Markov Chain Monte Carlo Methods, a survey with some frequent misunderstandings

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Abstract

In this chapter, we review some of the most standard tools used in Bayesian computation, along with vignettes on standard misunderstandings of these approaches taken from Q & A’s on the forum Cross-validated answered by the first author.

Acronyms: EM, MCMC, QMC, ABC, SMC, PDMP, HMC, NUTS, PMC.

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1 Introduction

When analysing a complex probability distribution or facing an unsolvable integration problem, as in most of Bayesian inference, Monte Carlo methods on a large variety of solutions, mostly based on the ability to simulate a sequence of random variables and subsequently call for the law of large numbers. Techniques based on the simulation of Markov chains are a special case of these methods, in which the current simulation value (and its probability) are used to switch to a different simulation value (hence the Markovian nature of such techniques). While the working principle of MCMC methods was proposed almost as early as the original Monte Carlo algorithms, the variety and efficiency of these methods has grown significantly since Gelfand and Smith (1990) (re)introduced them to the statistical community and in particular to its Bayesian component (Berger, 1985).

Given a likelihood function defined as a function of the parameter associated with the probability mass function or density function of the observations ($x_{\text{obs}}$), $L(\theta|x_{\text{obs}})$, a Bayesian approach means relying on a so-called prior distribution on the parameters, from which the resulting posterior distribution defined by

$$
\pi(\theta|x_{\text{obs}}) = \frac{L(\theta|x_{\text{obs}})\pi(\theta)}{\int_{\Theta} L(\theta|x_{\text{obs}})\pi(\theta')d\theta'}
$$

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is derived. The denominator is sometimes called the marginal likelihood and is denoted by \( m_\pi(x^{\text{obs}}) \). While most Bayesian procedures are by nature uniquely defined, the practice of this theory exposes various computational problems.

"Why is it necessary to sample from the posterior distribution if we already know the posterior distribution?" [cross-validated:307882]

When one states that we “know the posterior distribution”, the meaning of knowledge is unclear. “Knowing” a function of \( \theta \) to be proportional to the posterior density, namely

\[
\pi(\theta)f(x^{\text{obs}}|\theta)
\]

as for instance the completely artificial following target

\[
\pi(\theta|x) \propto \exp\left\{-||\theta - x||^2 - ||\theta + x||^4 - ||\theta - 2x||^6\right\}, \ x, \theta \in \mathbb{R}^{18},
\]

does not mean a quick resolution for approximating the following entities

- the posterior expectation of a function of \( \theta \), e.g., \( E[h(\theta)|x] \), posterior mean that operates as a Bayesian estimator under standard losses;
- the optimal decision under an arbitrary utility function, decision that minimises the expected posterior loss;
- a 90\% or 95\% range of uncertainty on the parameter(s), a sub-vector of the parameter(s), or a function of the parameter(s), aka HPD region \( \{h = h(\theta); \pi^b(h) \geq h\} \) where \( \pi^b(\cdot) \) denotes the marginal posterior distribution of \( h \);

The above quantities are only examples of the infinity of usages made of a posterior distribution. In all cases but the most simple ones, the answers are mathematically derived from the posterior but cannot be found without analytical or numerical steps, like Monte Carlo and Markov chain Monte Carlo (MCMC) methods.

The existing solutions to this computing challenge are roughly divisible into deterministic and stochastic approaches. The former include Laplace’s approximation, expectation propagation (Gelman et al., 2014) and Bayesian variational methods (Jaakkola and Jordan, 2000). The resulting approximation error then is usually unknown and cannot be corrected from additional calculations. The alternative of Monte Carlo methods leads to approximations that converge when the computational effort becomes infinite. We will focus on the latter.

"Why is variational Bayesian mixture model an alternative to MCMC? What are the similarities?" [cross-validated:386093]

Variational Bayes inference is a weak form of empirical Bayesian inference (Berger, 1985), in the sense that it estimates some parameters of the prior from the data for a simplified version of the true posterior, most often of a conjugate form. The variational Bayes approach to a Bayesian latent variable model (Jaakkola and Jordan, 2000) is producing a pseudo-posterior distribution on the parameters of the model; including the latent variables \( Z \), by imposing a certain dependence structure (or graphical model) and estimating its hyperparameters of this model by a maximising algorithm akin to the EM algorithm (Dempster et al., 1977).

There is thus no clear direct connection with MCMC, since the variational Bayes posterior is made of standard distributions, thus does not require simulation, but has hyperparameters that must be derived by an optimisation program, hence the call to an EM-like algorithm.
2 Monte Carlo methods

Monte Carlo approximations (Robert and Casella, 2004) are based on the Law of Large Numbers (LLN) in the sense that an integral like

\[ I_h := \mathbb{E}_P(h(X)) \]

is the limiting value of an empirical average

\[ \frac{1}{N} \sum_{i=1}^{N} h(x_i) \xrightarrow{P} I_h \]

when \( x_1, x_2, \cdots \) are i.i.d. random variables with probability distribution \( P \). In practice, the sample \( x_1, x_2, \cdots \), is produced by a pseudo-random generator (Rubinstein, 1981)

"How can you draw samples from the posterior distribution without first knowing the properties of said distribution? [cross-validated:307882]

In Bayesian settings, Monte Carlo methods are based on the assumption that the product (2) can be numerically computed (hence is known) for a given \( (\theta, x^{\text{obs}}) \), where \( x^{\text{obs}} \) denotes the observation, \( \pi(\cdot) \) the prior, and \( f(x^{\text{obs}}|\theta) \) the likelihood. This does not imply an in-depth knowledge about this function of \( \theta \). Still, from a mathematical perspective the posterior density is completely and entirely determined by Bayes’ formula, hence derived from the product (2). Thus, it is not particularly surprising that simulation methods can be found using solely the input of the product (2). The most amazing feature of Monte Carlo methods is that some methods like Markov chain Monte Carlo (MCMC) algorithms do not formally require anything further than this computation of the product, when compared with accept-reject algorithms for instance, which call for an upper bound. A related software like Stan (Carpenter et al., 2017) operates on this input and still delivers high end performances with tools like NUTS (Hoffman and Gelman, 2014) and HMC, including numerical differentiation.

A side comment is that the normalising constant of the posterior (1) is not particularly useful for conducting Bayesian inference in that, were one to “know” its exact numerical value in addition to the product (2), \( \mathcal{Z} = 3.17232 \times 10^{-23} \) say, one would not have made any progress towards finding Bayes estimates or credible regions. (The only exception when this constant matters is in conducting Bayesian model comparison.)

"If we do not know the normalising constant for a posterior distribution, why does it imply we can only sample dependent draws?" [cross-validated:182525]

This is mostly unrelated: missing normalising constant and dependence have no logical connection. That is to say, one may have a completely defined density and yet be unable to produce i.i.d. samples, or one may have a density with a missing constant and nonetheless be able to produce i.i.d. samples.

