousands (Braun and McAuliffe, 2010; Kabisa et al., 2016; Wand, 2017; Koop and Korobilis, 2018). Moreover, even though the method requires the evaluation of $p(\mathbf{y}|\boldsymbol{\theta})$ (through the need to evaluate $p(\boldsymbol{\theta},\mathbf{y}) = p(\mathbf{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})$ in (23)) we note that certain hybrid methods, which mix simulation with likelihood evaluation, can be used to partially overcome this feature. See, for example, Ong et al. (2018), who use stochastic gradient variational inference methods to approximate a version of the BSL posterior (appropriate when $p(\mathbf{y}|\boldsymbol{\theta})$ is intractable); or Tran et al. (2017) who extend the VB approach to intractable

likelihoods via pseudo-marginal principles. A melding of the VB-type algorithm known as *expectation propagation* with ABC occurs in Barthelm and Chopin (2014) and Barthelmé et al. (2018), also in settings where the likelihood cannot be evaluated. (See Vehtari et al., 2020, for a recent perspective on expectation propagation for large data and large parameter sets.)

Finally, the link between (22) and (23) makes it clear that maximizing (23) to yield $q^*(\boldsymbol{\theta})$ produces, as a by-product, a lower bound on the logarithm of the 'evidence', or marginal likelihood, $p(\mathbf{y})$. Hence, $\text{ELBO}[q^*(\boldsymbol{\theta})]$ serves as an estimate of the quantity which, as shown in Section 6.1, underpins model choice.

Recently, several authors have analyzed the asymptotic properties of VB methods; see, for example, Wang and Blei (2019a,b) and Zhang and Gao (2017). The most complete treatment can be found in Zhang and Gao, wherein the authors demonstrate that the rate at which the VB posterior concentrates is bounded above by the following two components: *i)* the concentration rate of the exact posterior, and *ii)* the approximation error incurred by the chosen variational family. This novel decomposition highlights the fundamental importance of the variational family that is used to approximate the posterior, something that is not present in other results on the asymptotic behavior of VB. Interestingly, while Zhang and Gao deliver a convenient upper bound in a general context, they also demonstrate that in specific examples, such as Gaussian sequence models and sparse linear regression models, the VB posterior can display concentration rates that are actually faster than those obtained by the exact posterior, owing to the fact that VB performs a type of 'internal regularization' as a consequence of the algorithm's optimization step.[35]

### 5.3.4  Integrated nested Laplace (INLA)

We complete our review of 21st century approximate computational methods with a reminder of a computational innovation from the 18th! In 1774, in a quest to illustrate posterior consistency, Laplace produced an asymptotic (in $n$) approximation to a particular posterior probability. Not only did this result represent the first step in the development of Bayesian asymptotic *theory*, it also provided a simple practical solution to the *computation* of general posterior expectations; one that (as highlighted in Section 4.1) continued to play an important role in Bayesian analysis prior to the eventual dominance of simulation methods.

In 1986, Tierney and Kadane revived and formalized the Laplace approximation: using it to yield an asymptotic approximation (of a given order) of any posterior expectation of the form of (4), including (in the multiple parameter case) marginal posterior densities.[36] Two decades later, Rue et al. (2009) took the method further: adapting it to approximate marginal posteriors (and general expectations like those in (4)) in latent Gaussian models (LGMs). With the authors using a series of *nested* Laplace approximations, allied with low-dimensional numerical *integration*, they termed their method *integrated nested Laplace,* or INLA for short. Since the LGM class encompasses a large range of empirically relevant models - including, generalized linear models, non-Gaussian state space (or hidden Markov) models,

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[35]Huggins et al. (2019) propose a method for validating the accuracy of VB posterior approximations using alternative (nonasymptotic) principles. See also Yu et al. (2019) (and earlier references therein) for practical validation approaches that are relevant to approximate posteriors in general.

[36]See also Tierney et al. (1989).

and spatial, or spatio-temporal models - a computational method tailored-made for such a setting is sufficiently broad in its applicability to warrant detailed consideration herein. In common with VB, and as follows from the use of Laplace approximations evaluated at modal values, INLA eschews simulation for *optimization* (in addition to using low-dimensional deterministic integration methods).

Deferring to Rue et al. (2009), Martino and Riebler (2019) and Wood (2019) for all details (including of the LGM structure), we provide here the *key* steps of INLA. We diverge from the less structured format we have, in the main, adopted for describing computational algorithms, by using numbered points to present these steps. To adhere to our goal of notational consistency, we reference the $p$-dimensional vector of static parameters in the LGM as $\boldsymbol{\theta}$, the $n$-dimensional vector of latent, random parameters as $\mathbf{z}$, and the $n$-dimensional vector of observed data as $\mathbf{y}$,[37] and express the model as:

$$
\begin{aligned}
\mathbf{y}|\mathbf{z},\boldsymbol{\theta} &\sim \textstyle\prod_{i=1}^{n} p(y_i|z_i,\boldsymbol{\theta}) \\
\mathbf{z}|\boldsymbol{\theta} &\sim \boldsymbol{N}(\mathbf{0}, Q^{-1}(\boldsymbol{\theta})) \\
\boldsymbol{\theta} &\sim p(\boldsymbol{\theta}),
\end{aligned}
$$

where $Q(\boldsymbol{\theta})$ is the precision matrix of the latent Gaussian field, assumed - for computational feasibility - to be sparse. The goal of the authors is to approximate the marginal posteriors; $p(\theta_j|\mathbf{y})$, $j = 1, 2, .., p$, and $p(z_i|\mathbf{y})$, $i = 1, 2, .., n$. The problems envisaged are those in which $p$ is small and $n$ is large (potentially in the order of millions), with MCMC algorithms deemed to be possibly unsuitable as a consequence, due to the scale of both $\mathbf{z}$ and $\boldsymbol{y}$.

