On computational tools for Bayesian data analysis

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Abstract

While the previous chapter (Robert and Rousseau, 2010) addressed the foundational aspects of Bayesian analysis, the current chapter details its practical aspects through a review of the computational methods available for approximating Bayesian procedures. Recent innovations like Monte Carlo Markov chain, sequential Monte Carlo methods and more recently Approximate Bayesian Computation techniques have considerably increased the potential for Bayesian applications and they have consequently opened new avenues for Bayesian inference, first and foremost Bayesian model choice.

Keywords: Bayesian inference, Monte Carlo methods, MCMC algorithms, Approximate Bayesian Computation techniques, adaptivity, latent variables models, model choice.

1 Introduction

The previous chapter (Robert and Rousseau, 2010) has (hopefully) stressed the unique coherence of Bayesian data analysis—the complete inferential spectrum (estimators, predictors, tests, confidence regions, etc.) is derived from a unique perspective, once both a loss function and a prior distribution are constructed—, but it has not addressed the complex issues related to the practical implementation of this analysis that usually involves solving integration, optimisation and implicit equation problems, most often simultaneously.

This computational challenge offered by Bayesian inference has led to a specific branch of Bayesian statistics concerned with these issues, from the early approximations of Laplace to the numerical probability developments of the current days. In particular, the past twenty years have witnessed a tremendous surge in computational Bayesian statistics, due to the introduction of powerful approximation methods like Markov chain (MCMC) and sequential Monte Carlo techniques. To some extent, this branch of Bayesian statistics is now so intricately connected with Bayesian inference that some notions like Bayesian model choice and Bayesian model comparison hardly make sense without it.

The probabilistic nature of the objects, involved in those computational challenges, as well as their potentially high dimension, led the community to opt for simulation based, rather than numerical, solutions. While numerical techniques are indeed used to solve some optimisation or some approximation setups, even producing specific approaches like variational Bayes (Jaakkola and Jordan 2000), the method of choice is simulation, i.e. essentially the use of computer generated random variables and the reliance on the Law of Large Numbers. For instance, all major softwares that have been built towards Bayesian data analysis like WinBUGS and JAGS, are entirely depending upon simulation approximations. We will therefore abstain from describing any further the nu-
merical advances found in this area, referring the reader to Spall (2003) and Gentle (2009) for proper coverage.

In this chapter, we thus discuss simulated-based computational methods in connection with a few model choice examples (Section 2), separating non-Markovian (Section 3) from Markovian (Section 1) solutions. For detailed entries on Bayesian computational statistics, we refer the reader to Chen et al. (2000), Liu (2001) or Robert and Casella (2004, 2009), pointing out that books like Albert (2009) and Marin and Robert (2007) encompass both Bayesian inference and computational methodologies in a single unifying perspective.

2 Computational difficulties

In this section, we consider two particular types of statistical models with computational challenges that can only be processed via simulation.

2.1 Generalised linear models

Generalised linear models (McCullagh and Nelder 1989) are extensions of the standard linear regression model. In particular, they bypass the compulsory selection of a single transformation of the data that must achieve the possibly conflicting goals of normality and linearity, goals which are imposed by the linear regression model but that are impossible to achieve for binary or count responses.

Generalised linear models formalise the connection between a response variable \( y \in \mathbb{R} \) and a vector \( x \in \mathbb{R}^p \) of explanatory variables. They assume that the dependence of \( y \) on \( x \) is partly linear in the sense that the conditional distribution of \( y \) given \( x \) is defined in terms of a linear combination \( x^T \beta \) of the components of \( x \) (\( x^T \) being the transpose of \( x \)),

\[
y | x, \beta \sim f(y | x^T \beta).
\]

We use the notation \( y = (y_1, \ldots, y_n) \) for a sample of \( n \) responses and

\[
X = [x_1 \ldots x_p] = \begin{bmatrix} x_{11} & x_{12} & \ldots & x_{1p} \\ x_{21} & x_{22} & \ldots & x_{2p} \\ x_{31} & x_{32} & \ldots & x_{3p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \ldots & x_{np} \end{bmatrix}
\]

for the \( n \times p \) matrix of corresponding explanatory variables, possibly with \( x_{11} = \ldots = x_{n1} = 1 \) (\( y \) and \( x \) correspond to generic notations for single-response and covariate vectors, respectively).

A generalized linear model is specified by two functions:

(i) a conditional density \( f \) on \( y \) conditional on \( x \) that belongs to an exponential family and that is parameterized by an expectation parameter \( \mu = \mu(x) = E[y|x] \) and possibly a dispersion parameter \( \phi > 0 \) that does not depend on \( x \); and

(ii) a link function \( k \) that relates the mean \( \mu = \mu(x) \) of \( f \) and the covariate vector, \( x \), through \( k(\mu) = (x^T \beta) \), \( \beta \in \mathbb{R}^p \).

For identifiability reasons, the link function \( k \) is a one-to-one function and we have

\[
E[y|x, \beta, \phi] = k^{-1} (x^T \beta).
\]

We can thus write the (conditional) likelihood as

\[
\ell(\beta, \phi | y, X) = \prod_{i=1}^{n} f(y_i | x_i^T \beta, \phi).
\]

In practical applications like econometrics or genomics, \( p \) can be very large and even larger than the number of observations \( n \). Bayesian data analysis on \( \beta \) and possibly \( \phi \) proceeds through the posterior distribution of \( (\beta, \phi) \) given \( (X, y) \):

\[
\pi(\beta, \phi | X, y) \propto \prod_{i=1}^{n} f(y_i | x_i^T \beta, \phi) \pi(\beta, \phi | X) \tag{1}
\]

which is never available as a standard distribution outside the normal linear model. Indeed, the choice of the prior distribution \( \pi(\beta, \phi | X) \) depends on the prior information available to the modeller. In cases when
\(\phi = 1\), we will use the default solution advocated in [Marin and Robert (2007)], namely the extension of Zellner’s g-prior that was originally introduced for the linear model, as discussed in the previous chapter:

\[
\beta | X \sim \mathcal{N} \left( 0, n (X^T X)^{-1} \right).
\]

The motivation behind the factor \(n\) is that the information brought by the prior is scaled to the level of a single observation. Even this simple modeling does not avoid the computational issue of exploiting the posterior density \(\Pi\).

**Example 1.** A specific if standard case of generalised linear model for binary data is the *probit model*:

\[
P(Y = 1 | x) = 1 - P(Y = 0 | x) = \Phi(x^T \beta),
\]

where \(\Phi\) denotes the standard normal cumulative distribution function. Under the g-prior \(\pi(\beta | X)\) presented above, the corresponding posterior distribution, proportional to

\[
\pi(\beta | X) \prod_{i=1}^{n} \Phi(x_i^T \beta)^{y_i} \Phi(-x_i^T \beta)^{1-y_i}, \tag{2}
\]

is available in closed form, up to the normalising constant, but is not a standard distribution and thus cannot be easily handled!

In this chapter, we will use as illustrative data the Pima Indian diabetes study available in R (R Development Core Team 2008) as the Pima.tr dataset with 332 women registered and consider a probit model predicting the presence of diabetes from three predictors, the glucose concentration (glu), the diastolic blood (bp) pressure and the diabetes pedigree function (ped).

\[
P(y = 1 | x) = \Phi(x_1 \beta_1 + x_2 \beta_2 + x_3 \beta_3).
\]

A maximum likelihood estimate of the regression coefficients is provided by R glm function as

\[
\text{Estimate} \quad \text{Std. Error} \quad z \text{ value} \quad \text{Pr}(>|z|)
\]

- \(\text{glu} \quad 0.012616 \quad 0.002406 \quad 5.244 \quad 1.57e-07 \quad ***\)
- \(\text{bp} \quad -0.029050 \quad 0.004094 \quad -7.096 \quad 1.28e-12 \quad ***\)
- \(\text{ped} \quad 0.350301 \quad 0.208806 \quad 1.678 \quad 0.0934 \quad .\)

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Signif. codes: ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1

Null deviance: 460.25 on 332 degrees of freedom
Residual deviance: 386.73 on 329 degrees of freedom
AIC: 392.73

Number of Fisher Scoring iterations: 4

the final column of stars indicating a possible significance of the first two covariates from a classical viewpoint.