If one knows a density \( f(\cdot) \) up to a normalising constant, \( f(x) \propto p(x) \), there are instances when one can draw independent samples, using for instance [accept-reject algorithms][1]: if one manages to find another density \( g \) such that

1. one can simulate from \( g \)
2. there exists a known constant \( M \) such that

\[ p(x) \leq Mg(x) \]
then the algorithm

Repeat
   simulate \( y \sim g(y) \)
   simulate \( u \sim \mathcal{U}(0,1) \)
until \( u < p(y)/Mg(y) \)

produces i.i.d. simulations from \( f \), even though one only knows \( p \).

For instance, if one wants to generate a Beta \( \text{Be}(a + 1, b + 1) \) distribution from scratch (with \( a, b \geq 1 \)), the density up to a normalising constant is

\[
p(x) = x^a(1-x)^b \mathbb{I}_{(0,1)}(x)
\]

which is bounded by 1. Thus, we can use \( M = 1 \) and \( g(x) = 1 \), the density of the uniform distribution in an accept-reject algorithm that produces a sample (with random size) that is i.i.d. from the Beta \( \text{Be}(3.3, 4.4) \) distribution. In practice, finding such a \( g \) may prove a formidable task and an easier approach is to produce simulations (asymptotically) from \( f \) by MCMC algorithms.

When direct simulation from \( P \), for instance a posterior distribution, is impossible, alternative stochastic solutions must be sought. A wide collection of such methods goes under the name of importance sampling, relying on a convenient if somewhat arbitrary auxiliary distribution.

"What is importance sampling? [cross-validated:254114]"

The intuition behind importance sampling is that a well-defined integral, like

\[
\mathcal{I} = \int_X h(x) \, dx
\]

can be expressed as an expectation for a wide range of probability distributions with density \( f \):

\[
\mathcal{I} = \mathbb{E}_f[H(X)] = \int_X H(x) f(x) \, dx
\]

where \( H \) is determined by \( h \) and \( f \). (Note that \( H(\cdot) \) is usually different from \( h(\cdot) \).) The choice

\[
H(x) = h(x)/f(x)
\]

leads to the equalities \( H(x) f(x) = h(x) \) and \( \mathcal{I} = \mathbb{E}_f[H(X)] \)—under some restrictions on the support of \( f \), meaning \( f(x) > 0 \) when \( h(x) \neq 0 \). Hence, there is no unicity in the representation of an integral as an expectation, but on the opposite an infinite array of such representations, some of which are better than others once a criterion to compare them is adopted. For instance, it may mean choosing \( f \) towards reducing the variance of the estimator.

Once this elementary property is understood, the implementation means simulating via a pseudo-random generator—an i.i.d. sample \( (x_1, \ldots, x_n) \) distributed from \( f \) and using the average of the \( H(x_i) \) as an unbiased approximation, \( \hat{\mathcal{I}} \). Depending on the choice of the distribution \( f \), this estimator \( \hat{\mathcal{I}} \) may or may not have a finite variance. However, there always exist choices of \( f \) that allow for a finite variance and even for an arbitrarily small variance (albeit those choices may be unavailable in practice). And there also exist choices of \( f \) that make the importance sampling estimator \( \hat{\mathcal{I}} \) a very poor approximation of \( \mathcal{I} \). This includes all the choices where the variance gets infinite, even though Chatterjee and Diaconis (2018) compare importance samplers with infinite variance. Figure 1 is taken from the first author’s blog discussion of the paper and illustrates the poor convergence of infinite variance estimators.

A decisive appeal in using importance sampling is that the weight function \( w \) can be known up to a multiplicative constant, which most often occurs when sampling
from a given posterior in Bayesian inference. Indeed, the multiplicative constant can be estimated by \( \frac{1}{N} \sum_{i=1}^{N} w(X_i) \) and it is straightforward to deduce that the normalised (if biased) estimator

\[
\sum_{i=1}^{N} \frac{h(X_i)w(X_i)}{\sum_{i=1}^{N} w(X_i)}
\]

consistently approximates the integral of interest.

The importance distribution \( Q \) selected for the associated approximation significantly impacts the quality of the method. The sequence of pseudo-random variables that stands at the core of the method remains at this stage i.i.d. but the next section describes a new class of sampling algorithms, based on Markov chains, which produce correlated samples to approximate the target distribution or the integrals of interest.

The term “sampling” is somewhat confusing in that it does not intend to provide samples from a given distribution.

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**Can importance sampling be used as an actual sampling mechanism?**

The difficulty is that the resulting (re)sample is not marginally distributed from \( p \). While

\[
E_q[h(Y)p(Y)/q(Y)] = E_p[h(Y)]
\]

for any integrable function \( h(\cdot) \), weighting and resampling an i.i.d. sample \( (Y_1, \ldots, Y_n) \) from \( q \) does not produce a sample distributed from \( p \), even marginally. The reason for the discrepancy is that the weighting-resampling step implies dividing the \( p(Y_i)/q(Y_i) \) by the random sum of the weights, i.e., the index \( i \) is selected with probability

\[
\frac{p(Y_i)/q(Y_i)}{\sum_j p(Y_j)/q(Y_j)}
\]
Figure 2: Failed simulation of a Student’s $t_5$ distribution with mean $N(2, 1/\sqrt{2})$ distribution when simulating $10^7$ realisations using $10^7$ realisations from a standard Normal importance distribution (with thinner tails).

Figure 3: Recovery of a Normal $N(2, 1/\sqrt{2})$ distribution when simulating $10^7$ realisations from a standard Normal importance distribution (with fatter tails).

which modifies the marginal distribution of the resampled rv’s, especially when the sum has an infinite variance.

Figure 2 provides an illustration when $p$ is the density of a Student’s $t_5$ distribution with mean 3 and $q$ is the density of a standard Normal distribution. The original Normal sample fails to cover the rhs of the tail of the Student’s $t$ and hence that the weighted-resampled sample cannot recover with a manageable number of simulations. Obviously, as shown in Figure 3, when the target $q$ has fatter tails than $p$, the method converges reasonably fast.

“What is the difference between Metropolis Hastings, Gibbs, Importance, and Rejection sampling?” [cross-validated:185921]

These methods all produce samples from a given distribution, with density $f$ say, either to get an idea about this distribution, or to solve an integration or optimisation problem related with $f$. Instances include finding the value of

$$\int_X h(x)f(x)dx$$

or the mode of the distribution of $h(X)$ when $X \sim f(x)$ or a quantile of this distribution.

Here are a few generic points that do not cover the complexity of the issue:

1. **Accept-reject methods** are intended to provide an i.i.d. sample from $f_i$, as explained above. The pros are that there is no approximation in the method: the outcome is truly an i.i.d. sample from $f$. The cons are many: (i) designing the algorithm by finding an envelope of $f$ that can be generated may be very costly in human time; (ii) the algorithm may be inefficient in computing time, i.e., requires many uniforms to produce a single $x$; (iii) those performances are decreasing with the dimension of $X$. In short, such methods cannot be used for simulating one or a few simulations from $f$ unless they are already available in a computer language like R.