Beginning with the expression of $p(\boldsymbol{\theta}|\mathbf{y})$ as

$$
p(\boldsymbol{\theta}|\mathbf{y}) = \frac{p(\mathbf{z}, \boldsymbol{\theta}|\mathbf{y})}{p(\mathbf{z}|\boldsymbol{\theta}, \mathbf{y})} \propto \frac{p(\mathbf{z}, \boldsymbol{\theta}, \mathbf{y})}{p(\mathbf{z}|\boldsymbol{\theta}, \mathbf{y})} = \frac{p(\mathbf{y}|\mathbf{z},\boldsymbol{\theta})p(\mathbf{z}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{z}|\boldsymbol{\theta}, \mathbf{y})}, \tag{25}
$$

and recognizing that the proportionality sign arises due to the usual lack of integrating constant (over $\mathbf{z}$ and $\boldsymbol{\theta}$), the steps of the algorithm (in its simplest form) are as follows:

1. On the assumption that all components of the model can be evaluated and, hence, that the numerator is available, approximate $p(\boldsymbol{\theta}|\mathbf{y})$ in (25) as

$$
\widetilde{p}(\boldsymbol{\theta}|\mathbf{y}) \propto \frac{p(\mathbf{y}|\widehat{\mathbf{z}}(\boldsymbol{\theta}),\boldsymbol{\theta})p(\widehat{\mathbf{z}}(\boldsymbol{\theta})|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p_G(\widehat{\mathbf{z}}(\boldsymbol{\theta})|\boldsymbol{\theta}, \mathbf{y})}, \tag{26}
$$

where the denominator represents a Gaussian approximation of $p(\mathbf{z}|\boldsymbol{\theta}, \mathbf{y})$, $p_G(\mathbf{z}|\boldsymbol{\theta}, \mathbf{y}) = N(\widehat{\mathbf{z}}(\boldsymbol{\theta}), \widehat{\Sigma}(\boldsymbol{\theta}))$, evaluated at the mode, $\widehat{\mathbf{z}}(\boldsymbol{\theta})$, of $p(\mathbf{z}, \boldsymbol{\theta}, \mathbf{y})$ (at a given value of $\boldsymbol{\theta}$); and where $\widehat{\Sigma}(\boldsymbol{\theta})$ is the inverse of the Hessian of $-\log p(\mathbf{z}, \boldsymbol{\theta}, \mathbf{y})$ with respect to $\mathbf{z}$, also evaluated at $\widehat{\mathbf{z}}(\boldsymbol{\theta})$. The expression in (26) can obviously be further simplified to

$$
\widetilde{p}(\boldsymbol{\theta}|\mathbf{y}) \propto p(\mathbf{y}|\widehat{\mathbf{z}}(\boldsymbol{\theta}),\boldsymbol{\theta})p(\widehat{\mathbf{z}}(\boldsymbol{\theta})|\boldsymbol{\theta})p(\boldsymbol{\theta}) \left|\widehat{\Sigma}(\boldsymbol{\theta})\right|^{1/2}. \tag{27}
$$

With appropriate adjustments made for notation, and noting that the expression is given up to the integrating constant only, (27) can be seen to be identical to the Laplace approximation of a marginal density in Tierney and Kadane (1986, equation (4.1)).[38]

---

[37]The model allows for each element of $\mathbf{y}$ to be of dimension $d \geq 1$; however we keep our description simple by assuming $d = 1$.

[38]Rue et al. (2009) discuss the circumstances in which the order of approximation proven in Tierney and Kadane (1986) applies to the LGM setting.

2. Define the marginal posterior for the *ith* element of $\mathbf{z}$ as

$$\widetilde{p}(z_i|\mathbf{y}) = \int_\Theta \widetilde{p}(z_i|\boldsymbol{\theta},\mathbf{y})\widetilde{p}(\boldsymbol{\theta}|\mathbf{y})d\boldsymbol{\theta}. \tag{28}$$

A second application of a Laplace approximation would yield

$$\widetilde{p}(z_i|\boldsymbol{\theta},\mathbf{y}) \propto p(\mathbf{y}|\widehat{\mathbf{z}}_{-i}(\boldsymbol{\theta},z_i),\boldsymbol{\theta})p(\widehat{\mathbf{z}}_{-i}(\boldsymbol{\theta},z_i)|\boldsymbol{\theta})p(\boldsymbol{\theta})\left|\widehat{\Sigma}_{-i}(\boldsymbol{\theta},z_i)\right|^{1/2}, \tag{29}$$

where $\widehat{\mathbf{z}}_{-i}(\boldsymbol{\theta},z_i)$ is the mode of $p(\mathbf{z}_{-i},z_i,\boldsymbol{\theta},\mathbf{y})$ (at given values of $\boldsymbol{\theta}$ and $z_i$, with $\mathbf{z}_{-i}$ denoting all elements of $\mathbf{z}$ other than the *ith*); and where $\widehat{\Sigma}_{-i}(\boldsymbol{\theta},z_i)$ is the inverse of the Hessian of $-\log p(\mathbf{z}_{-i},z_i,\boldsymbol{\theta},\mathbf{y})$ with respect to $\mathbf{z}_{-i}$, also evaluated at $\widehat{\mathbf{z}}_{-i}(\boldsymbol{\theta},z_i)$. Computation of (29) for each $z_i$ would, however, involve $n$ optimizations (over $\mathbf{z}_{-i}$) plus $n$ specifications of the high-dimensional matrix $\widehat{\Sigma}_{-i}(\boldsymbol{\theta},z_i)$. Rue et al. (2009) avoid this computational burden by modifying the approximation in (29) in a number of alternative ways, all details of which are provided in the references cited above. Once a representation of $\widetilde{p}(z_i|\boldsymbol{\theta},\mathbf{y})$ is produced, (28) is computed using a deterministic numerical integration scheme defined over a grid of values for the low-dimensional $\boldsymbol{\theta}$.

3. Define the marginal posterior for the *jth* element of $\boldsymbol{\theta}$ as

$$\widetilde{p}(\theta_j|\mathbf{y}) = \int_{\Theta_{-j}} \widetilde{p}(\boldsymbol{\theta}|\mathbf{y})d\boldsymbol{\theta}_{-j}, \tag{30}$$

where $\boldsymbol{\theta}_{-j}$ denotes all elements of $\boldsymbol{\theta}$ excluding $\theta_j$. The integral in (30) is computed using deterministic integration over $\boldsymbol{\theta}_{-j}$.

4. If required, approximate the marginal likelihood, $p(\mathbf{y})$, by computing the normalizing constant in (27),

$$\int_\Theta p(\mathbf{y}|\widehat{\mathbf{z}}(\boldsymbol{\theta}),\boldsymbol{\theta})p(\widehat{\mathbf{z}}(\boldsymbol{\theta})|\boldsymbol{\theta})p(\boldsymbol{\theta})\left|\widehat{\Sigma}(\boldsymbol{\theta})\right|^{1/2}d\boldsymbol{\theta},$$

using deterministic integration over $\boldsymbol{\theta}$.

All steps of the algorithm are provided in a dedicated package, R-INLA, for the general LGM framework, with particular packages also available for implementing INLA in more specific models nested within the LGM class; see Martino and Riebler (2019) for a listing of all such packages.