This type of model is characteristic of conditional models where there exist a plethora of covariates \(x_i\)—again, potentially more than there are observations—and one of the strengths of Bayesian data analysis is to be able to assess the impact of those covariates on the dependent variable \(y\). This obviously is a special case of model choice, where a given set of covariates is associated with a specific model. As discussed in the previous chapter, the standard Bayesian solution in this setting is to compute posterior probabilities or Bayes factors for all models in competition. For instance, if a single covariate, \(x_3\) (ped) say, is under scrutiny, the Bayes factor associated with the null hypothesis \(H_0: \beta_3 = 0\) is

\[
B_{01}^\pi = \frac{m_0(y)}{m_1(y)} \tag{3}
\]

where \(m_0\) and \(m_1\) are the marginal densities under the null and the alternative hypotheses, i.e.

\[
m_i(y) = \int f(y | \beta, X_i) \pi_i(\beta | X_i) d\beta,
\]

\(\pi_0\) being the g-prior excluding the covariate \(x_3\).

If we denote by \(X_0\) the \(332 \times 2\) matrix containing the values of glu and bp for the 332 individuals and by \(X_1\) the \(332 \times 3\) matrix containing the values of the covariates glu, bp and ped, the Bayes factor \(B_{01}\) is given by

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As will become clearer in Section 3.3, Bayes factor approximations are intrinsically linked with the normalising constants of the posterior distributions of the models under competition. We already stressed in Robert and Rousseau (2010) that this is a special case when normalising constants matter!
using the shortcut notation that $A_i.$ is the $i$-th line of the matrix $A$.

The approximation of those marginal densities, which are not available outside the normal model (see, e.g., Marin and Robert 2007, Chapter 3), is thus paramount to decide about the inclusion of available covariates.

In this setting of selecting covariates in a conditional model, an additional and non-negligible computational difficulty is that the number of hypotheses to be tested is $2^p$ if each of the $p$ covariates is under scrutiny. When $p$ is large, it is simply impossible to envision all possible subsets of covariates and a further level of approximation must be accepted, namely that only the most likely subsets will be visited by an approximation method.

### 2.2 Challenging likelihoods

A further degree of difficulty in the computational processing of Bayesian models is reached when the likelihood function itself cannot be computed in a reasonable amount of time. Examples abound in econometrics, physics, astronomy, genetics, and beyond. The level of difficulty may be that the computation time of one single value of the likelihood function requires several seconds, as in the cosmology analysis of Wraith et al. (2009) where the likelihood is represented by an involved computer program. It may also be that the only possible representation of the likelihood function is as an integral over a possibly large number of latent variables of a joint (unobserved) likelihood.

**Example 2.** (Continuation of Example 1) Although the likelihood of a probit model is available in closed form, this probit model can be represented as a natural latent variable model. If we introduce an artificial sample $z = (z_1, \ldots, z_n)$ of $n$ independent latent variables associated with a standard regression model, i.e. such that $z_i | \beta \sim N(x_i^T \beta, 1)$, where the $x_i$'s are the $p$-dimensional covariates and $\beta$ is the vector of regression coefficients, then $y = (y_1, \ldots, y_n)$ defined by $y_i = 1_{z_i > 0}$ is a probit sample. Indeed, given $\beta$, the $y_i$'s are independent Bernoulli rv’s with $P(Y_i = 1|x_i, \beta) = \Phi (x_i^T \beta)$.

Such latent variables models are quite popular in most applied fields. For instance, a stochastic volatility model (Jacquier et al. 1994; Chib et al. 2002) includes as many (volatility) latent variables as observations. In a time series with thousands of periods, this feature means a considerable increase in the complexity of the problem, as the volatilities cannot be integrated analytically and thus need to be simulated. Similarly, phylogenetic trees (REF) that reconstruct ancestral histories in population genetics are random trees and a nuisance parameter for inference about evolutionary mechanisms, but, once more, they cannot be integrated.

**Example 3.** Capture-recapture experiments are used in ecology to assess the size and the patterns of a population of animals by a series of captures where captured animals are marked, i.e. individually identified as having been captured once, and released. The occurrence of recaptures is then informative about the whole population. A longer description is provided in Marin and Robert (2007, Chapter 5), but we only consider here a three stage open population capture-recapture model, where there is a probability $q$ for each individual in the population to leave the population between each capture episode. Due to this possible emigration of animals, the associated likelihood involves unobserved indicators and we study here the case where only the individuals captured during the first capture experiment are marked and subsequent recaptures are registered. This model is thus described via the summary statistics

$$
\begin{align*}
    n_1 & \sim \mathcal{B}(N,p), \\
    r_1 | n_1 & \sim \mathcal{B}(n_1, q), \\
    r_2 | n_1, r_1 & \sim \mathcal{B}(n_1 - r_1, q), \\
    c_2 | n_1, r_1 & \sim \mathcal{B}(n_1 - r_1, p), \\
    c_3 | n_1, r_1, r_2 & \sim \mathcal{B}(n_1 - r_1 - r_2, p),
\end{align*}
$$
where only the first capture size, \( n_1 \), the first recapture size, \( c_2 \), and the second recapture size, \( c_3 \), are observed. The numbers of marked individuals removed at stages 1 and 2, \( r_1 \) and \( r_2 \), are not observed and are therefore latent variables of the model. If we incorporate those missing variables within the parameters, the likelihood \( \ell(N, p, q, r_1, r_2| n_1, c_2, c_3) \) is given by

\[
\left( \frac{N}{n_1} \right)^{n_1} (1 - p)^{N-n_1} \left( \frac{n_1}{r_1} \right)^{q^{r_1}(1 - q)^{n_1-r_1}} \times \left( \frac{n_1 - r_1}{c_2} \right)^{p^{c_2}(1 - p)^{n_1-r_1-c_2}} \times \left( \frac{n_1 - r_1}{r_2} \right)^{q^{r_2}(1 - q)^{n_1-r_1-r_2}} \times \left( \frac{n_1 - r_1 - r_2}{c_3} \right)^{p^{c_3}(1 - p)^{n_1-r_1-r_2-c_3}}
\]

and, if we use the improper prior \( \pi(N, p, q) = N^{-1} I_{[0,1]}(p) I_{[0,1]}(q) \), the posterior on the \( (N, p, q, r_1, r_2| n_1, c_2, c_3) \) is available up to a constant.

Summing over all possible values of \( (r_1, r_2) \) to obtain the posterior associated with the “observed” likelihood creates some difficulties when \( n_1 \) is large. Indeed, this summation typically introduces a lot of numerical errors.

The dataset associated with this example is extracted from Marin and Robert’s (2007) Chapter 5 eurordip dataset and is related to a population of birds called European dippers. For the 1981 captures, we have \( n_1 = 22, c_2 = 11, \) and \( c_3 = 6 \). \( \Box \)

The following example is a different case where the likelihood is missing a term that cannot be reconstructed by completion and thus requires a custom-built solution.

**Example 4.** The \( k \)-nearest-neighbour procedure is a classification procedure that uses a training dataset \( \{y_i, x_i\}_{1 \leq i \leq n} \) for prediction purposes. The observables \( y_i \) are class labels, \( y_i \in \{1, \ldots, G\} \), while the \( x_i \) are covariates, possible of large dimension. When observing a new covariate \( x_{n+1} \), the corresponding unobserved label \( y_{n+1} \) is predicted as the most common class label found in the \( k \) nearest neighbours of \( x_{n+1} \) in \( X = \{x_1, \ldots, x_n\} \), the neighbours of a covariate vector being defined by the usual Euclidean norm. Cucala et al. (2009) have proposed a probabilistic model for this classification mechanism. They first propose to model the distribution of \( y \):

\[
f(y|X, \beta, k) = \exp \left( \frac{\beta}{k} \sum_{i \sim k} \delta_{y_i}(y) + \sum_{i \sim k} \delta_{y_i}(y) \right) \Big/ Z(\beta, k)
\]

where \( \delta_{y}(y) \) denotes the Kroenecker delta, \( Z(\beta, k) \) is the normalising constant of the density and where \( \ell \sim i \) means that the summation is taken over the observations \( x_i \) for which \( x_i \) is a \( k \)-nearest neighbour.

The motivation for this modelling is that the full conditionals corresponding to (4) are given by

\[
f(y_i|y_{-i}, X, \beta, k) \propto \exp \left( \frac{\beta}{k} \sum_{i \sim k} \delta_{y_i}(y) + \sum_{i \sim k} \delta_{y_i}(y) \right).
\]

The normalising constant \( Z(\beta, k) \) cannot therefore be expressed in closed form. Indeed, the computation of this constant calls for a summation over \( G^n \) terms.