2. **Markov chain Monte Carlo (MCMC) methods** are extensions of i.i.d. simulations methods when i.i.d. simulation is too costly. They produce a sequence of simulations $(x_t)_t$ which limiting distribution is the distribution $f$. The pros are that (i) less information about $f$ is needed to implement the method; (ii) $f$ may be only known up to a normalising constant or even as an integral

$$f(x) \propto \int_z \tilde{f}(x,z)dz$$
and still be associated with an MCMC method; (iii) there exist generic MCMC algorithms to produce simulations \((x_t)\), that require very little calibration; (iv) dimension is less of an issue as large dimension targets can be broken into conditionals of smaller dimension (as in Gibbs sampling). The cons are that (i) the simulations \((x_t)\), are correlated, hence less informative than i.i.d. simulations; (ii) the validation of the method is only asymptotic, hence there is an approximation in considering \(x_t\) for a fixed \(t\) as a realisation of \(f\); (iii) convergence to \(f\) (in \(t\)) may be so slow that for all practical purposes the algorithm does not converge; (iv) the universal validation of the method means there is an infinite number of potential implementations, with an equally infinite range of efficiencies.

3. Importance sampling methods are originally designed for integral approximations, namely generating from the wrong target \(g(x)\) and compensating by an importance weight \(f(x)/g(x)\). The resulting sample is thus weighted, which makes the comparison with the above awkward. Importance sampling can be turned into importance sampling resampling by using an additional resampling step based on the weights, still failing to produce an exact simulation from the target as discussed above. The pros of importance sampling are that (i) generation from an importance target \(g\) can be cheap and recycled for different targets \(f\); (ii) the “right” choice of \(g\) can lead to huge improvements compared with regular or MCMC sampling; (iii) importance sampling is more amenable to numerical integration improvement, like for instance quasi-Monte Carlo integration; (iv) it can be turn into adaptive versions like population Monte Carlo and sequential Monte Carlo. The cons are that (i) resampling induces inefficiency (which can be partly corrected by reducing the noise as in systematic resampling or qMC); (ii) the “wrong” choice of \(g\) can lead to huge losses in efficiency and even to infinite variance; (iii) importance has trouble facing large dimensions and its efficiency diminishes quickly with the dimension; (iv) the method may be as myopic as local MCMC methods in missing important regions of the support of \(f\).

A final warning is that there is no such thing as an optimal simulation method. Even in a specific setting like approximating an integral \(\mathcal{I}\), costs of designing and running different methods intrude as to make a global comparison very delicate, if at all possible, while, from a formal point of view, they can never beat the zero variance answer of returning the constant “estimate”. For instance, simulating from \(f\) is very rarely if ever the best option. This does not mean that methods cannot be compared, but that there always is a possibility for an improvement, which usually comes with additional costs.
3 Markov chain Monte Carlo methods

Markov chain Monte Carlo (MCMC) algorithms are now standard computing tools for analysing Bayesian complex models, even though practitioners may still face difficulties with its implementations. The concept behind MCMC is quite simple in that it creates a sequence of dependent variables that converge (in distribution) to the distribution of interest (also called target). In that sense, MCMC algorithms are robust or universal, as opposed to the most standard Monte Carlo methods which require direct simulations from the target distribution.

"Is Markov chain based sampling the “best” for Monte Carlo sampling? Are there alternative schemes available?" [cross-validated:131455]

There is no reason that MCMC sampling is the “best” Monte Carlo method! Usually, it is on the opposite worse than i.i.d. sampling, at least in terms of variance of the resulting Monte Carlo estimators

\[
\frac{1}{T} \sum_{t=1}^{T} h(X_t)
\]

Indeed, while this average converges to the expectation \( E_\pi[h(X)] \) when \( \pi \) is the stationary and limiting distribution of the Markov chain \((X_t)\), there are at least two drawbacks in using MCMC methods:

1. The chain needs to “reach stationarity”, meaning that it needs to forget about its starting value \( X_0 \). In other words, \( t \) must be “large enough” for \( X_t \) to be distributed from \( \pi \). Sometimes “large enough” may exceed by several orders of magnitude the computing budget available for the experiment.

2. The values \( X_t \) are correlated, leading to an asymptotic variance that involves

\[
\text{var}_\pi(X) + 2 \sum_{i=1}^{\infty} \text{cov}_\pi(X_0, X_i)
\]

which generally exceeds \( \text{var}_\pi(X) \) and hence requires longer simulations than for an i.i.d. sample, as well as more involved evaluation techniques.

This being said, MCMC is very useful for handling settings where regular i.i.d. sampling is impossible or too costly and where importance sampling is quite difficult to calibrate, in particular because of the dimension of the random variable to be simulated. However, sequential Monte Carlo methods (Lin et al., 2001) like particle filters may be more appropriate in dynamical models, where the data comes by bursts that need immediate attention and may even vanish (i.e., cannot be stored) after a short while.

From the early 1950’s, MCMC methods (see, e.g. Cappé and Robert, 2000; Green et al., 2015; Robert and Casella, 2010) have been utilised to handle complex target distributions by simulation, where the meaning of complexity depends on the target density, the size of the associated data, the dimension of the object to be simulated, or on the allocated budget. For instance, the density \( p(x) \) is only expressed as a multidimensional integral that is analytically intractable,

\[
p(x) = \int \omega(x, \xi) d\xi.
\]

An evaluation of this density requires the simulation of the whole vector \((x, \xi)\).

In these cases when \( \xi \) has a dimension at least as large as the data, this involves a significant increase in the dimension of the simulated object and hence
deeper computational difficulties, like handling the new target \( \omega(x, \xi) \). An MCMC algorithm provides an alternative solution to this computational issues through a simulated Markov chain evolving in the augmented space without requiring further information on the density \( p \).

The connection between Markov chain and Markov chain Monte Carlo?"[cross-validated:169518]

The connection between both concepts is that Markov chain Monte Carlo (MCMC) methods rely on Markov chain theory to produce simulations and Monte Carlo approximations from a complex target distribution \( \pi \).

In practice, these simulation methods output a sequence \( X_1, \ldots, X_N \) that is a Markov chain, i.e., such that the distribution of \( X_i \) given the whole past \( \{X_{i-1}, \ldots, X_1\} \) only depends on \( X_{i-1} \).

In other words,

\[
X_i = f(X_{i-1}, \epsilon_i)
\]

where \( f \) is a function specified by the algorithm and the target distribution \( \pi \) and the \( \epsilon_i \)'s are i.i.d.. The (ergodic) theory guarantees that \( X_i \) converges (in distribution) to \( \pi \) as \( i \) gets to \( \infty \).