## 5.4   MCMC Algorithms Revisited

Despite the rich pickings now on offer with all of the new (including approximate) computational methods, it is *far* from the case that the stalwart of the late 20th century - MCMC - has run its race! Hence, we complete this section with a brief overview of the many key advances in MCMC that have been made, subsequent to the appearance of the first algorithms. Brevity is adopted, not because this segment of the literature is not ripe with developments; in fact, attempts to improve the performance of the original (Gibbs and MH) schemes began early, have been continual, and engage a substantial number of researchers. Rather, we choose to be brief simply because the fundamental principles of the

newer advances remain *essentially* faithful to the original principles of MCMC, and those principles have already been covered herein.[39]

Indeed, we begin with three reminders about MCMC algorithms:

1. *First*, an *MC*-MC algorithm is just that - a *Markov chain* Monte Carlo algorithm. As such, an MCMC scheme - by design - produces a *local* exploration of the target posterior, with the location in the parameter space of any simulated draw being *dependent* on the location of the previous draw, in a manner that reflects the specific structure of the algorithm. Most notably, an MCMC algorithm with a high degree of dependence will potentially be slow in exploring the high mass region of the target posterior (or the 'target set', in the language of Betancourt, 2018), with this problem usually being more severe the larger is the dimension of the parameter space.[40] Looked at through another lens: for $M$ MCMC draws, the greater the degree of (typically positive) dependence in those draws, the less efficient is the MCMC-based estimate of (4), relative to an estimate based on $M$ *i.i.d.* draws from the target. This loss of efficiency is measured by the so-called *inefficiency factor (IF)*, defined (in the case of scalar $g(\boldsymbol{\theta})$) as the ratio of the *MCMC standard error*, $\sigma_{MCMC} = \sqrt{Var(g(\boldsymbol{\theta}))[1 + 2\sum_{l=1}^{\infty}\rho_l]/M}$ to the standard error associated with $M$ *i.i.d.* draws, $\sqrt{\sigma_{MC}^2}$, with $\sigma_{MC}^2$ as given in (12), where $\rho_l$ is the lag-$l$ autocorrelation of the draws of $g(\boldsymbol{\theta})$ over the history of the chain. This ratio, in turn, defines the *effective sample size* of the MCMC algorithm, $ESS = M/[1 + 2\sum_{l=1}^{\infty}\rho_l]$. Improving the efficiency of an MCMC algorithm, for any given value of $M$, thus equates to increasing $ESS$ to its maximum possible value of $M$ by reducing the dependence in the draws.

2. *Second*: an MC-*MC* algorithm is also a Markov chain *Monte Carlo* algorithm. That is, under appropriate regularity it produces a $\sqrt{M}$-consistent estimate of (4), whatever the degree of dependence in the chain, with the dependence affecting the constant term implicit in the $O(M^{-1/2})$ rate of convergence, but not the rate itself. Hence, in principle, any MCMC algorithm, no matter how inherently inefficient, can produce an estimate of (4) that is arbitrarily accurate, simply though an increase in $M$. However, an increase in $M$ entails an increase in *computational cost*, measured, say, by *computing clock-time*. The extent of this increase depends, in turn, on the (per-iteration) cost of generating a (proposal/candidate) draw and, with an MH step, the cost of calculating the acceptance probability. Both component costs will (for any algorithm) clearly increase with the number of unknowns that need to be simulated, and assessed, at each iteration. Either cost, or both, will also increase with the sample size, given the need for pointwise evaluation of the likelihood function across the elements of **y**.

3. *Third*: the very concept of efficiency is relevant only if the Markov chain is (asymptotically in $M$) *unbiased*, which depends critically on draws being produced from the correct invariant distribution.

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[39]We acknowledge here a slight inconsistency in our approach, by having allocated (above) a full section to pseudo-marginal MCMC methods, methods that also remain faithful to the fundamental principles of MCMC. However, the goals of the pseudo-marginal literature are arguably broader than just improving algorithmic performance, as we have touched on in Section 5.2.2.

[40]See Betancourt (2018) for a discussion of high-dimensional parameter spaces, and the challenges they can present to MCMC algorithms.

That is, the production of an *accurate* MCMC-based estimate of (4) depends, not just on reducing the degree of dependence in the chain, or on increasing the number of draws, but on ensuring that the chain *actually* explores the target set, and thereby avoids bias in the estimation of (4).[41]

Hence, all advances in MCMC - *at their core* - aim to increase the effectiveness with which an algorithm explores the high mass region of the target posterior and, hence, the accuracy with which (4) is estimated, by doing one (or more) of three things: reducing dependence in the chain, reducing the computational cost per iteration of the chain (thus enabling more draws to be produced), or eliminating bias. Focus is increasingly directed towards developing algorithms that *scale well*, in terms of the dimension of the data and/or the number of unknowns.

With our goal of brevity in mind, we simply *list* the main contenders here, including certain key references or reviews, deflecting both to those papers, and to the broad overviews of modern developments in MCMC in Robert et al. (2018) and Dunson and Johndrow (2019) for all details. We categorize the methods according to whether improved performance is achieved (*primarily*): *i)* via the exploitation of more geometric information about the target posterior; *ii)* by better choice of proposal distribution; *iii)* by the use of parallel, batched, subsample, coupled or ensemble sampling methods; or *iv)* by more effective use of any given set of draws, however obtained:

*i)* Hamiltonian Monte Carlo (HMC) (Neal, 2011a; Carpenter et al., 2017; Betancourt, 2018); no U-turn sampling (NUTS) (Hoffman and Gelman, 2014);[42] Metropolis-Adjusted Langevin algorithm (MALA) (Roberts et al., 1996; Roberts and Rosenthal, 1998); stochastic gradient MCMC (Nemeth and Fearnhead, 2019); piecewise deterministic Markov processes (PDMP) (Bierkens et al., 2018; Fearnhead et al., 2018; Bierkens et al., 2019).

*ii)* Optimal scaling of random-walk MH (Roberts et al., 1997); Adaptive sampling (Nott and Kohn, 2005; Roberts and Rosenthal, 2009; Rosenthal, 2011); Simulated tempering and parallel tempering (Geyer, 1991; Marinari and Parisi, 1992; Gramacy et al., 2010, Geyer, 2011a; Tawn et al., 2020); Delayed rejection sampling (Tierney and Mira, 1998); Delayed acceptance sampling (Christen and Fox, 2005; Golightly et al., 2015; Wiqvist et al., 2018; Banterle et al., 2019); Multiple try MCMC (Liu et al., 2000; Bédard et al., 2012; Martino, 2018; Luo and Tjelmeland, 2019); Tempered Gibbs Sampling (TGS) (Zanella and Roberts, 2019).