Based on (5), the predictive distribution of a new observation \( y_{n+1} \) given its covariate \( x_{n+1} \) and the training sample \( \{y, X\} \) is, for \( g = 1, \ldots, G \),

\[
P(y_{n+1} = g|x_{n+1}, y, X, \beta, k) \propto \exp \left( \frac{\beta}{k} \sum_{\ell \sim k} \delta_g(y_{\ell}) + \sum_{(n+1) \sim k} \delta_{y_i}(g) \right),
\]

where

\[
\sum_{\ell \sim k} \delta_g(y_{\ell}) \quad \text{and} \quad \sum_{(n+1) \sim k} \delta_{y_i}(g)
\]

are the numbers of observations in the training dataset from class \( g \) among the \( k \) nearest neighbours of \( x_{n+1} \) and among the observations for which \( x_{n+1} \) is a \( k \)-nearest neighbour, respectively. \( \Box \)
3 Monte Carlo Methods

The generic approach for solving computational problems related with Bayesian analysis is to use simulation, i.e. to produce via a computer program a sample from the posterior distribution and to use the simulated sample to approximate the procedures of interest. This approach goes under the generic name of Monte Carlo methods, in reference to the casino of Monaco (Metropolis 1987). Recall that a standard Bayesian estimate is the posterior expectation of functions $h(\theta)$ of the parameter,

$$I = \int_{\Theta} h(\theta) \pi(\theta | y) \, d\theta.$$

A formal Monte Carlo algorithm associated with the target $I$ proceeds as follows:

**Basic Monte Carlo Algorithm**

For a computing effort $N$

1) Set $i = 1$,

2) Generate independent $\theta^{(i)}$ from the posterior distribution $\pi(\cdot | y)$,

3) Set $i = i + 1$,

4) If $i \leq N$, return to 2).

The corresponding crude Monte Carlo approximation of $I$ is given by:

$$\hat{I}_{MC} = \frac{1}{N} \sum_{i=1}^{N} h(\theta^{(i)}).$$

When the computing effort $N$ grows to infinity, the approximation $\hat{I}_{MC}$ converges to $I$ and the speed of convergence is $1/\sqrt{N}$ if $h$ is square-integrable against $\pi(\cdot | y)$ (Robert and Casella 2004). The assessment of this convergence relies on the Central Limit Theorem, as described in Robert and Casella (2009, Chapter 4).

3.1 Importance sampling and resampling

A generalisation of the basic Monte Carlo algorithm stems from an alternative representation of the above integral $I$, changing both the integrating density and the integrand:

$$I = \int_{\Theta} \frac{h(\theta) \pi(\theta | y)}{g(\theta)} g(\theta) \, d\theta,$$

where the support of the posterior distribution $\pi(\cdot | y)$ is included in the support of $g(\cdot)$.

**Importance Sampling Scheme**

For a computing effort $N$

1) Set $i = 1$,

2) Generate independent $\theta^{(i)}$ from the importance distribution $g(\cdot)$,

3) Calculate the importance weight $\omega^{(i)} = \frac{\pi(\theta^{(i)} | y)}{g(\theta^{(i)})}$.

4) Set $i = i + 1$,

5) If $i \leq N$, return to 2).

The corresponding importance sampling approximation of $I$ is given by

$$\hat{I}_{IS} = \frac{1}{N} \sum_{i=1}^{N} \omega^{(i)} h(\theta^{(i)}).$$

From a formal perspective, the posterior density $g(\theta) = \pi(\theta | y)$ is a possible (and the most natural) choice for the importance function $g(\cdot)$, leading back to the basic Monte Carlo algorithm. However, (6) states that a single integral may be approximated in infinitely many ways. Maybe surprisingly, the choice of the posterior $g(\theta) = \pi(\theta | y)$ is generally far from being the most efficient choice of importance function. While the representation (6) holds in wide generality (the only requirement is that the support of $\pi(\cdot | x)$ should be included in the one of $g(\cdot)$), the choice of $g(\cdot)$ is fundamental to provide good approximations of $I$. Poor choices of $g(\cdot)$ lead to unreliable approximations: for instance, if

$$\int_{\Theta} h^{2}(\theta) \omega^{2}(\theta) g(\theta) \, d\theta$$
is infinite, the variance of the estimator \( \hat{\omega} \) is also infinite (Robert and Casella [2009], Chapters 3 and 4) and then \( \hat{\omega} \) cannot be used for approximation purposes.

We stress here that, while Monte Carlo methods do not formally suffer from the “curse of dimensionality” in the sense that, contrary to numerical methods, the error of the Monte Carlo estimators is always decreasing in \( 1/\sqrt{N} \), notwithstanding the dimension of the parameter space \( \Theta \), the difficulty increases with the dimension \( p \) of \( \Theta \) in that deriving satisfactory importance sampling distributions becomes more difficult as \( p \) gets larger. As detailed in Section 3.2, a solution for deriving satisfactory importance functions in large dimensions is to turn to iterative versions of importance sampling.

**Example 5** (Continuation of Example 4). In the case of the probit model, the posterior distribution, proportional to \( \pi(\beta|X, y) \) cannot be easily simulated, even though it is bounded from above by the prior density \( \pi(\beta|X) \).

In this setting, we propose to use as importance distribution a normal distribution with mean equal to the maximum likelihood (ML) estimate of \( \beta \) and with covariance matrix equal to the estimated covariance matrix of the ML estimate. While, in general, those normal distributions provide crude approximations to the posterior distributions, the specific case of the probit model shows this is an exceptionally good approximation to the posterior. For instance, if we compare the weights resulting from using this normal distribution with the weights resulting from using the prior distribution as importance function, the range of the former weights is much more concentrated than for the later weights, as shown by Figure 1. (Note that, due to the missing normalising constant in \( \pi(\beta|X, y) \), the weights are computed with the product \( \pi(\beta|X) \) as the target function.)

As noted in the above example, a common feature of Bayesian integration settings is that the normalising constant of the posterior distribution, \( m(y) \), cannot be computed in closed form. In that case, \( \omega(i) \) and \( \hat{\omega} \) cannot be used and they are replaced by the unnormalised version

\[
\omega(i) = m(y)\pi(\theta(i)|y)/g(\theta(i))
\]

and by the self-normalized version

\[
\hat{\omega}_{SNIS} = \sum_{i=1}^{N} \omega(i)h(\theta(i))/\sum_{i=1}^{N} \omega(i),
\]

respectively. The self-normalized \( \hat{\omega}_{SNIS} \) also converges to \( \mathbb{I} \) since \( \sum_{i=1}^{N} \omega(i) \) converges to the normalising constant \( m(y) \). The weights \( (i = 1, \ldots, T) \) are then called *normalised weights* and, since they sum up to one, they induce a probability distribution on the sample of \( \theta(i) \)'s. When choosing an importance function, the adequation with the posterior distribution needs to get higher as the dimension \( p \) increases. Otherwise, very few weights \( \pi(i) \) are different from 0 and even the largest weight, which is then close to 1, may correspond to an unlikely value for the posterior distribution, its closeness to 1 being then an artifact of the renormalisation and not an indicator of its worth. A related measure of performance of the importance function is given by the *effective sample size*

\[
\text{ESS}_N = 1/\sum_{i=1}^{N} (\pi(i))^2.
\]

For a uniformly weighted sample, \( \text{ESS}_N \) is equal to \( N \), while, for a completely degenerated sample where all importance weights but one are zero, \( \text{ESS}_N \) is equal to 1. The effective sample size thus evaluates the size of the iid sample equivalent to the weighted sample and allows for a direct comparison of samplers.

**Example 6** (Continuation of Example 5). For the two schemes tested in the probit model of Example 5 using the same number \( N = 10,000 \) of simulations, the effective sample sizes are \( T_1 = 6291.45 \) and \( T_2 = 9.77 \) for the ML based and prior normal importance functions, respectively.
While importance sampling is primarily an integral approximation methodology, it can also be used for simulation purposes, via the sampling importance resampling (SIR) methodology of Rubin (1988). Given a weighted sample \((\theta^{(1)}, \omega^{(1)}), \ldots, (\theta^{(N)}, \omega^{(N)})\) simulated from \(q(\cdot)\), it is possible to derive a sample approximately distributed from the target distribution \(\pi(\cdot|x)\), \(\tilde{\theta}^{(1)}, \ldots, \tilde{\theta}^{(M)}\), by resampling from the instrumental sample \(\theta^{(1)}, \ldots, \theta^{(N)}\) using the importance weights, that is,

\[
\tilde{\theta}^{(i)} = \theta^{(J_i)}, \quad 1 \leq i \leq M,
\]

where the random variables \(J_1, \ldots, J_M\) are distributed as

\[
P(J_i = j | \theta^{(1)}, \ldots, \theta^{(N)}) = \pi^{(i)}(\cdot|\cdot)
\]

(see, e.g., Robert and Casella 2009, Chapter 3).