The easiest example of an MCMC algorithm is the slice sampler: at iteration \( i \) of this algorithm, do

1. simulate \( \epsilon_i^1 \sim U(0, 1) \)
2. simulate \( X_i \sim U(\{x; \pi(x) \geq \epsilon_i^1 \pi(X_{i-1})\}) \) (which amounts to generating a second independent \( \epsilon_i^2 \))

For instance, if the target is a Normal \( \mathcal{N}(0, 1) \) distribution the above translates as

1. simulate \( \epsilon_i^1 \sim U(0, 1) \)
2. simulate \( X_i \sim U(\{x; x^2 \leq -2 \log(\sqrt{2\pi} \epsilon_i^1)\}) \), i.e.,

\[
X_i = \pm \epsilon_i^2 \{-2 \log(\sqrt{2\pi} \epsilon_i^1)\varphi(X_{i-1})\}^{1/2}
\]

with \( \epsilon_i^2 \sim U(0, 1) \)

Figure 5 is a representation of the output, showing the right fit to the \( \mathcal{N}(0, 1) \) target and the evolution of the Markov chain \( (X_i) \). And Figure 6 zooms on the evolution of the Markov chain \( (X_i, \epsilon_i^1 \pi(X_i)) \) over the last 100 iterations, which follows vertical and horizontal moves of the Markov chain under the target density curve.

The validation of the method (e.g., Robert and Casella [2004]) proceeds by estab-
lishing that the resulting Markov chain is ergodic (e.g., Meyn and Tweedie 1993), meaning that it converges to the distribution corresponding to $\pi$, making the starting value of the chain irrelevant. Akin to basic Monte Carlo methods, MCMC samples (usually) enjoy standard limit theorems.

3.1 Metropolis-Hastings algorithms

The Metropolis–Hastings algorithm is the “Swiss knife” of MCMC methods in that it offers a form of universal solution to the construction of an appropriate Markov chain. The algorithm requires a proposal distribution, with density $q(x'|x)$ and proceeds one step at a time based on simulations proposed from this distribution and accepted or rejected by a Metropolis–Hastings ratio, as described in Algorithm 1.

Algorithm 1 Metropolis-Hastings algorithm

Input: starting point $X_0$, proposal distribution $q$ and number of iterations $N$.

for $n = 1, 2, \ldots, N$ do

Sample $X' \sim q(\cdot | X_{n-1})$

Compute the acceptance probability $\alpha(X_{n-1}, X')$, where

$$\alpha(X_{n-1}, X') = \min \left\{ 1, \frac{p(X') q(X_{n-1}|X')}{p(X_{n-1}) q(X'|X_{n-1})} \right\}$$

Sample $U \sim U[0,1]$;

if $U < \alpha(X_{n-1}, X')$ then

$X_n \rightarrow X'$

else

$X_n \rightarrow X_{n-1}$

end if

end for

The accept–reject step in this algorithm is fundamental in that it turns $p$ into its stationary distribution, assuming the resulting Markov kernel is irreducible, provided the chain $(X_n)$ is irreducible, meaning it has a positive probability of hitting any part of the support of $p$ on a finite number of steps. Stationary follows from the transition satisfying the detailed balance condition, corresponding to the chain being reversible in time, see, e.g., Robert and Casella 2004. A special case when $q$ is symmetric, i.e., $q(x|y) = q(y|x)$ is called random walk MCMC and the acceptance probability only involves the targeted $p$.

"What is the deeper intuition behind the symmetric proposal distribution in the Metropolis-Hastings Algorithm?" [cross-validated:262216]

1. The Normal and Uniform are symmetric probability density functions themselves, is this notion of “symmetry” the same as the “symmetry” above?

2. Is there an intuitive way of seeing the deeper meaning behind the symmetry formula above?

Both Normal and Uniform distributions are symmetric around their mean. But the symmetry in Metropolis-Hastings signifies that $q(x|y) = q(y|x)$ which makes the ratio cancel in the Metropolis-Hastings acceptance probability. If one uses a Normal distribution not centered at the previous

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1 in reference to N. Metropolis, with whom the algorithm originated (Metropolis et al. 1953) and K. Hastings, for his generalisation (Hastings 1970)
value in the Metropolis-Hastings proposal (as e.g. in the Langevin version), the Normal distribution remains symmetric as a distribution but the proposal distribution is no longer symmetric and hence it must appear in the Metropolis-Hastings acceptance probability.

There is no particular depth in this special symmetric case, it simply makes life easier by avoiding the ratio of the proposals. It may save time or it may avoid computing complex or intractable densities. Note also that the symmetry depends on the parameterisation of the model: if one changes the parameterisation, a Jacobian appears and kills the symmetry.

The independent Metropolis Algorithm using the proposal \( X' \sim f_V(x) \) should have \( \alpha(X_0, X'_0) = 1 \) and hence the chain always equal to \( X'_0 \). (cross-validated:396704]

The confusion stems from a misunderstanding of the notation \( X' \sim f_V \) which means both (a) \( X' \) is a random variable with density \( f_V \) and (b) \( X' \) is created by a pseudo-random generation algorithm that reproduces a generation of a random variable with density \( f_V \). Each time a generation \( X'_i \sim f_V \) occurs in the algorithm, a new realisation of a random variable with density \( f_V \) occurs, which is independent from all previous realisations, hence different from these previous realisations. Equivalently, stating that the \( X'_i \) are all identically distributed from the same distribution \( f_V \) does not mean that their realisations all are numerically identical.

The starting point of the Metropolis-Hastings algorithm is arbitrary, either fixed \( X_0 = 0 \) for instance or random, for instance \( X_0 \sim f_V \) (a notation meaning that \( X_0 \) is distributed from \( f_V \)). This starting value is always accepted. For \( i = 1 \), one generates \( X'_1 \sim f_V \) (meaning that \( X'_1 \) is distributed from \( f_V \), independently and thus different from \( X_0 \))

\[
X_1 = \begin{cases} 
X'_1 & \text{if } U_1 \leq \alpha_1 = \min \left( \frac{f_V(X'_1)}{f_V(X)} \frac{f_V(X)}{f_V(X'_1)} \right, 1 \\
X_0 & \text{if } U_1 > \alpha_1
\end{cases}
\]

and \( \alpha_1 \neq 1 \) in general. Hence sometimes \( X_1 \) is accepted and sometimes not. The same applies to the following steps. To make a toy illustration on how the algorithm applies, take \( f_V \) to be the density of a \( \mathcal{N}(0, 1) \) distribution and \( f_V \) to be the density of a \( \mathcal{N}(1, 1) \) distribution. A sequence of i.i.d. generations from \( f_V \) is for instance (by a call to \( \text{R norm} \))

\[
0.45735433, -0.99178415, -1.08312586, -0.85762451, 0.92186197, -0.50442298, ...
\]

(note that they are all different) and a sequence of generations from \( \mathcal{U} \) is for instance (by a call to \( \text{R runif} \))

\[
0.441328, 0.987837, 0.386258, 0.316593, 0.195910, 0.2772669, ...
\]