*iii)* Parallelized MCMC (Jacob et al., 2011; Wang and Dunson, 2013); subposterior (batched) methods (Neiswanger et al., 2013; Scott et al., 2016); subsampling methods based on pseudo-marginal

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[41]It is acknowledged in the literature that MCMC algorithms produce potentially strong biases in their initial phase of 'convergence' to the typical set from an initial point in the parameter space. However, under appropriate regularity, such biases are transient, and their impact on the estimation of (4) able to be eliminated by discarding a sufficiently large number of 'burn-in' or 'warm-up' draws from the computation. (See Robert and Casella, 2004, and Gelman and Shirley, 2011, for textbook discussions of convergence, including diagnostic methods.) Some of the more recent literature is concerned with removing this transitory bias after a finite number of iterations; e.g. Jacob et al. (2020). Other literature is concerned with ensuring that an MCMC algorithm does not yield a bias that is *non-transitory* due to the inability of the algorithm to effectively explore the target set at all (within a meaningful time frame); see e.g. Betancourt (2018).

[42]As described in Neal (2011a), simulation methods based on Hamiltonian dynamics can actually be viewed as having as long a history as MCMC itself. The more modern manifestations of HMC, however, including NUTS, can be viewed as Markov chain algorithms that simply explore the parameter space more effectively than (say) a default random walk scheme. The probabilistic programming platform Stan (Carpenter et al., 2017) enables implementation of NUTS, in addition to certain variants of VB.

MCMC (Bardenet et al., 2017; Quiroz et al., 2018b, and Quiroz et al., 2019); unbiased MCMC via coupling (Glynn and Rhee, 2014; Middleton et al., 2018; Jacob et al., 2020); unbiased MCMC for doubly-intractable problems using pseudo-marginal principles (Lyne et al., 2015); ensemble MCMC (Iba, 2000; Cappé et al., 2004; Neal, 2011b).

iv) Thinning (Owen, 2017); Rao-Blackwellization (Casella and Robert, 1996; Robert and Casella, 2004; Douc and Robert, 2011).

# 6 The Role of Computation in Model Choice and Prediction

Thus far, our focus has been on computing the posterior expectation in (4) defined in the context of an assumed model, $p(\mathbf{y}|\boldsymbol{\theta})$. Other than the brief reference made to the lower bound on the marginal likelihood, $p(\mathbf{y})$, yielded by the VB procedure, and to the deterministic approximation of $p(\mathbf{y})$ produced by INLA, the issue of model uncertainty itself (and the quantification thereof) has not been addressed; nor has the specific case in which the expectation in (4) defines a predictive distribution. We touch on these topics in the following sections, emphasizing the particular role played by computation in these settings. In so doing we break with the overarching approach adopted in the paper of presenting computational developments chronologically; simply presenting a brief summary of the methods that are currently in use, several of which had their genesis in the 1990s, and some of which are much more recent.

In Section 6.1 model uncertainty is managed by treating each model in the assumed model space separately, and using the set of *posterior model probabilities* so produced to make decisions. In Section 6.2 model uncertainty is directly incorporated into the computational method via the principle of augmentation, with inference about the model being a direct outcome. In Section 6.3 we look at Bayesian prediction, under both single and multiple unknown models.

## 6.1 Model Uncertainty and Marginal Likelihood Computation

We begin by adopting the simplest possible characterization of model uncertainty, where the model space is spanned by two models, $M_1$ and $M_2$, with prior probabilities, $p(M_1)$ and $p(M_2)$ respectively. A simple application of the Bayesian calculus leads to the following expression for the ratio of posterior model probabilities (or *posterior odds ratio*):

$$\frac{p(M_1|\mathbf{y})}{p(M_2|\mathbf{y})} = \frac{p(M_1)}{p(M_2)} \times \frac{p(\mathbf{y}|M_1)}{p(\mathbf{y}|M_2)}, \tag{31}$$

where

$$p(\mathbf{y}|M_k) = \int_{\Theta_k} L(\boldsymbol{\theta}_k|\mathbf{y})p(\boldsymbol{\theta}_k)d\boldsymbol{\theta}_k, \tag{32}$$

and $\boldsymbol{\theta}_k$ is the unknown parameter (vector) for model $M_k$, $k = 1, 2$. The density in (32) defines, equivalently, the *marginal likelihood*, the *marginal data density*, or the *evidence* of model $M_k$, and the ratio of the two such densities on the right-hand-side of (31) defines the *Bayes factor*.

Computation of $p(M_1|\mathbf{y})$ and $p(M_2|\mathbf{y})$ proceeds via (31) allied with the restriction that $p(M_1|\mathbf{y})+$ $p(M_2|\mathbf{y}) = 1$.[43] *Model choice* can be performed by invoking decision-theoretic arguments, and minimizing expected posterior loss. This leads to $M_1$ being chosen if $p(M_1|\mathbf{y})/p(M_2|\mathbf{y})$ exceeds the ratio of losses of 'Type 2' and 'Type 1' errors. *Model averaging* can also be used, whereby the posterior expectation of a quantity of interest is computed for both models, then *averaged*, using $p(M_1|\mathbf{y})$ and $p(M_2|\mathbf{y})$ as the weights (an example of which is given in Section 6.3).[44]

Key to all of this is the evaluation of the two integrals in (32). Once again, analytical solutions to (32) are available only for certain special cases; and computation of some sort is required otherwise. Whilst the VB approach to computing $E(g(\boldsymbol{\theta})|\boldsymbol{y})$ within the context of a given model yields, as a bi-product, a lower bound on the evidence for that model, we focus in this section on methods that target the marginal likelihood *directly*. We do not reproduce here the INLA-based method for computing $p(\mathbf{y})$ that has been described in Section 5.3.4.

Notably, the integral in (32) does *not* constitute a special case of (4); i.e. it is not a *posterior* expectation but, rather, is a *prior* expectation; and this has two consequences. *First*, the two expectations in (32), and the Bayes factor that they define, are *well-defined* only if the prior for the parameters under both models are *proper* density functions. Hence, Bayes factors, and the posterior odds ratios that they imply, cannot be computed with impunity under (typically improper) non-informative, or objective, priors.[45] Attempts to incorporate objective prior information into Bayes factors have been made (see Strachan and van Dijk, 2014, for a recent treatment, and relevant referencing); however the convention in the literature remains one of adopting informative, proper priors in the computation of posterior model probabilities.