### 3.2 Sequential importance sampling

In general, importance sampling techniques require a rather careful tuning to be of any use, especially in large dimensions. While MCMC methods (Section 1) are a ready-made solution to this problem, given that they can break the global distribution into distributions with smaller dimensions, the recent literature has seen an extension of importance sampling that adaptively calibrates some importance functions towards more similarity with the target density (Cappé et al. 2004, Del Moral et al. 2006, Douc et al. 2007a, Cappé et al. 2008). The method is called sequential Monte Carlo (SMC) because it evolves along a time axis either through the target—as in regular sequential statistical problems—or through the importance function, and also population Monte Carlo (PMC), following Iba (2000), because it produces populations rather than points. Although the idea has connections with the earlier particle filter literature (Gordon et al. 1993, Doucet et al. 2001, Cappé et al. 2004), the main principle of this method is to build a sequence of increasingly better—against a performance criterion that may be the entropy divergence from the target distribution or the variance of the corresponding estimator of a fixed integral—proposal distributions through a sequence of simulated samples (which thus behave like populations). Given that the validation

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4 This simulated population is then used to devise new and hopefully improved importance (or proposals) functions.
of the technique is still based on sampling importance resampling principles, the resulting dependence on past samples can be arbitrarily complex, while the approximation to the target remains valid (unbiased) at each iteration and while it does not require asymptotic convergence as MCMC methods do (see Section 4). A very recent connection between both approaches can be found in Andrieu et al. (2010) and the discussion therein.

While the following algorithm does appear as a repeated (or sequential) sampling importance resampling algorithm (Rubin 1988), the major update is the open choice of \( q \) in the first step, since \( q \) can depend on all past simulated samples as well as on the index of the currently simulated value. For instance, in Cappé et al. (2008), mixtures of standard kernels are used with an update of the weights and of the parameters of those kernels at each iteration in such a way that the entropy distance of the corresponding importance sampling estimator to the target are decreasing from one iteration to the other.

### General Population Monte Carlo Algorithm

For a computing effort \( N \)

1. Generate \( (\theta_{i,0})_{1 \leq i \leq N} \) iid \( q_0 \) and compute \( \omega_{i,0} = \pi(\theta_{i,0}|y)/q_0(\theta_{i,0}) \),
2. Generate \( (J_{i,0})_{1 \leq i \leq N} \) iid \( \mathcal{M}(1, (\varpi_{i,0})_{1 \leq i \leq N}) \) and set \( \theta_{i,0} = \theta_{J_{i,0},0} \) (1 \( \leq i \leq N \)),
3. Set \( t = 1 \),
4. Conditionally on past \( \theta_{i,j} \)'s and \( \theta_{i,j} \)'s, generate independently \( \theta_{i,t} \sim q_{i,t} \) and compute \( \omega_{i,t} = \pi(\theta_{i,t}|y)/q_{i,t}(\theta_{i,t}) \),
5. Generate \( (J_{i,t})_{1 \leq i \leq N} \) iid \( \mathcal{M}(1, (\varpi_{i,t})_{1 \leq i \leq N}) \) and set \( \theta_{i,t} = \theta_{J_{i,t},t} \) (1 \( \leq i \leq N \)),
6. Set \( t = t + 1 \),
7. If \( t \leq N \) return to 4).

In this representation, while the choice of \( q_{i,t} \) is completely open, a convenient case is when the \( \theta_{i,t} \)'s are simulated either from a non-parametric kernel-like proposal of the form

\[
\sum_{j=1}^{n} \theta_{j,t-1} K_i(\theta_{j,t-1}, \theta),
\]

where \( K_i \) is a Markov kernel modified at each iteration (Douc et al. 2007b) or from a mixture of the form

\[
\sum_{j=1}^{n} \theta_{j,t-1} g_j(\theta_{j,t-1} | \xi_{j,t-1}),
\]

where \( g_j \) is a standard distribution from an exponential family parameterised by \( \xi \), both parameters and weights being updated at each iteration (Cappé et al. 2008). An illustration of the performances of this PMC algorithm for a cosmological target is given in Wraith et al. (2009), while an ABC extension has been introduced by Beaumont et al. (2009).

Since PMC produces at each iteration a valid approximation to the target distribution, the populations \( \theta_{i,t} \) produced at each of those iterations should not be dismissed for approximation purposes. Cornuet et al. (2009) have developed a nearly optimal strategy recycling all past simulations, based on the multiple mixture technique of Owen and Zhou (2000) and called adaptive multiple importance sampling (AMIS).

### 3.3 Approximations of the Bayes factor

As already explained above, when testing for an null hypothesis (or a model) \( H_0 : \theta \in \Theta_0 \) against the alternative hypothesis (or the alternative model) \( H_1 : \theta \in \Theta_1 \), the Bayes factor is defined by

\[
B_{01}(y) = \frac{\int_{\Theta_0} f_0(y|\theta_0) \pi_0(\theta_0) d\theta_0}{\int_{\Theta_1} f_1(y|\theta_1) \pi_1(\theta_1) d\theta_1}.
\]

The computation of Monte Carlo approximations of the Bayes factor (3) has undergone rapid changes in the last decade as illustrated by the book of Chen et al. (2000) and the recent survey of Robert and
Marin (2010). We assume here that the prior distributions under both the null and the alternative hypotheses are proper, as, typically they should be. (In the case of common nuisance parameters, a common improper prior measure can be used on those, see Berger et al. (1998), Marin and Robert (2007). This complicates the computational aspect, as some methods like crude Monte Carlo cannot be used at all, while others are more prone to suffer from infinite variance.) In that setting, the most elementary approximation to \( B_{01}(y) \) consists in using a ratio of two standard Monte Carlo approximations based on simulations from the corresponding priors. Indeed, for \( i = 0, 1 \):

\[
\int_{\Theta_i} f_i(y|\theta) \pi_i(\theta) d\theta = \mathbb{E}_{\pi_i} [f(y|\theta)].
\]

Then, if \( \theta_{0,1}, \ldots, \theta_{0,n_0} \) and \( \theta_{1,1}, \ldots, \theta_{1,n_1} \) are two independent samples generated from the prior distributions \( \pi_0 \) and \( \pi_1 \), respectively,

\[
\frac{n_0^{-1} \sum_{j=1}^{n_0} f_0(y|\theta_{0,j})}{n_1^{-1} \sum_{j=1}^{n_1} f_1(y|\theta_{1,j})}
\]

is a strongly consistent estimator of \( B_{01}(y) \).

Defining two importance distributions with densities \( g_0 \) and \( g_1 \), with the same supports as \( \pi_0 \) and \( \pi_1 \), respectively, we have:

\[
B_{01}(y) = \frac{\mathbb{E}_{g_0} [f_0(y|\theta) \pi_0(\theta)/g_0(\theta)]}{\mathbb{E}_{g_1} [f_1(y|\theta) \pi_1(\theta)/g_1(\theta)].}
\]

Therefore, given two independent samples generated from distributions \( g_0 \) and \( g_1 \), respectively, \( \theta_{0,1}, \ldots, \theta_{0,n_0} \) and \( \theta_{1,1}, \ldots, \theta_{1,n_1} \), the corresponding importance sampling estimate of \( B_{01}(y) \) is

\[
\frac{n_0^{-1} \sum_{j=1}^{n_0} f_0(y|\theta_{0,j}) \pi_0(\theta_{0,j})/g_0(\theta_{0,j})}{n_1^{-1} \sum_{j=1}^{n_1} f_1(y|\theta_{1,j}) \pi_1(\theta_{1,j})/g_1(\theta_{1,j})}.\]

Compared with the standard Monte Carlo approximation above, this approach offers the advantage of opening the choice of the representation in that it is possible to pick importance distributions \( g_0 \) and \( g_1 \) that lead to a significant reduction in the variance of the importance sampling estimate.