(note that they are all different). Applying the algorithm with starting value \( X_0 = 0 \) means considering

\[
\frac{f_V(X'_1)}{f_V(X)} \frac{f_V(X)}{f_V(X'_1)} = 0.9582509/0.6065307 = 1.579889 > 1
\]

which implies that \( X_1 = X'_1 = 0.45735433 \). Then

\[
\frac{f_V(X'_2)}{f_V(X)} \frac{f_V(X)}{f_V(X'_2)} = 0.2249709/0.9582509 = 0.2347724 < U_2 = 0.987837
\]

which implies that \( X_2 = X_1 \). The algorithm can be applied step by step to the sequences provided above, which leads to

\[
\begin{align*}
\frac{f_V(X'_3)}{f_V(X)} \frac{f_V(X)}{f_V(X'_3)} &= 0.2053581/0.9582509 = 0.2143051 < U_3 \quad Z_3 = Z_1 \\
\frac{f_V(X'_4)}{f_V(X)} \frac{f_V(X)}{f_V(X'_4)} &= 0.2572712/0.9582509 = 0.2684800 < U_4 \quad Z_4 = Z_1 \\
\frac{f_V(X'_5)}{f_V(X)} \frac{f_V(X)}{f_V(X'_5)} &= 1.5247980/0.9582509 = 1.591230 > 1 \quad Z_5 = V_5
\end{align*}
\]
Figure 7: Independent Metropolis sequence with a proposal \( f_V \) equal to the density of a \( \mathcal{N}(0, 1) \) distribution and a target \( f_Y \) being the density of a \( \mathcal{N}(1, 1) \) distribution.

producing a sequence as in Figure 7 (notice the flat episodes in the graph, which correspond to a sequence of rejections).

As a final remark, the only potentially confusing part in the description in Casella and Berger (1990) is the very first sentence where the random variables \( Y \) and \( V \) are not needed. It could have been clearer to state “Let \( f_Y \) and \( f_V \) be two densities with common support.”

Since the purpose of MCMC methods like the Metropolis-Hastings algorithm is to simulate realisations from \( p \), their performances are highly variable. These obviously depends on the connection between \( p \) and \( q \). For instance, the Metropolis-Hastings algorithm is an i.i.d. sampler when \( q(\cdot|X_n) = p(\cdot) \), a choice that is rarely available. Although it may happen that the Markov chain \((X_n)\) achieves negative correlations between successive and further terms of the series, making it em more efficient than i.i.d. sampling [Liu et al., 1995], it is more common that there exists a positive covariance between simulations (sometimes for all transforms, see Liu et al., 1994). This feature means a lesser efficiency of the algorithm which thus requires a greater number of simulations to achieve the same accuracy as the i.i.d. approach (regardless of the differences in computing time). In general, the MCMC algorithm may require a large number of iterations to escape the attraction of the starting point \( X_0 \) and to converge. There is a real danger that some versions of these algorithms do not converge within the allotted time (in practice if not in theory).

“What is the Metropolis-Hastings acceptance ratio for a truncated proposal?” [cross-valdated:345291]

If a Metropolis-Hastings algorithm uses a truncated Normal as proposal, e.g., the positive Normal \( \mathcal{N}^+(\mu_{t-1}, \sigma^2) \), the associated Metropolis-Hastings acceptance ratio is

\[
\frac{\pi(\mu')}{\pi(\mu_{t-1})} \times \frac{\varphi(\{\mu_{t-1} - \mu'\}/\sigma)}{\varphi(\{\mu' - \mu_{t-1}\}/\sigma)} \times \frac{\Phi(\mu_{t-1}/\sigma)}{\Phi(\mu'/\sigma)}
\]

when \( \mu' \sim \mathcal{N}^+(\mu_{t-1}, \sigma^2) \) is the proposed value and \( \pi \) denotes the target of the simulation (e.g., the posterior distribution). This ratio simplifies into

\[
\frac{\pi(\mu')}{\pi(\mu_{t-1})} \frac{\Phi(\mu_{t-1}/\sigma)}{\Phi(\mu'/\sigma)}
\]

hence the truncation impacts the Metropolis-Hastings acceptance ratio.

Figure 8 provides an illustration for the target density

\[
\pi(\mu) \propto \exp\{- (\log \mu - 1)^2\} \exp\{- (\log \mu - 3)^4/4\}
\]

when using \( \sigma = .1 \) as the scale in the truncated Normal.
“What to do when rejecting a proposed point in MCMC?” [cross-validated:123113]

The validation of the Metropolis-Hastings algorithm relies on repeating the current value in the Markov chain if the proposed value is rejected. One should not consider the list of accepted* points as one’s sample but instead the Markov chain with transition

\[ X_{t+1} = Y_{t+1} \]

\[ = X_t \]

if \( U_{t+1} \leq \frac{\pi(Y_{t+1})}{\pi(X_t)} \)

otherwise

(assuming a symmetric proposal distribution). The repetition of the current value in the event of a rejection is what makes the algorithm valid, i.e., why \( \pi \) is the stationary distribution.

It is always possible to study the distribution of the accepted and of the rejected values, with some recycling possible by Rao-Blackwellisation [Casella and Robert 1996], but this study is more advanced and far from necessary to understand the algorithm.

How to account for impossible proposed values? [cross-validated:51808]

It is indeed a popular belief that something needs to be done to account for restricted supports. However, there is no mathematical reason for doing so. The Metropolis-Hastings acceptance probability

\[ \rho(x_t, y_{t+1}) = \min(1, \pi(y_{t+1})q(x_t|y_{t+1})/\pi(x_t)q(y_{t+1}|x_t)) \]

with \( y_t \sim q(y_{t+1}|x_t) \) can handle cases when \( y_t \) is outside the support of \( \pi \) by extending this support, defining \( \pi(y) = 0 \) outside the original support. Hence, if \( \pi(y_{t+1}) = 0 \), then \( \rho(x_t, y_{t+1}) = 0 \), which means the proposed value is automatically rejected and \( x_{t+1} = x_t \).