The *second* consequence relates to computation: the most direct approach to computing (32) via simulation, namely drawing $\boldsymbol{\theta}_k$ from $p(\boldsymbol{\theta}_k)$, and averaging $L(\boldsymbol{\theta}_k|\mathbf{y})$ over the draws, is typically inaccurate, as $p(\boldsymbol{\theta}_k)$ will not necessarily have high mass in the high-mass region of the likelihood function. All simulation-based estimates of (32) thus use draws of $\boldsymbol{\theta}_k$ that are informed by the data in some way, to improve accuracy. However, the fact that (32) is not a posterior moment means that *direct* computation of it as the mean of some function $g(\boldsymbol{\theta})$ over draws simulated from $p(\boldsymbol{\theta}|\mathbf{y})$ (or some representation of it) is not feasible. Different, more *indirect* uses of simulation are needed.

Several alternative methods for simulation-based estimation of (32) have been proposed, in addition to - and sometimes combined with - either partial analytical solutions or asymptotic (Laplace) approximations. We refer the reader to Kass and Raftery (1995), Geweke (1999), Chib (2011) and Fourment et al. (2018) for reviews. We simply emphasize below three distinct uses of simulation, all of which nest, or can be linked to, a range of specific methods, not all of which we cover here. We adopt section headings that indicate the over-arching *principle* underlying each approach.

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[43]The extension to multiple ($K > 2$) models is obvious: the information from $K - 1$ odds ratios is combined with the summation restriction.

[44]Textbook illustrations of various versions of these steps can be found in Zellner (1971), Koop (2003) and Robert (2007).

[45]If an inherently improper prior is rendered proper by arbitrary truncation, the Bayes factor itself will be arbitrary, and the posterior probabilities assigned to the two alternative models, meaningless.

### 6.1.1 Importance sampling

As noted at the beginning of Section 3.4, the original motivation of Hammersley and Handscomb (1964) in using IS to compute integrals was that of variance reduction. The focus of those authors was on computing $\phi = \int_0^1 f(x)dx$, for some function $f(.)$. What they termed a 'crude' Monte Carlo estimator was simply $\widehat{\phi} = \frac{1}{M}\sum_{i=1}^{M} f(x^{(i)})$, based on $M$ i.i.d. draws, $x^{(i)}$, from a uniform distribution on $(0,1)$, with sampling variance $\sigma^2/M$, where $\sigma^2$ is the variance of the scalar $f(x)$. In other words, $\phi$ can be re-expressed as $\phi = \int f(x)p(x)dx$, with $p(x)$ the density of the uniform distribution on $(0,1)$, and with $\widehat{\phi}$ being the natural estimate of the expectation of $f(x)$ with respect to $p(x)$. The problem is that $p(x)$ that does not necessarily target the parts of the support where $f(x)$ is 'important'. This leads to a sampling variance that is larger than it *could* be. As the authors highlight, judicious choice of an importance density, $q(x)$, defined on $(0,1)$, and estimation of $\phi = \int \frac{f(x)p(x)}{q(x)}q(x)dx$ by $\widehat{\phi} = \frac{1}{M}\sum_{i=1}^{M} \frac{f(x^{(i)})p(x^{(i)})}{q(x^{(i)})}$ can lead to a smaller sampling variance than $\sigma^2/M$.

The problem of computing (32) can be viewed in the same way, with draws from the prior, $p(\boldsymbol{\theta}_k)$, yielding values of $L(\boldsymbol{\theta}_k|\mathbf{y})$ (our '$f(x)$') that are unimportant; hence the benefit of invoking IS principles. Defining $w^{(i)} = L(\boldsymbol{\theta}_k^{(i)}|\mathbf{y})p(\boldsymbol{\theta}_k^{(i)})/q(\boldsymbol{\theta}_k^{(i)}|\mathbf{y})$, $i = 1, 2, ..., M$, for draws, $\boldsymbol{\theta}_k^{(i)}$, from some suitable importance density $q(\cdot|\mathbf{y})$ (usually explicitly dependent on the data), an IS approach produces

$$\widehat{p}(\mathbf{y}|M_k) = \frac{1}{M}\sum_{i=1}^{M} w^{(i)}. \tag{33}$$

Subject to regularity on $q(\cdot|\mathbf{y})$, the usual asymptotic (in $M$) arguments can be invoked to prove the consistency and asymptotic normality of (33) as an estimator of $p(\mathbf{y}|M_k)$ (see Geweke, 1999). Note that, on the assumption that $L(\boldsymbol{\theta}_k^{(i)}|\mathbf{y})$ and $p(\boldsymbol{\theta}_k^{(i)})$ are available in closed form, and that $q(\cdot|\mathbf{y})$ is known in in its entirety (i.e. including its integrating constant), no additional normalization step (like that in (13)) is required. See Geweke (1989b), Gelfand and Dey (1994) and Raftery (1996) for early examples of this approach, and Geweke (1999) for illustration of a non-i.i.d. version, based on draws from an MH candidate distribution, $q(\cdot|\mathbf{y})$, that is dependent on the previous draw of $\boldsymbol{\theta}_k$ in the Markov chain.

The general principle of IS has, of course, two aspects to it: i) the use of draws simulated from the importance density to compute a weighted mean; and ii) evaluation of the importance density in the weight. The so-called 'reciprocal IS' (RIS) method (Gelfand and Dey, 1994; Frühwirth-Schnatter, 2004) uses the second aspect, whilst taking draws from the posterior itself. Simple calculations can be used to show that, for some $q(\cdot|\mathbf{y})$ that is contained in the support of $p(\boldsymbol{\theta}_k|\mathbf{y})$, and defining $g(\boldsymbol{\theta}_k) = q(\boldsymbol{\theta}_k|\mathbf{y})/[L(\boldsymbol{\theta}_k|\mathbf{y})p(\boldsymbol{\theta}_k)]$,

$$E(g(\boldsymbol{\theta}_k)|\mathbf{y}) = [p(\mathbf{y}|M_k)]^{-1}. \tag{34}$$

Again, under regularity, including on the support of $q(\boldsymbol{\theta}_k|\mathbf{y})$, any set of draws from $p(\boldsymbol{\theta}_k|\mathbf{y})$, can be used to estimate (34), and its reciprocal used as an estimate of the marginal likelihood itself. The 'harmonic mean estimator' of Newton and Raftery (1994) is a special case of (34) in which $q(\boldsymbol{\theta}_k|\mathbf{y}) = p(\boldsymbol{\theta}_k)$. The major computational problems that arise when the prior has fatter tails than the posterior (Neal, 1994, 1999) have led to this method being largely eschewed in the literature. The 'bridge sampler', on the other hand, provides a more robust version of (34) by exploiting draws from *both* the posterior and the weight density, $q(\boldsymbol{\theta}_k|\mathbf{y})$ (Meng and Wong, 1996; Meng and Schilling, 2002; Frühwirth-Schnatter, 2004;

Gronau et al., 2017). More recent versions of the RIS method retain draws from the posterior, but use VB approximations of $p(\boldsymbol{\theta}_k|\mathbf{y})$ to define $q(\boldsymbol{\theta}_k|\mathbf{y})$ (Fourment et al., 2018; Hajargasht and Woźniak, 2018).