In the special case when the parameter spaces of both models under comparison are identical, i.e., \( \Theta_0 = \Theta_1 \), a bridge sampling approach (Meng and Wong 1996) is based on the general representation

\[
B_{01}(y) = \frac{\int f_0(y|\theta) \pi_0(\theta) \alpha(\theta) \pi_1(\theta|y) d\theta}{\int f_1(y|\theta) \pi_1(\theta) \alpha(\theta) \pi_0(\theta|y) d\theta}
\]

\[
\approx \frac{n_1^{-1} \sum_{j=1}^{n_1} f_0(y|\theta_{1,j}) \pi_0(\theta_{1,j}) \alpha(\theta_{1,j})}{n_0^{-1} \sum_{j=1}^{n_0} f_1(y|\theta_{0,j}) \pi_1(\theta_{0,j}) \alpha(\theta_{0,j})}
\]

where \( \theta_{0,1}, \ldots, \theta_{0,n_0} \) and \( \theta_{1,1}, \ldots, \theta_{1,n_1} \) are two independent samples coming from the posterior distributions \( \pi_0(\theta|y) \) and \( \pi_1(\theta|y) \), respectively. That applies for any positive function \( \alpha \) such that the upper integral exists. Some choices of \( \alpha \) can lead to very poor performances of the method in connection with the harmonic mean approach (see below), but there exists a quasi-optimal solution, as provided by Gelman and Meng (1998):

\[
\alpha^*(y) \propto \frac{1}{n_0 \pi_0(\theta|y) + n_1 \pi_1(\theta|y)}.
\]

This optimum cannot be used per se, since it requires the normalising constants of both \( \pi_0(\theta|y) \) and \( \pi_1(\theta|y) \). As suggested by Gelman and Meng (1998), an approximate but practical version uses iterative versions of \( \alpha^* \), the current approximation of \( \alpha^* \) being used to produce a new bridge sampling approximation of \( B_{01}(y) \), which in its turn is used to set a new approximation of \( \alpha^* \). Note that this solution recycles simulations from both posteriors, which is quite appropriate since one model is selected via the Bayes factor, instead of using an importance weighted sample common to both approximations. We will see below an alternative representation of the bridge factor that bypasses this difficulty (if difficulty there is!).

Those derivations are however restricted to the case when both models have the same complexity and
thus they do not apply to embedded models, when 
\( \Theta_0 \subset \Theta_1 \) in such a way that \( \theta_1 = (\theta, \psi) \), i.e. when
the submodel corresponds to a specific value \( \psi_0 \) of \( \psi \):
\( f_0(y|\theta) = f_1(y|\theta, \psi_0) \).

The extension of the most advanced bridge sampling
tactics to such cases requires the introduction of a
density between both parameter spaces. Indeed, if we augment
\( \pi_0(\theta|y) \) with \( \omega(\psi|\theta, y) \), we obtain a joint distribution
with density \( \pi_0(\theta|y) \times \omega(\psi|\theta, y) \) on \( \Theta_1 \). The Bayes
factor \( B_{01}(y) \) can then be expressed as
\[
\int_{\Theta_1} f_1(y|\theta, \psi) \pi_0(\theta) \alpha(\theta, \psi) \pi_1(\theta, \psi|y) d\theta \omega(\psi|\theta, y) d\psi,
\]
(8)
because it is clearly independent from the choice of both
\( \alpha(\theta, \psi) \) and \( \omega(\psi|\theta, y) \). Obviously, the performances
of the approximation
\[
(n_1)^{-1} \sum_{j=1}^{n_1} f_1(y|\theta_{1,j}, \psi_0) \pi_0(\theta_{1,j}) \omega(\psi_{1,j}|\theta_{1,j}, y) \alpha(\theta_{1,j}, \psi_{1,j})
\]
\[
(n_0)^{-1} \sum_{j=1}^{n_0} f_1(y|\theta_{0,j}, \psi_0) \pi_1(\theta_{0,j}) \omega(\psi_{1,j}|\theta_{0,j}, y) \alpha(\theta_{0,j}, \psi_{0,j}),
\]
where \( (\theta_{0,1}, \psi_{0,1}), \ldots, (\theta_{0,n_0}, \psi_{0,n_0}) \) and
\( (\theta_{1,1}, \psi_{1,1}), \ldots, (\theta_{1,n_1}, \psi_{1,n_1}) \) are two independent samples generated from distributions
\( \pi_0(\theta|y) \times \omega(\psi|\theta, y) \) and \( \pi_1(\theta, \psi|y) \), respectively, do
depend on this completion by the pseudo-posterior
as well as on the function \( \alpha(\theta, \psi) \). [Chen et al. 2000]
establish that the asymptotically optimal choice for
\( \omega(\psi|\theta, y) \) is the obvious one, namely
\[
\omega(\psi|\theta, y) = \pi_1(\psi|\theta, y),
\]
which most often is unavailable in closed form (es-
specially when considering that the normalising constant
of \( \omega(\psi|\theta, y) \) is required in (8)).

Another approach to approximating the marginal
likelihood is based on harmonic means. If \( \theta_{i,j} \sim \pi_1(\cdot) \)
\( (i = 1, 2, j = 1, \ldots, N) \), the prior distribution, then
\[
\frac{1}{N} \sum_{j=1}^{N} \frac{1}{f_i(y|\theta_{i,j})}
\]
is an unbiased estimator of \( 1/m_i(y) \) [Newton and
Raftery 1994]. This generic harmonic mean is too
often associated with an infinite variance to ever be
recommended [Neal 1994], but the representation
[Gelfand and Dey 1994] \( (i = 0, 1) \)
\[
\mathbb{E}_{\pi_i} \left[ \frac{\varphi_i(\theta)}{\pi_i(\theta)f_i(y|\theta)} \middle| y \right] = \int \frac{\varphi_i(\theta)\pi_i(\theta)f_i(y|\theta)}{\pi_i(\theta)f_i(y|\theta)m_i(y)} d\theta
\]
holds, no matter what the density \( \varphi_i \) is, provided
\( \varphi_i(\theta_i) = 0 \) when \( \pi_i(\theta_i)f_i(y|\theta_i) = 0 \). This
representation is remarkable in that it allows for a direct
processing of Monte Carlo (or MCMC) output from
the posterior distribution \( \pi_i(\theta_i|y) \). As with
importance sampling approximations, the variability of
the corresponding estimator of \( B_{01}(y) \) will be small if
the distributions \( \varphi_i \) \( (i = 0, 1) \) are close to the
posterior distributions. However, as opposed to usual
importance sampling constraints, the density \( \varphi_i \) must have lighter—rather than fatten—
tails than \( \pi_i(\cdot)f_i(y|\cdot) \) for the approximation of the marginal \( m_i(x) \)
\[
\left[ N^{-1} \sum_{j=1}^{N} \frac{\varphi_i(\theta_{i,j})}{\pi_i(\theta_{i,j})f_i(y|\theta_{i,j})} \right]^{-1},
\]
when \( \theta_{i,j} \sim \pi_i(\theta|y) \), to enjoy finite variance. For instance,
using \( \varphi_i \)'s with constrained supports derived from
a Monte Carlo sample, like the convex hull of the
simulations corresponding to the 10% or to the
25% HPD regions—that again is easily derived from
the simulations—is both completely appropriate and
implementable [Robert and Wraith 2009].

Example 7 (Continuation of Example 5). In the case
of the probit model, if we use as distributions
\( \varphi_i \) the normal distributions with means equal to the
ML estimates and covariance matrices equal to the
estimated covariance matrices of the ML estimates,
the results of Robert and Marin [2010], obtained
over 100 replications with \( N = 20,000 \) simulations
each are reproduced in Figure 2. They compare
both approaches—harmonic mean and importance
sampling—to the approximation of the Bayes factor.
testing for the significance of the ped covariate and show a very clear proximity between both importance solutions in this special case, even though the importance sampling estimate is much faster to compute. Simulation from the posterior distribution is obtained by an MCMC algorithm described in Section 4.