Consider the following illustration.

```r
target=function(x) (x>0)*(x<1)*dnorm(x,mean=4)
mcmc=rep(0.5,10^5)
for (t in 2:10^5){
  prop=mcmc[t-1]+rnorm(1,.1)
  if (runif(1)<target(prop)/target(mcmc[t-1]))
    mcmc[t]=prop
  else
    mcmc[t]=mcmc[t-1]
}
that is targeting a truncated normal distribution using a Gaussian random walk proposal with support the entire real line. Then the algorithm is properly converging as shown by the fit in Figure[9]

Unbiased MCMC [xianblog:25/08/2017]

Jacob et al. (2020) propose an unbiased MCMC technique based on coupling. Associating MCMC with unbiasedness is rather challenging since MCMC are rarely producing simulations from the exact target, unless specific tools like renewal can be produced in an efficient manner.

The central idea is coupling of two (MCMC) chains, associated with the debiasing formula used by Glynn and Rhee (2014). Having the coupled chains meet at some time with probability one implies that the debiasing formula does not need a (random) stopping time. The coupling time is sufficient. Furthermore, several estimators can be derived from the same coupled Markov chain simulations, obtained by starting the averaging at a later time than the first iteration. The average of these (unbiased) averages results into a weighted estimate that weights more the later differences. Although coupling is also at the basis of perfect simulation methods, the analogy between this debiasing technique and perfect sampling is hard to fathom, since the coupling of two chains is not a perfect sampling instant. (Something obvious in retrospect is that the variance of the resulting unbiased estimator is at best the variance of the original MCMC estimator.)

When discussing the implementation of coupling in Metropolis and Gibbs settings, the authors produce a simple optimal coupling algorithm, a form of accept-reject also found in perfect sampling. While I did not fully understood the way two random walk Metropolis steps are coupled, in that the normal proposals seem at odds with the boundedness constraints, coupling is clearly working in this setting, while renewal does not. In toy examples like the Efron and Morris (1973) baseball data and the Gelfand and Smith (1990) pump failure data, the parameters of the algorithm can be optimised against the variance of the averaged averages. And this approach proves highly useful in the case of the cut distribution.

3.2 Gibbs sampling

Historically, this form of MCMC algorithm is distinguished from the other types of MCMC methods for being both justified by other arguments and used for a specific class of models (Robert and Casella 2004).

“Why would one use Gibbs sampling instead of Metropolis-Hastings?” [cross-validated:244573]

The question does not have an answer in that a Metropolis-Hastings sampler can be almost anything, including a Gibbs sampler. The primary reason why Gibbs sampling was introduced was to break the curse of dimensionality (which impacts both rejection and importance sampling) by producing a sequence of low dimension simulations that still converge to the right target. Even though the dimension of the target impacts the speed of convergence. Metropolis-Hastings samplers are designed to create a Markov chain (like Gibbs sampling) based on a proposal (like importance and rejection sampling) by correcting for the wrong density through an acceptance-rejection step. But an important point is that they are not opposed: namely, Gibbs sampling may require Metropolis-Hastings steps when facing complex if low-dimension conditional targets,
while Metropolis-Hastings proposals may be built on approximations to (Gibbs) full conditionals. In a formal definition, Gibbs sampling is a special case of Metropolis-Hastings algorithm with a probability of acceptance of one.

Usually, Gibbs sampling—understood as running a sequence of low-dimensional conditional simulations—is favoured in settings where the decomposition into such conditionals is easy to implement and fast to run. In settings where such decompositions induce multimodality and hence a difficulty to move between modes (latent variable models like mixture models come to mind), using a more global proposal in a Metropolis-Hastings algorithm may produce a higher efficiency. But the drawback stands with choosing the proposal distribution in the Metropolis-Hastings algorithm.

3.3 Hamiltonian Monte Carlo

A more advanced (and still popular) form of MCMC algorithm is Hamiltonian Monte Carlo (HMC) [Duane et al., 1987; Neal 1999, 2011]. While a special case of continuous time samplers, it can be implemented in discrete time and is actually behind the successful Stan package [Carpenter et al., 2017]. The construction of the process relies on an auxiliary variable $v$ that augments the target into

$$
\rho(x, v) = p(x) \varphi(v|x) \propto \exp\{-H(x, v)\},
$$

where $\varphi(v|x)$ is the conditional density of $v$ given $x$. This density obviously enjoys $p(v)$ as its marginal and while it could be anything, the so-called momentum $v$ is usually chosen of the same dimension as $v$, with $\varphi(v|x)$ often taken as a Normal density. The associated Hamiltonian equations

$$
\frac{dx_t}{dt} = \frac{\partial H}{\partial v}(x_t, v_t), \quad \frac{dv_t}{dt} = -\frac{\partial H}{\partial x}(x_t, v_t),
$$

which keeps the Hamiltonian target $H(\cdot)$ constant over time, as

$$
\frac{dH(x_t, v_t)}{dt} = \frac{\partial H}{\partial v}(x_t, v_t) \frac{dv_t}{dt} + \frac{\partial H}{\partial x}(x_t, v_t) \frac{dx_t}{dt} = 0.
$$

Since there is no randomness in the above process, the HMC algorithm is completed with random changes of the momentum according to the correct conditional distribution, $v_t \sim \varphi(v|x_t)$, at times driven by a Poisson process $\{\tau_n\}_n$.

As noted above, the choice of the conditional density $\varphi(v|x_t)$ often is a Gaussian density with either a constant covariance matrix $M$ calibrated from the target covariance or as a local curvature depending on $x$ in the version of Girolami and Calderhead [2011] called Riemannian Hamiltonian Monte Carlo. See, e.g., Livingstone et al. [2017] for an analysis of the impact of different types of kinetic energy on Hamiltonian Monte Carlo performances.

When the fixed covariance matrix is equal to $M$, the Hamilton equations write as

$$
\frac{dx_t}{dt} = M^{-1}v_t, \quad \frac{dv_t}{dt} = \nabla \log p(x_t),
$$

where the last term is the score function. The velocity of the HMC process is thus connected to the gradient of the log-target.

In practice, implementing this rather simple remark proves rather formidable in that there is no direct approach for methodology for simulating this continuous time process, since the above equations cannot be intractable. A natural resolution
associates a numerical solver like Euler’s method, usually unstable, with a numerical solver naturally suited to these equations.

This general method is called a symplectic integrator (Betancourt, 2017) with implementation in the constant covariance case resorting to time-discretisation leapfrog steps

\[
\begin{align*}
v_{t+\epsilon/2} &= v_t + \epsilon \nabla \log p(x_t)/2, \\