On a related thread, note that SMC has often been advocated for estimating the evidence (Doucet et al., 2000; Fiel and Wyse, 2012; Everitt et al., 2020). Similarly, techniques incorporating the intractable marginal likelihood as a supplementary parameter can be traced back to Geyer (1993), with more recent occurrences like noise-contrastive estimation (Gutmann and Hyvärinen, 2012), being based on a so-called 'logistic trick' that turns the approximation of the evidence into the estimation of the intercept of a logistic classification program. See also Barthelm and Chopin (2015) and Lyne et al. (2015) for related work.

### 6.1.2 Multiple runs of MCMC

Given the definition of $p(\boldsymbol{\theta}_k|\mathbf{y})$, we can produce a representation of the marginal likelihood as:

$$p(\mathbf{y}|M_k) = \frac{L(\boldsymbol{\theta}_k|\mathbf{y})p(\boldsymbol{\theta}_k)}{p(\boldsymbol{\theta}_k|\mathbf{y})}. \tag{35}$$

The insight of Chib (1995) was to recognize that (35) *holds for all* $\boldsymbol{\theta}$. Hence, an estimate of $p(\mathbf{y}|M_k)$ is simply produced as: $\widehat{p}(\mathbf{y}|M_k) = L(\boldsymbol{\theta}_k^*|\mathbf{y})p(\boldsymbol{\theta}_k^*)/p(\boldsymbol{\theta}_k^*|\mathbf{y})$, where the convention is to take $\boldsymbol{\theta}_k^*$ as some high posterior value. Whilst the (common) availability of the likelihood and prior in closed form renders the ordinates of the factors in the numerator readily accessible in most cases, the denominator and, indeed, the value of $\boldsymbol{\theta}_k^*$ itself are, by the very nature of the problem, inaccessible without further work. However, defining $\boldsymbol{\theta}_k^* = (\theta_{k,1}^*, \theta_{k,2}^*, ..., \theta_{k,p_k}^*)'$, the joint posterior (evaluated at $\boldsymbol{\theta}_k^*$) can be decomposed as:

$$p(\boldsymbol{\theta}_k^*|\mathbf{y}) = p(\theta_{k,1}^*|\theta_{k,2}^*, ..., \theta_{k,p_k}^*, \mathbf{y})p(\theta_{k,2}^*|\theta_{k,3}^*, ..., \theta_{k,p_k}^*, \mathbf{y})...p(\theta_{k,p_k}^*|\mathbf{y}). \tag{36}$$

The last term on the right-hand-side of (36) can simply be estimated in the usual way using a full run of an MCMC sampler. The remaining conditionals can be estimated from *additional* applications of the same simulation scheme, but with the appropriate sets of parameters *held fixed*. Modification of the original (pure Gibbs) approach proposed in Chib (1995) to cater for full conditionals that are not available in closed form, by using MH steps, is detailed in Chib and Jeliazkov (2001). The approach, however, quickly becomes computationally impractical as the dimension of $\boldsymbol{\theta}_k$ grows.

### 6.1.3 Nested sampling

Nested sampling (Skilling, 2007) is yet another method for producing a simulation-based estimate of $p(\mathbf{y}|M_k)$. Whilst it gained an immediate foothold in astronomy (Mukherjee et al., 2006) - possibly due to the availability of dedicated software like MultiNest and Dynesty - it has not gained wide acceptance beyond that field. A cartoon description of the method is as the simulation version of Lebesgue integration, in that $M$ points are simulated on slices of the likelihood function (delineated by points $t$, $t-1$ in the support of $\boldsymbol{\theta}$), $\{\boldsymbol{\theta};\ L(\boldsymbol{\theta}_{t-1}|\mathbf{y}) \leq L(\boldsymbol{\theta}|\mathbf{y}) \leq L(\boldsymbol{\theta}_t|\mathbf{y})\}$, with each slice having approximately a prior probability, $\exp\{-(t-1)/M\} - \exp\{-(t-1)/M\}$, of occurring. As first shown in Chopin and Robert (2010), nested sampling is a Monte Carlo method with a $\sqrt{M}$ speed of convergence, whose performance relies on the ability to efficiently simulate parameters within the above slices, which is challenging when these are not connected.

## 6.2 Reversible Jump MCMC

All methods described above for computing $p(\mathbf{y}|M_k)$ have one thing in common: the marginal likelihood for *each* model is tackled as a separate computational exercise. Once each $p(\mathbf{y}|M_k)$ is computed, the posterior model probabilities follow, and model choice, or model averaging, can proceed.

As an alternative to this approach, uncertainty about the model can be used to *augment* the set of unknowns, and a posterior sampler designed to target this augmented space. This is the basic principle adopted in a range of papers, including those that focus on variable selection in regression models, and the number of components in finite mixture models; and we refer the reader to George (2000), Marin et al. (2005) and Chib (2011) for reviews and important references. We focus here on one particular approach only, that of Green (1995): being illustrative as it is of the general approach, and representing as it does a key step in the historical development of MCMC algorithms.

Green (1995) characterizes the problem of an unknown model as one in which the dimension of the (model-specific) unknowns *varies*, depending on which model is in play. He thus designs an MCMC sampler that is allowed to *jump* between parameter spaces of differing dimensions; coining the term: 'reversible jump MCMC' (RJMCMC). At its core though, Green's approach is one of augmentation, and can be viewed as a particular application of the original idea of Tanner and Wong (1987), with the extra complexity of dimension variation as the sampler traverses the augmented space.