A final approach to the approximation of Bayes factors that is worth exploring is Chib’s (1995) method. First, it is a direct application of Bayes’ theorem: given $y \sim f_i(y|\theta)$, we have that

$$m_i(y) = \frac{f_i(y|\theta) \pi_i(\theta)}{\pi_i(\theta|y)},$$

for all $\theta$’s (since both the lhs and the rhs of this equality are constant in $\theta$). Therefore, if an arbitrary value $\theta^*$, is selected and if a good approximation to $\pi_i(\theta^*|y)$ is available, denoted $\hat{\pi}_i(\theta^*|y)$, Chib’s (1995) approximation to the marginal likelihood (and hence to the Bayes factor) is

$$m_i(y) = \frac{f_i(y|\theta^*) \pi_i(\theta^*)}{\hat{\pi}_i(\theta^*|y)}. \tag{9}$$

In a general setting, $\hat{\pi}_i(\theta^*|y)$ may be the normal approximation based on the MLE, already used in the importance sampling, bridge sampling and harmonic mean solutions, but this is unlikely to be accurate in a general framework. A second solution is to use a nonparametric approximation based on a preliminary MCMC sample, even though the accuracy may also suffer in large dimensions. In the special setting of latent variables models introduced in Section 2.2, Chib’s (1995) approximation is particularly attractive as there exists a natural approximation to $\pi_k(\theta|y)$, based on the Rao–Blackwell (Gelfand and Smith 1990) estimate

$$\hat{\pi}_k(\theta^*|y) = \frac{1}{N} \sum_{j=1}^{N} \pi_k(\theta^*|y, z_j),$$

where the $z_j$’s are the latent variables simulated by the MCMC sampler. The estimate $\hat{\pi}_k(\theta^*|y)$ is indeed a parametric unbiased approximation of $\pi_k(\theta^*|y)$ that converges with rate $O(1/\sqrt{N})$. It obviously requires the full conditional density $\pi_k(\theta^*|y, z)$ to be available in closed form (constant included) but, for instance, this is the case for the probit model of Example 1.

Example 8 (Continuation of Example 7). Figure 3 reproduces the results of Robert and Marin (2010) obtained for 100 replications of Chib’s approximations of $B_{01}(y)$ for the same test as in Example 7 with $N = 20,000$ simulations for each approximation of $m_i(y)$ ($i = 0, 1$). While Chib’s method is usually very reliable and dominates importance sampling, the incredibly good approximation provided by the asymptotic normal distribution implies that, in this highly special case, Chib’s method is dominated by both the importance sampling and the harmonic mean estimates.

While the methods presented above cannot ranked in a fixed order for all types of problems, the conclusion of Robert and Marin (2010) is worth repeating here. In cases when a good approximation $g(\cdot)$ to the true posterior distribution of a model is available, it should be used in a regular importance sampling evaluation of the marginal likelihood. Given
that this good fit rarely occurs in complex and new settings, more generic solutions like Chib’s (1995) should be used, whenever available. (When used with a bounded support on the $\phi_i$’s, the harmonic mean approximation can be considered as a generic method.) At last, when faced with a large number or even an infinity of models to compare, the only available solution is to use model jump techniques like reversible jump MCMC (Green 1995).

4 Markov chain Monte Carlo methods

4.1 Basics

Given the difficulties involved in constructing an efficient importance function in complex setting, Markov chain Monte Carlo (MCMC) methods (Gelfand and Smith 1990, Robert and Casella 2004, 2009, Marin and Robert 2007) try to overcome some of the limitations of regular Monte Carlo methods (particularly dimension-wise) by simulating a Markov chain with stationary (and limiting) distribution.

There exist fairly generic ways of producing such chains, including the Metropolis–Hastings and Gibbs algorithms defined below. Besides the fact that stationarity of the target distribution is enough to justify a simulation method by Markov chain generation, the idea at the core of MCMC algorithms is that local exploration, when properly weighted, can lead to a valid (global) representation of the distribution of interest. This includes for instance using only component-wise (and hence small-dimensional) simulations—that escape (to some extent) the curse of dimensionality—as in the Gibbs sampler.

This very short introduction may give the impression that MCMC simulation is only superficially different from other Monte Carlo methods. When compared with alternatives such as importance sampling, MCMC methods differ on two issues:

5 The theoretical foundations of MCMC algorithms are both sound and simple: as stressed by Tierney (1994) and Mengersen and Tweedie (1996), the existence of a stationary distribution almost immediately validates the principle of a simulation algorithm based on a Markov kernel.
1. the output \((\theta^{(t)})\) of an MCMC algorithm is only asymptotically distributed from the target distribution. While this usually is irrelevant, in that the \(\theta^{(t)}\)'s are very quickly distributed from that target, it may also happen that the algorithm fails to converge in the prescribed number of iterations and thus that the resulting estimation is biased.

2. the sequence \((\theta^{(t)})\) being a Markov chain, the \(\theta^{(t)}\)'s are correlated and therefore this modifies the evaluation of the asymptotic variance as well as the effective sample size associated with the output.

We also note here that trying to produce an iid sequence out of a MCMC method is highly inefficient and thus not recommended.

### 4.2 Metropolis–Hastings algorithm

The Metropolis–Hastings algorithm truly is the generic MCMC method in that it offers a straightforward and universal solution to the problem of simulating from an arbitrary\(^6\) posterior distribution \(\pi(\theta|x) \propto f(y|\theta)\pi(\theta)\): starting from an arbitrary point \(\theta_0\), the corresponding Markov chain explores the surface of this posterior distribution using an internal Markov kernel (proposal) \(q(\theta^{(t-1)}|\theta)\) that progressively visits the whole range of the possible values of \(\theta\). This internal Markov kernel should be irreducible with respect to the target distribution (that is, the Markov chain associated with the proposal \(q(\cdot|\cdot)\) should be able to visit the whole support of the target distribution). The reason why the resulting chain does converge to the target distribution despite the arbitrary choice of \(q(\theta^{(t-1)}|\theta)\) is that the proposed values are sometimes rejected by a step that relates with the accept-reject algorithm.

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\(^6\)The only restriction is that this function is known up to a normalising constant.

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#### Metropolis–Hastings Algorithm

For a computing effort \(N\)

1. Choose \(\theta^{(0)}\),

2. Set \(t = 1\),

3. Generate \(\theta'\) from \(q(\cdot|\theta^{(t-1)})\),

4. Generate \(u\) from \(U_{[0,1]}\),

5. If \(u \leq \frac{\pi(\theta') f(y|\theta') q(\theta^{(t-1)}|\theta')}{\pi(\theta^{(t-1)}) f(y|\theta^{(t-1)}) q(\theta|\theta^{(t-1)})}\),

   set \(\theta^{(t)} = \theta'\) else \(\theta^{(t)} = \theta^{(t-1)}\),

6. Set \(t = t + 1\),

7. If \(t \leq N\) return to 3).

A generic choice for \(q(\theta^{(t-1)}|\theta)\) is the random walk proposal: \(q(\theta|\theta^{(t-1)}|\theta) = g(\theta - \theta^{(t-1)})\) with a symmetric function \(g\), which provides a simplified acceptance probability. Indeed, in that case, step 5 of the previous algorithm is replaced with: if

\[
u \leq \frac{\pi(\theta') f(y|\theta')}{\pi(\theta^{(t-1)}) f(y|\theta^{(t-1)})},\]

set \(\theta^{(t)} = \theta'\) else \(\theta^{(t)} = \theta^{(t-1)}\).

This ensures that values \(\theta'\) that are more likely than the current \(\theta^{(t-1)}\) are always accepted while values that are less likely are sometimes accepted.

**Example 9** (Continuation of Example 1). If we consider the Pima Indian diabetes dataset with only its first two covariates, the parameter \(\beta\) is of dimension 2 and the random walk proposal can be easily implemented. We use for \(g\) a normal distribution with covariance matrix the asymptotic covariance matrix \(\Sigma\) of the MLE and the proposed value \(\beta'\) is then simulated at iteration \(t\) as

\[
\beta' \sim N_2(\beta^{(t-1)}, \Sigma).
\]

The MLE may also be used as starting value for the chain. Figure 4 illustrates the behaviour of the Metropolis–Hastings algorithm for this dataset, the lhs graph describing the path of the subchain \((\beta^{(100t)})\) and the rhs detailing the first component.
for $5000 \leq t \leq 6000$. Although this is not clearly visible on the rhs graph, the acceptance rate of the algorithm is close to 50%, which means that half of the proposed $\beta$’s are rejected.

Using a covariance matrix that is five times larger leads to an acceptance rate of 25%, while the larger $10\hat{\Sigma}$ produces an acceptance rate of 15%.

Finding the proper scale is not always as straightforward as in Example 8 and asymptotic normal approximations to the posterior distribution may be very inefficient. While the Metropolis–Hastings algorithm recovers better from facing large-dimensional problems than standard importance sampling techniques, this still is a strong limitation to its use in large-dimensional setups.