x_{t+\epsilon} &= x_t + \epsilon M^{-1} v_{t+\epsilon/2}, \\
v_{t+\epsilon} &= v_{t+\epsilon/2} + \epsilon \nabla \log p(x_{t+\epsilon})/2,
\end{align*}
\]

which symmetrises the two-step move, with \(\epsilon\) standing for the time-discretisation step. The proposed value of \(v_0\) is generated from the true Gaussian target. The correction to the discretisation approximation involves a Metropolis–Hastings step over the pair \((x_{t+\epsilon}, v_{t+\epsilon})\) which reintroduces some reversibility into the picture.

Time-discretising the Hamiltonian dynamics in the leapfrog integrator involves two quantities, \(\epsilon\) and \(T\) the trajectory length. One empirically sound calibration of these parameters is found in the “no-U-turn sampler” of Hoffman and Gelman (2014) which selects the value of \(N\) by primal-dual averaging and produces the trajectory length \(T\) as the length of the chain is takes for the path to fold back.

Algorithm 2 Leapfrog \((x_0, v_0, \epsilon, L)\)

\[
\text{Input: starting position } x_0, \text{ starting momentum } v_0, \text{ step-size } \epsilon, \text{ steps } L
\]

\[
\text{for } \ell = 0, 1, \ldots, L - 1 \text{ do}
\]

\[
\begin{align*}
v_{\ell+1/2} &= v_{\ell} + \epsilon \nabla \log p(x_{\ell}) \\
x_{\ell+1} &= x_{\ell} + \epsilon M^{-1} v_{\ell+1/2} \\
v_{\ell+1} &= v_{\ell+1/2} + \epsilon \nabla \log p(x_{\ell+1})
\end{align*}
\]

\[
\text{end for}
\]

\[
\text{Output: } (x_L, v_L)
\]

Algorithm 3 Hamiltonian Monte Carlo algorithm

\[
\text{Input: step-size } \epsilon, \text{ steps of leapfrog integrator } L, \text{ starting position } x_0, \text{ desired number of iterations } N.
\]

\[
\text{for } n = 1, \ldots, N \text{ do}
\]

\[
\begin{align*}
\text{Sample } v_{n-1} &\sim \phi(v); \\
\text{Compute } (x^*, v^*) &\leftarrow \text{Leapfrog}(x_{n-1}, v_{n-1}, \epsilon, L); \\
\text{Compute the acceptance ratio } \alpha, \text{ where}
\end{align*}
\]

\[
\alpha = \min \{1, \exp(-H(x^*, -v^*)/\exp(-H(x_{n-1}, v_{n-1})) \}
\]

\[
\text{Sample } u \sim \mathcal{U}[0, 1];
\]

\[
\text{if } u < \alpha \text{ then}
\]

\[
x_n \leftarrow x^*
\]

\[
\text{else}
\]

\[
x_n \leftarrow x_{n-1}
\]

\[
\text{end if}
\]

\[
\text{end for}
\]

In practice, it is important to note that discretising Hamiltonian dynamics introduces two free parameters, the step size \(\epsilon\) and the trajectory length \(T\), both to be calibrated. As an empirically successful and popular variant of HMC, the “no-U-turn sampler” (NUTS) of Hoffman and Gelman (2014) adapts the value of \(\epsilon\) based on primal-dual averaging. It also eliminates the need to choose the trajectory length.
via a recursive algorithm that builds a set of candidate proposals for a number of forward and backward leapfrog steps and stops automatically when the simulated path retraces.

Unbiased HMC [xianblog:25/09/2017]

Heng and Jacob (2019) propose to achieve unbiased Hamiltonian Monte Carlo by coupling, following Jacob et al. (2020) discussed earlier. The coupling within the HMC amounts to running two HMC chains with common random numbers, plus subtleties.

“As with any other MCMC method, HMC estimators are justified in the limit of the number of iterations. Algorithms which rely on such asymptotics face the risk of becoming obsolete if computational power keeps increasing through the number of available processors and not through clock speed.” Heng and Jacob (2019)

The main difficulty here is to have both chains meet (exactly) with large probability, since coupled HMC can only bring these chain close to one another. The trick stands in using both coupled HMC and coupled Hastings-Metropolis kernels, since the coupled MH kernel allows for exact meetings when the chains are already close, after which they remain forever identical. The algorithm is implemented by choosing at random between the kernels at each iteration. (Unbiasedness follows by the Glynn-Rhee trick, which is eminently well-suited for coupling.) As pointed out from the start of the paper, the appeal of this unbiased version is that the algorithm can be (embarrassingly) parallelised since all processors in use return estimators that are i.i.d. copies of one another, hence easily merged into a better estimator.

4 Approximate Bayesian computation

The methods surveyed above share the common feature of exploiting the shape of the target density, $p(\cdot)$, namely that it is known exactly or known up to a normalising constant $p(x) \propto \tilde{p}(x)$ or yet known as the marginal of another density

$$p(x) = \int_y q(x, y) \, dy.$$ 

It may however occur that the density of the target is not numerically available, in the sense that computing $p(x)$ or $\tilde{p}(x)$ is not feasible in a reasonable time or that completing $p(\cdot)$ into $q(\cdot)$ involves a massive increase in the dimension of the problem. This obviously causes difficulties in applying, e.g., MCMC methods. A particularly common case occurs in the Bayesian analysis of intractable likelihoods.

“What would be a good example of a really simple model that has an intractable likelihood?” [cross-validated:127180]

Given an original Normal dataset

$$x_1, \ldots, x_n \overset{iid}{\sim} N(\theta, \sigma^2),$$

the reported data is made of the two-dimensional summary

$$S(x_1, \ldots, x_n) = (\text{med}(x_1, \ldots, x_n), \text{mad}(x_1, \ldots, x_n)),$$

where $\text{mad}(x_1, \ldots, x_n)$ is the median average deviation of the sample, which is not sufficient and which does not have a closed form joint density.
Besides this simple example, there are numerous occurrences of ill-defined likelihoods that cannot be computed, from latent variable models, including hidden Markov models, to likelihoods with a missing normalising term depending on the parameter, including Ising models [Potts 1952] and other non-standard exponential families, to densities defined as solutions of differential equations, via their characteristic function, like α-stable distributions [Peters et al. 2012], or via their quantile function like Tukey’s g-and-k distributions [Haynes et al. 1997].

A different kind of algorithms is required for handling such situations. They are called ‘likelihood-free’ or approximate Bayesian computation (ABC) methods, as they do not require the likelihood function and provide an approximation of the original posterior distribution.

“What does it mean for an inference or optimisation method to be ‘likelihood-free’.”
[cross-validated:383731]

Specifically, likelihood-free methods are a rewording of the ABC algorithms, where ABC stands for approximate Bayesian computation. This intends to cover inference methods that do not require the use of a closed-form likelihood function, but still intend to study a specific statistical model. They are free from the computational difficulty attached with the likelihood but not from the model that produces this likelihood. See for instance the recent handbook by Sisson et al. (2019).

The basic ABC algorithm is based on the following principle: given a target posterior proportional to $\pi(\theta)f(x_{\text{obs}}|\theta)$, when the likelihood function $f(x_{\text{obs}}|\theta)$ is not available in closed form, jointly simulating