In brief, Green (1995) assumes a countable collection of candidate models $\mathcal{M} = \{M_1, M_2, ...\}$, indexed by $k = 1, 2, .....$. Each model has a $p_k$-dimensional set of unknown parameters $\boldsymbol{\theta}_k$, where each $p_k$ may well be a different integer. Using obvious notation for the DGP and prior for the *kth* model, and the prior $p(k)$ for the model index itself, the target of the RJMCMC algorithm is then: $p(k, \boldsymbol{\theta}_k|\mathbf{y}) = p(\mathbf{y}|k, \boldsymbol{\theta}_k)p(\boldsymbol{\theta}_k|k)p(k)/p(\mathbf{y})$. The RJMCMC sampler moves between any two parameters spaces by creating temporary auxiliary variables that bring the dimensions of the augmented spaces to be equal, with a reversibility constraint on the proposed moves between these models. Such draws from the joint space of $\{k, \boldsymbol{\theta}_k\}$ can be used to compute any particular $E(g(\boldsymbol{\theta}_k)|\mathbf{y})$ of interest. Indeed, the draws can also be used to compute an expectation of the form: $E(g(k)|\mathbf{y})$, which nests the marginal posterior probability attached to the *kth* model: $p(k|\mathbf{y})$. That is, posterior model probabilities are an automatic outcome of the simulation scheme. Moreover, the computation of *any* expectation of interest incorporates all uncertainty associated with both the parameters of each model and the model itself; hence *model averaging* is automatic. See Green (2003), Fan and Sisson (2011) and Geyer (2011b) for reviews of RJMCMC, including: all theoretical and implementation properties of the algorithm, its links to other 'multi-model' samplers, and the scope of its application.

## 6.3 Computation in Bayesian Prediction

With the single exception of computing of Bayes factors, we have presented all computational methods as a means of performing one particular task: computing the posterior expectation in (4) when no analytical solution is available. Hence, in principle we have already covered the activity of prediction, as this is simply a special case of (4), when $g(\boldsymbol{\theta}) = p(y_{n+1}^*|\boldsymbol{\theta}, \mathbf{y})$, for some point $y_{n+1}^*$ in the support of $y_{n+1}$.

However, it can be argued that Bayesian prediction is more than just a 'special case' of the general Bayesian computational problem.[46] Predicting outcomes that have not yet been observed is arguably the most stringent test to which any model can be put; and the evolution of the large field of prediction (or forecasting) - with Bayesian methods forming part of that - is testament to the singular importance of this particular statistical activity. Hence, our allocation to it of a separate section.

Conditional on an assumed model being 'correctly specified' - i.e. $p(\mathbf{y}|\boldsymbol{\theta})$ coinciding with the true DGP - the 'gold standard' for Bayesian prediction is:

$$p(y_{n+1}^*|\mathbf{y}) = \int_{\Theta} p(y_{n+1}^*|\boldsymbol{\theta}, \mathbf{y})p(\boldsymbol{\theta}|\mathbf{y})d\boldsymbol{\theta}. \tag{37}$$

This density summarizes all uncertainty about $y_{n+1}$, conditional on both the assumed model - which underpins the structure of both the conditional predictive, $p(y_{n+1}^*|\boldsymbol{\theta}, \mathbf{y})$, and the posterior itself - and the prior beliefs that inform $p(\boldsymbol{\theta}|\mathbf{y})$. Point and interval predictions of $y_{n+1}$, and indeed any other distributional summary, can be extracted from (37). In the case where the model itself is uncertain, and a finite set of models, $M_1, M_2,...,M_K$, is assumed to span the model space, the principle of *model averaging* can be used to produce a 'model-averaged' predictive, $p_{MA}(y_{n+1}^*|\mathbf{y})$ as

$$p_{MA}(y_{n+1}^*|\mathbf{y}) = \sum_{k=1}^{K} p(y_{n+1}^*|\mathbf{y}, M_k)p(M_k|\mathbf{y}), \tag{38}$$

where $p(y_{n+1}^*|\mathbf{y}, M_k)$ denotes the density in (37), but conditioned explicitly on the *kth* model in the set. In the typical case where (37) and (38) are unavailable analytically, *any* of the computational methods that have been discussed thus far could be used to compute either $p(y_{n+1}^*|\mathbf{y})$ or $p_{MA}(y_{n+1}^*|\mathbf{y})$, and any summaries thereof. In some ways then, this could be viewed as completing the Bayesian prediction story.

However, recent work has posed the following important question. In cases (such as those highlighted in Section 5.3) where the exact posterior, $p(\boldsymbol{\theta}|\mathbf{y})$, is inaccessible for a given model, and the exact predictive in (37) is thus also unavailable, what is lost - in terms of predictive accuracy - by adopting an approximation to $p(\boldsymbol{\theta}|\mathbf{y})$ and, hence, $p(y_{n+1}^*|\mathbf{y})$? And the answer so far is: not much! In particular, Frazier et al. (2019a) document that an 'approximate predictive' produced by replacing $p(\boldsymbol{\theta}|\mathbf{y})$ with an ABC-based posterior, is numerically indistinguishable in many cases from the exact predictive. Further, under certain conditions, the exact and approximate predictives are shown to be asymptotically (in $n$) equivalent. Related work exploring prediction in approximate inference settings appears in Park and Nassar (2014), Canale and Ruggiero (2016), Koop and Korobilis (2018), Quiroz et al. (2018a) and Kon Kam King et al. (2019).

Finally, Loaiza-Maya et al. (2019) address the arguably more challenging question. How does one even think about Bayesian prediction - and the use of computation therein - when one acknowledges that, in reality: *i)* any given model is misspecified; and *ii)* any finite set of models does not span the truth. The authors propose what they term *focused Bayesian prediction*, in which the likelihood function in the standard Bayesian up-date is replaced by a criterion that captures a user-specified measure of predictive accuracy. Focusing on *the loss that matters* is indeed found to produce superior predictive performance relative to using a misspecified likelihood up-date.

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[46]SMC actually covers prediction as a natural component of the particle filter, due to its temporal nature. This is one of the three goals usually associated with such filters, along with filtering and smoothing.

Indeed, this issue of model misspecification, and the associated move towards more problem-specific loss-based Bayesian up-dates, is identified in Section 7 as one of the key challenges being addressed in the most recent computational literature.

# 7 The Future

Our journey with Bayesian computation began in *1763*: with a posterior probability defined in terms of a scalar $\theta$, whose solution challenged Bayes. We now end our journey in *2020*: having referenced posterior distributions defined over thousands, possibly millions of unknowns, and computational problems with a degree of complexity - and scale - to match. Along the way, we have seen the huge variety of imaginative computational solutions that have been brought to bear on all such problems, over the span of 250 years. A natural question to ask then is: 'what is there left to do?'