4.3 Gibbs sampling

In contrast, the alternative Gibbs sampler is an attractive algorithm for large-dimensional problems because it naturally fits the hierarchical structures often present in Bayesian models and more generally in graphical and latent variable models. The fundamental strength of the Gibbs sampler is its ability to break a joint target distribution like $\pi(\theta_1, \ldots, \theta_p | y)$ in the corresponding conditional distributions $\pi_i(\theta_i | y, \theta_{-i})$ $(i = 1, \ldots, n)$ and to simulate successively from these low-dimensional targets:

$p$-component systematic scan Gibbs sampler

For a computing effort $N$

1) Choose $\theta^{(0)}$.

2) Set $t = 1$.

3) Generate $\theta_1^{(t)}$ from $\pi_1 \left( \theta_1 | y, \theta_{-1}^{(t-1)} \right)$.

4) Generate $\theta_2^{(t)}$ from $\pi_2 \left( \theta_2 | y, \theta_1^{(t-1)} \theta_{-1:2}^{(t-1)} \right)$.

5) \ldots

6) Generate $\theta_p^{(t)} \sim \pi_p \left( \theta_p | y, \theta_{1: (p-1)}^{(t)} \right)$.

7) Set $t = t + 1$.

8) If $t \leq N$ return to 3).

While this algorithm seems restricted to mostly hierarchical multidimensional models, the special case of the slice sampler (Robert and Casella, 2004, Chapter 8) shows that the Gibbs sampler applies in a wide variety of models.

Example 10. (Continuation of Example 2) As noted in Example 2, the probit model allows for a latent variable representation based on the artificial normal variable $z_t$ connected with the observed variable $y_t$.

This representation opens the door to a Gibbs sampler (Albert and Chib 1993) aimed at the joint posterior distribution of $(\beta, z)$ given $y$. Indeed, the conditional distribution of the latent variable $z_t$ given $\beta$ and $y_t$,

$$z_t | y_t, \beta \sim \begin{cases} N_+ (x_t^T \beta, 1, 0) & \text{if } y_t = 1, \\ N_- (x_t^T \beta, 1, 0) & \text{if } y_t = 0, \end{cases} \quad (10)$$

is clearly available. The corresponding full conditional on the parameters is given by the standard

---

7 This rate happens to be almost optimal for small dimensions (Gelman et al. 1996).

8 Here, $N_+ (x_t^T \beta, 1, 0)$ denotes the normal distribution with mean $x_t^T \beta$ and variance 1 that is left-truncated at 0, while $N_- (x_t^T \beta, 1, 0)$ denotes the symmetrical normal distribution that is right-truncated at 0.
Figure 4: Random-walk Metropolis–Hastings algorithm applied to the Pima Indian diabetes dataset. The left graph describes the path of the subchain ($\beta^{(100i)}$). The right graph shows the path of the first component chain $\beta_1^{(t)}$ for $5000 \leq t \leq 6000$.

The normal distribution (which does not depend on $y$)

$$
\beta | z \sim \mathcal{N}
\left(\frac{n}{n+1} (X^T X)^{-1} X^T z, \frac{n}{n+1} (X^T X)^{-1}\right).
$$

Therefore, given the current value of $\beta$, one cycle of the Gibbs algorithm produces a new value for $z$ as simulated from the conditional distribution (10), which, when substituted into (11), produces a new value for $\beta$. Although it does not impact the long-term properties of the sampler, the starting value of $\beta$ may once again be taken as the maximum likelihood estimate to avoid (useless) burning steps in the Gibbs sampler.

The implementation of this Gibbs sampler is straightforward. There is no parameter to calibrate (as opposed to the scale in the random-walk Metropolis–Hastings scenario). When comparing Figure 4 and 5, the raw plot of the sequence ($\beta_1^{(t)}$) shows that the mixing behaviour of the Gibbs sampling chain is superior to the one for the Metropolis–Hastings chain.

4.4 Hybrid solutions

Mixing both Metropolis–Hastings and Gibbs algorithms often result in better performances like faster convergence of the resulting Markov chain, the former algorithm being often used for global exploration of the target and the later for local improvement.

A classic hybrid algorithm replaces a non-available Gibbs update by a Metropolis–Hastings step. Another hybrid solution alternates Gibbs and Metropolis–Hastings proposals. The corresponding algorithms are valid: they produce ergodic Markov chains with the posterior target as stationary distribution.

**Example 11** (Continuation of Example 5). For $p = 1$, the probit model can be over-parameterised as

$$
\mathbb{P}(Y_i = 1|x_i) = 1 - \mathbb{P}(Y_i = 0|x_i) = \Phi(x_i \beta/\sigma),
$$

while only depending on $\beta/\sigma$. Using a proper prior like

$$
\pi(\beta, \sigma^2|x) = \pi(\beta|x)\pi(\sigma^2|x)
\propto \sigma^{-4} \exp\{-1/\sigma^2\} \exp\{-\beta^2/50\},
$$
Figure 5: Gibbs sampling algorithm applied to the Pima Indian diabetes dataset. The left graph describes the path of the subchain \((\beta^{(100t)})\). The right graph shows the path of the first component chain \(\beta_1^{(t)}\) for \(5000 \leq t \leq 6000\).

the corresponding Gibbs sampler simulates \(\beta\) and \(\sigma^2\) alternatively, from

\[
\pi(\beta | x, y, \sigma) \propto \prod_{i=1}^{n} \Phi(x_i \beta / \sigma)^{y_i} \Phi(-x_i \beta / \sigma)^{1-y_i} \pi(\beta | x)
\]

and

\[
\pi(\sigma^2 | x, y, \beta) \propto \prod_{i=1}^{n} \Phi(x_i \beta / \sigma)^{y_i} \Phi(-x_i \beta / \sigma)^{1-y_i} \pi(\sigma^2 | x)
\]

respectively. Since both of these conditional distributions are non-standard, we replace the direct simulation by one-dimensional Metropolis–Hastings steps\(^9\) using normal \(N(\beta^{(t)}, 1)\) and log-normal \(LN(\log \sigma^{(t)}, .04)\) random walk proposals, respectively. (The scales were found by trial-and-error.)

For a simulated dataset of 1,000 points, the contour plot of the log-posterior distribution is given in Figure 6, along with the last 1,000 points of a corresponding MCMC sample after 100,000 iterations. This graph shows a very satisfactory repartition of the simulated parameters over the likelihood surface, with higher concentrations near the largest posterior regions.

\(^9\)In this Metropolis-within-Gibbs strategy, note that a single step of a Metropolis–Hastings move is sufficient to validate the algorithm, since stationarity, not convergence, is the issue.

Let us note as a conclusion to this short section that an alternative meaning for hybrid solutions is the simultaneous use of different Markov kernels (Tierney).
A mixture of MCMC kernels does remain an MCMC kernel with the same stationary distribution and its performances are at least as good as the best component in the mixture. There is therefore very little to say against advocating this extension.

4.5 Scaling and adaptivity

A difficulty with Metropolis–Hastings algorithms, including random walk versions, is the calibration of the proposal distribution: this proposal must be sufficiently related to the target distribution so that, in a reasonable number of steps, the whole support of this distribution can be visited. If the scale of the random walk proposal is too small, this will not happen as the algorithm stays “too local” and, if for instance there are several modes on the target, the algorithm may remain trapped within one modal region because it cannot reach other modal regions with jumps of too small a magnitude.

Example 12. For a sample \( y_1, \ldots, y_n \) from the mixture distribution

\[
p \mathcal{N}(\mu_1, \sigma^2) + (1 - p) \mathcal{N}(\mu_2, \sigma^2)
\]

where both \( p \) and \( \sigma^2 \) are known, the posterior distribution associated with the prior \( \mathcal{N}(0, 10\sigma^2) \) on both \( \mu_1 \) and \( \mu_2 \) is multimodal, with a major mode close to the true value of \( \mu_1 \) and \( \mu_2 \) (when \( n \) is large enough) and a secondary and spurious mode (that stems from the nonidentifiable case \( p = 0.5 \)). When running a random walk Metropolis–Hastings algorithm on this model, with a normal proposal \( \mathcal{N}_2((\mu_1^{(t)}, \mu_2^{(t)}), \tau \mathbf{I}_2) \), a small scale \( \tau \) prevents the Markov chain from visiting the major mode. Figure 7 compares two choices of \( \tau \) for the same dataset: for \( \tau = 1 \), the spurious mode can be escaped but for \( \tau = .3 \) the chain remains trapped in that starting mode.