Judging from the wealth of contributions to '*Bayes Comp 2020*', in January 2020,[47] the answer to that question is: 'a great deal!'; and *most certainly* as pertains to matters of scale. Indeed, of the 129 abstracts recorded on the conference website, 16 make explicit use of the term *scalability* (or something comparable); 10 refer to the ability of a proposed computational method to deal effectively with *large data sets*, and 22 refer to *high-dimensional problems* of one form or another.[48] Whilst not attempting to cover here the precise nature of these contributions, we comment that there are attempts to *scale* most categories of computational methods reviewed in this paper, and that the scope of the empirical problems to which these advances are applied - from probabilistic topic models, health studies on hypertension and sepsis, problems in neuroimaging, genomics, biology, epidemiology, ecology, psychology and econometrics, through to probabilistic record linkage and geographic profiling - is extremely broad.

But if *scale* may be viewed as a key focus of this selection of research, there is another theme that can also be discerned. A second glance at these conference proceedings and, indeed, at very recent *arXiv.org* submissions and journal publications, pinpoints a growing interest in the impact of *model misspecification* on computational methods.

To provide some context for why this latter topic may indeed be worthy of attention, we remind the reader of an important fact. With the exception of the prediction methodology of Loaiza-Maya et al. (2019) cited in the previous section, all problems for which Bayesian computational solutions have been sought in this review have something in common: *all* are characterized by an assumed DGP, $p(\mathbf{y}|\boldsymbol{\theta})$, or, at best, a finite set of such processes. Computational methods differ, yes, in terms of what features are required for these models (e.g. can they be *evaluated*, or not), and the role the models play in the computational algorithms (e.g. do they need to be *simulated*, or not); however, they are always there, lurking.

The intrinsic role played by $p(\mathbf{y}|\boldsymbol{\theta})$ is, of course, to be expected! This is a review of computational methods in conventional parametric Bayesian settings; and such settings require the assumption of a full parametric model to represent the likelihood function that appears in Bayes' theorem. This does prompt two questions though: *1)* what are the implications for computation if that parametric model is *misspecified*; i.e. if the likelihood function does not match the process that has generated the data?

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[47]http://users.stat.ufl.edu/~jhobert/BayesComp2020/Conf_Website/

[48]There is, of course, some double counting here as certain abstracts make more than one such reference.

And, *2)* what are the implications for computation if the conventional paradigm - based on a likelihood function - is eschewed altogether?

Underpinning the need to address *1)* and *2)* is the following logic: as the scale of data sets has increased, and as our ability to capture finer measurements on phenomena of interest has been honed, the models used to explain such data have grown in complexity. However, this does not imply that such models are in any sense 'closer to the truth' than the simpler models used in the past to explain isolated phenomena. Indeed, the old adage that 'all models are wrong [and] the scientist cannot obtain a "correct" one by excessive elaboration' (Box, 1976) is even more likely to apply to the ambitious modelling exercises that characterize modern statistics. Hence, the implications for Bayesian computation of misspecified likelihoods (question 1), *and* the implications for computation of pursuing non-likelihood-based inference (question 2) are increasingly pertinent.[49]

Remembering that our interest here is indeed on the *implications for computation per se* of both misspecified and non-likelihood settings, we note that specific attempts to address both questions *directly* are still quite small in number, if growing.[50] We complete our review by briefly summarizing *five* recent (sets of) papers in this vein:

i) *First*, Lyddon et al. (2019) and Syring and Martin (2019) use bootstrap principles, of one sort or another, to compute so-called *general Bayesian posteriors*, in which the likelihood function associated with an assumed (and potentially misspecified) model is replaced by a more general loss function that is not tied to a particular model specification. Huggins and Miller (2019) also use the bootstrap to construct so-called 'bagged' posteriors (*BayesBag*), and thereby conduct Bayesian inference that is robust to model misspecification.

ii) *Second*, Frazier et al. (2020) analyze the theoretical properties of ABC under model misspecification; outlining when ABC concentrates posterior mass on an appropriately defined pseudo-true value, and when it does not. The nonstandard asymptotic behaviour of the ABC posterior, including its failure to yield credible sets with valid frequentist coverage, is highlighted. The authors also devise techniques for diagnosing model misspecification in the context of ABC. Frazier and Drovandi (2019) devise a version of BSL that is robust to model misspecification, also developing diagnostic tools.

iii) *Third*, Wang and Blei (2019a) investigate VB under model misspecification. They demonstrate that the VB posterior both concentrates on the value that minimizes the Kullback-Leibler (KL) divergence from the true DGP, and is asymptotically normal; as is the VB posterior mean. These results generalize the asymptotic results for VB of Wang and Blei (2019b), derived under correct specification, to the misspecification case.

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[49]This point is elaborated on in more detail by Knoblauch et al. (2019), in particular with reference to problems in machine learning.

[50]We refer to Kleijn and van der Vaart (2012) and Muller (2013) for general treatments of Bayesian likelihood-based inference in misspecified models; and to Chernozhukov and Hong (2003), Bissiri et al. (2016), Gallant (2016), Giummolè et al. (2017), Holmes and Walker (2017), Chib et al. (2018), Loaiza-Maya et al. (2019) and Miller and Dunson (2019) for various generalizations of the standard Bayesian paradigm, including posterior up-dates driven by problem-specific loss (or moment) functions. It can be argued, however, that in none of these papers are the implications of model misspecification and/or non-likelihood up-dates for computation *per se* the primary focus.

*iv) Fourth*, Knoblauch et al. (2019) propose what they term *generalized variational inference,* by extending the specification of the Bayesian paradigm to accommodate general loss functions (thereby avoiding the reliance on potentially misspecified likelihoods) and building an optimization-based computational tool within that setting.

*v) Fifth*, building on earlier work in the context of HMC (and which is cited therein), Bornn et al. (2019) derive an MCMC scheme for sampling on the lower-dimensional manifold implied by the moment conditions that they adopt within a Bayesian framework. Whilst this work embeds the moments within a nonparametric Bayesian set-up - and we have not discussed computation in nonparametric settings in this review - we make note of this work as an example of a fundamental shift in computational design that is required when moving to a particular *non-likelihood* Bayesian up-date. Whilst not motivated by this same problem, the work on extending VB to manifolds by Tran et al. (2019) is also relevant here.

Bayesian computation in parametric models is thus beginning to confront - and adapt to - the reality of misspecified DGPs, and the generalizations beyond the standard likelihood-based up-date that are evolving. Allied with the growing ability of computational methods to also deal with the scale of modern problems, the future of the paradigm in the 21st century thus seems assured. And with this, the 18th century Bayes (and his loyal champion, Price) would no doubt be duly impressed!

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