The larger the dimension \( p \) is, the harder the determination of the scale is, because

a. the curse of dimensionality implies that there is an increasingly important part of the space with zero probability under the target;

Figure 7: Evolution of a random walk Metropolis–Hastings chain on a mixture log-posterior surface for \( n = 500 \) observations and (top) \( \tau = 1 \) and 1,000 iterations; (bottom) \( \tau = .3 \) and 10,000 iterations.
b. the knowledge and intuition about the modal regions get weaker (for complex distributions, it is impossible to identify none but a few of the modes);

c. the proper scaling of a random walk proposal involves a symmetric \((p, p)\) matrix. Even when diagonal, this matrix gets harder to scale as the dimension increases (unless one resorts to a Gibbs-like implementation, where each direction is scaled separately).

In addition to these difficulties, learning about the specificities of the target distribution while running an MCMC algorithm and tuning the proposal accordingly, i.e. constructing an adaptive MCMC procedure, is difficult because this cancels the Markov property of the original method and thus jeopardizes convergence. For instance, Figure 8 shows the discrepancy between an histogram of a simulated Markov chain and the theoretical limit (solid curve) when the proposal distribution at time \(T\) is a kernel approximation based on the first \(T - 1\) simulations of the “chain”. Similarly, using an on-line scaling of the algorithm against the empirical acceptance rate in order to reach a golden number like 0.234 (see Robert and Casella 2004, Note 7.8.4) is inherently flawed in that the attraction of a modal region may give a false sense of convergence and may thus lead to a choice of too small a scale, simply because other modes will fail to be visited during the scaling experiment.

However, there are algorithms that preserve ergodicity (convergence to the target) while implementing adaptivity. See, e.g., Gilks et al. (1998) who use regeneration to create block independence and preserve Markovianity on the paths rather than on the values, Haario et al. (1999, 2001) who derive a proper adaptation scheme by using a ridge-like correction to the empirical variance in very large dimensions for satellite imaging data, and Andrieu et al. (2005) who propose a general framework of valid adaptivity based on stochastic optimisation and the Robbins-Monro algorithm.

More recently, Roberts and Rosenthal (2007) consider basic ergodicity properties of adaptive Markov chain Monte Carlo algorithms under minimal assumptions, using coupling constructions. They prove convergence in distribution and a weak law of large numbers. Moreover, in Roberts and Rosenthal (2009), they investigate the use of adaptive MCMC algorithms to automatically tune the Markov chain parameters during a run. Examples include the adaptive Metropolis multivariate algorithm of Haario et al. (2001), Metropolis-within-Gibbs algorithms for nonconjugate hierarchical models, regionally adjusted Metropolis algorithms, and logarithmic scalings. Roberts and Rosenthal (2009) present some computer simulation results that indicate that the algorithms perform very well compared to non-adaptive algorithms, even in high dimensions.

5 Approximate Bayesian computation techniques

There exist situations where the likelihood function \(f(y|\theta)\) is overly expensive or even impossible to calculate, but where simulations from the density \(f(y|\theta)\) are reasonably produced. A generic class of such situations is made by latent variable models where the analytic integration of the latent variables is impossible, while handling the latent variables as additional parameters in a joint distribution causes any MCMC
to face convergence problems. Another illustration is given by inverse problems where computing the function $f(y|\theta)$ for a given pair $(y, \theta)$ involves solving a numerical equation. In such cases, it is almost impossible to use the computational tools presented in the previous section to sample from the posterior distribution $\pi(\theta|y)$. Approximate Bayesian computation (ABC) is an alternative to such techniques that only requires being able to sample from the likelihood $f(\cdot|\theta)$. It was first proposed for population genetic models (Beaumont et al. 2002) but applies in much wider generality.

### Likelihood free rejection sampling

For a computing effort $N$

1) Set $i = 1$,

2) Generate $\theta'$ from the prior distribution $\pi(\cdot)$,

3) Generate $z$ from the likelihood $f(\cdot|\theta')$,

4) If $\eta(z, \eta(y)) \leq \epsilon$, set $\theta_i = \theta'$ and $i = i + 1$,

5) If $i \leq N$, return to 2).

This likelihood free algorithm samples from the marginal in $z$ of the following joint distribution:

$$\pi_{\epsilon}(\theta, z|y) \propto \pi(\theta)f(z|\theta)I_{\rho_{\epsilon},\nu}(z)$$

with the tuning parameters as

- $\rho(\cdot, \cdot)$ a distance,
- $\eta(\cdot)$ a summary statistic,
- $\epsilon > 0$ a tolerance level,
- $P_{\rho_{\epsilon},\nu} = \{z|\rho(\eta(z), \eta(y)) < \epsilon\}$.

The idea behind ABC (Beaumont et al. 2002) is that the summary statistics coupled with a small tolerance should provide a good approximation of the posterior distribution:

$$\pi_{\epsilon}(\theta|y) = \int \pi_{\epsilon}(\theta, z|y)dz \approx \pi(\theta|y).$$

It has been shown in Marjoram et al. (2003) that it is possible to construct a Metropolis–Hastings algorithm that samples from $\pi_{\epsilon}(\theta, z|y)$, and the marginally from $\pi_{\epsilon}(\theta|y)$; this algorithm only requires the ability to sample from $f(\cdot|\theta)$. This is the likelihood free MCMC sampler:

### Likelihood free MCMC sampler

For a computing effort $N$

1) Use the likelihood free rejection sampling to get a realization $\theta^{(0)}$ from the ABC target distribution $\pi_{\epsilon}(\theta|y)$,

2) Set $t = 1$,

3) Generate $\theta'$ from the Markov kernel $q(\cdot|\theta^{(t-1)})$,

4) Generate $z$ from the likelihood $f(\cdot|\theta')$,

5) Generate $u$ from $U[0,1]$,

6) If $u \leq \frac{\pi(\theta')q(\theta^{(t-1)}|\theta')}{\pi(\theta^{(t-1)})q(\theta'|\theta^{(t-1)})}I_{\rho_{\epsilon},\nu}(z)$, set $\theta^{(t)} = \theta'$ else $\theta^{(t)} = \theta^{(t-1)}$,

7) Set $t = t + 1$,

8) If $t \leq N$ return to 3).

Rejection sampling and MCMC methods can perform poorly if the tolerance level $\epsilon$ is small. Consequently various sequential Monte Carlo algorithms have been constructed as an alternative to both methods. For instance, Beaumont et al. (2009) proposed an ABC version of the Population Monte Carlo algorithm presented above. The key idea is to decompose the difficult issue of sampling from $\pi_{\epsilon}(\theta, z|y)$ into a series of simpler subproblems. The algorithm begins at time 0 sampling from $\pi_{\epsilon_0}(\theta, z|y)$ with a large value $\epsilon_0$, then simulating from an increasing difficult sequence of target distribution $\pi_{\epsilon_i}(\theta, z|y)$, that is when $\epsilon_t < \epsilon_{t-1}$.

### Example 13 (Continuation of Example 8)

Figure 9 provides an illustration of the above algorithm when applied to the probit model with the three covariates described in Example 1. In this artificial case,
the ABC outcome can be compared with the MCMC “exact” simulation described above and the result is striking in that the ABC approximation is confounded with the exact posterior densities. The tuning of the ABC algorithm is to use $10^6$ simulations over 10 iterations, with bounds $\epsilon_t$ set as the 1% quantile of the simulated $\rho(\eta(z), \eta(y))$, $\rho$ chosen as the Euclidean distance, and $\eta(z)$ as the predictive distribution based on the current parameter $\beta$, made of the $\Phi(x_i^T \beta)$’s, while $\eta(y)$ is the predictive distribution based on the MLE $\hat{\beta}(y)$ made of the $\Phi(x_i^T \hat{\beta}(y))$’s. In this special case we are therefore avoiding the simulation of the observations themselves as predictive functions are available. This choice reduces the variability in the divergence between $\eta(z)$ and $\eta(y)$, and explains for the very good fit between the densities.

6 Final remarks

This tutorial is necessarily incomplete and biased: the insistence on model choice and on variable dimension models is also a reflection of the author’s own interests. Others would have rather chosen to stress the relevance of these simulation methods for optimal design [Müller 1999, Müller et al. 2004] in conjunction with simulated annealing (e.g. Andrieu and Doucet 2000, Doucet et al. 2002), for non-parametric regression (Holmes et al. 2002) or for the analysis of continuous time stochastic processes (Dellaportas et al. 2004, Beskos et al. 2006). That such a wealth of choices is available indicates that the field still undergoes a formidable expansion that should benefit a wide range of areas and disciplines and, conversely, that the continued attraction of new areas within the orbit of Bayesian computational methods backfeeds their creativity by introducing new challenges and new paradigms.

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