$$\theta' \sim \pi(\theta), z \sim f(z|\theta'),$$

until the auxiliary variable $z$ is equal to the observed value, $z = x_{\text{obs}}$ does produce a realisation from the posterior distribution without ever computing a numerical value of the likelihood function. It only requires that the model associated with this likelihood can be simulated, which often leads to the model being called a generative model.

“How can we prove that when accepting for $x = x_{\text{obs}}$ this algorithm, we sample from the true posterior?” [cross-validated:380076]

This case is the original version of the algorithm, as in Rubin (1984) and Tavaré et al. (1997). Assuming that

$$\mathbb{P}_\theta(Z = x_{\text{obs}}) > 0$$

the values of $\theta$ that come out of the algorithm are distributed from a distribution with density proportional to

$$\pi(\theta) \times \mathbb{P}_\theta(Z = x_{\text{obs}})$$

since the algorithm generates the pair $(\theta, 1_{Z = x_{\text{obs}}})$ with joint distribution

$$\pi(\theta) \times \mathbb{P}_\theta(Z = x_{\text{obs}})1_{Z = x_{\text{obs}}} \times \mathbb{P}_\theta(Z \neq x_{\text{obs}})1_{Z \neq x_{\text{obs}}}.$$

Conditioning on $1_{Z = x_{\text{obs}}} = 1$ leads to

$$\theta|1_{Z = x_{\text{obs}}} = 1 \sim \pi(\theta) \times \mathbb{P}_\theta(Z = x_{\text{obs}}) / \int \pi(\theta) \times \mathbb{P}_\theta(X = x_{\text{obs}}) \, d\theta$$

which is the posterior distribution.

3The notation $x_{\text{obs}}$ is intended to distinguish the observed sample from simulated versions of this sample.
As noted in the above vignette, the principle can only be implemented when \( P_\theta(Z = x^{\text{obs}}) > 0 \) and more accurately when the event \( Z = x^{\text{obs}} \) has a non-negligible chance to occur. This is however rarely the case in realistic settings, especially when \( Z \) is a continuous variable, and the first implementations \cite{Pritchard99} of the ABC algorithm replaced the constraint of equality \( z = x^{\text{obs}} \) a relaxed version,

\[
\varrho(z, x^{\text{obs}}) \leq \epsilon
\]

where \( \varrho \) is a distance and \( \epsilon > 0 \) is called the tolerance. This approximation step makes the concept applicable in a wider range of settings with an intractable, but it also implies that the simulated distribution is modified from the true posterior into

\[
\pi(\theta | \varrho(Z, x^{\text{obs}}) < \epsilon) \propto \pi(\theta) P_\theta \{ \varrho(Z, x^{\text{obs}}) < \epsilon \}.
\]

It helps to visualise this alternative posterior distribution as truly conditioning on the event \( \varrho(Z, x^{\text{obs}}) < \epsilon \) rather than \( x^{\text{obs}} \) as it gives a specific meaning to this distribution and explains the loss in information brought by the approximation.

In many settings, especially with large datasets, looking at a distance between the raw observed data and the raw simulated data is very inefficient. It is much more efficient \cite{Frazier18,Li18} to compare informative summaries of the data as the decrease in dimension allows for smaller tolerance, a higher signal to noise ratio, and outweighs the potential loss in information. A more common implementation of the algorithm is thus

\begin{algorithm}
\textbf{Algorithm 4} Likelihood-free (ABC) rejection sampler
\begin{algorithmic}
\FOR {i = 1 to N}
\REPEAT
\STATE generate \( \theta' \) from the prior distribution \( \pi(\cdot) \)
\STATE generate \( z \) from the likelihood \( f(\cdot | \theta') \)
\UNTIL \( \rho(\eta(z), \eta(x^{\text{obs}})) \leq \epsilon \)
\STATE set \( \theta_i = \theta' \)
\ENDFOR
\end{algorithmic}
\end{algorithm}

where \( \eta(\cdot) \) denotes a (not necessarily sufficient) statistic, usually (needlessly) called a summary statistic. While there is a huge literature \cite{Aeschbacher12,Blum13,Estoup12,Fearnhead12,Sisson19} on the choice of the summary statistic, compelling arguments \cite{Fearnhead12,Li18} lead to opt for summaries of the same dimension as the parameter \( \theta \).

While the motivation for simulating from the prior distribution is clear from a theoretical perspective, given that the probability of accepting in Algorithm 4 is approximately the intractable likelihood, it is also often poor in efficiency since the posterior is much more concentrated. Subsequent versions of ABC have thus aimed at alternative approaches to increase the efficiency of the method. For instance, the proposal distribution on \( \theta \) can be modified towards increase the frequency of \( x \)'s within the vicinity of \( x^{\text{obs}} \) \cite{Bortot07,Marjoram03}. Others have replaced the indicator function in Algorithm 4 with less rudimentary estimators of the likelihood \cite{Beaumont02,Blum10,Mengersen13}, interpreting the tolerance \( \epsilon \) as a bandwidth \cite{Frazier18,Li18} or a new component in the inferential framework \cite{Ratmann09}.

Computational advances have seen MCMC, SMC \cite{Beaumont09} and Gibbs \cite{Clarte19} versions of ABC. For instance, ABC-MCMC \cite{Marjoram07}
is based on the property that the Markov chain \((\theta^{(t)})\) created via the transition function

\[
\theta^{(t+1)} = \begin{cases} 
\theta' \sim K_\omega(\theta'|\theta^{(t)}) & \text{if } z \sim f(z|\theta') \text{ is such that } z = x_{\text{obs}} \\
\theta^{(t)} & \text{otherwise,}
\end{cases}
\]

enjoys the posterior \(\pi(\theta|x_{\text{obs}})\) as its stationary distribution. The corresponding algorithm is then

**Algorithm 5 Likelihood-free MCMC sampler**

Use Algorithm 4 to get \((\theta^{(0)}, z^{(0)})\)

\[
\text{for } t = 1 \text{ to } N \text{ do}
\]

\[
\begin{align*}
\theta' & \sim K_\omega(\cdot|\theta^{(t-1)}) \\
z' & \sim f(\cdot|\theta') \\
u & \sim \mathcal{U}(0, 1) \\
\text{if } u \leq \frac{\pi(\theta')K_\omega(\theta'|\theta^{(t-1)})}{\pi(\theta^{(t-1)}K_\omega(\theta'|\theta^{(t-1)})} \text{ then set } (\theta^{(t)}, z^{(t)}) = (\theta', z') \\
\text{else set } (\theta^{(t)}, z^{(t)}) = (\theta^{(t-1)}, z^{(t-1)}),
\end{align*}
\]

\[
\text{end if}
\]

\[
\text{end for}
\]

The choice of summary statistics in ABC method is paramount for the efficiency of the approximation and nowhere more than for model choice. Since the Bayes factor is given by

\[
B_{12}(x_{\text{obs}}) = \frac{\Pr(M_1|x_{\text{obs}})}{\Pr(M_2|x_{\text{obs}})} / \Pr(M_1) / \Pr(M_2)
\]

the ratio of frequencies of simulations from \(M_1\) and \(M_2\) that are accepted need be divided by the prior probabilities of \(M_1\) and \(M_2\) if these reflect the number of times each model is simulated. Apart from this, the approximation is valid. Using inappropriate summary statistics in this setting has been pointed out in [Didelot et al. (2011), Robert et al. (2011) and Marin et al. (2014)].

A special instance of (almost) intractable is the setting of “Big Data” problems where the size of the data makes computing the likelihood quite expensive. In such cases, ABC can be seen as a convenient approach to scalable Monte Carlo.

What difference does it make working with a big or small dataset in ABC? [cross-validated:424712]

It all depends on the structure of the dataset and the complexity of the model behind. In some settings the size of the data may be the reason for conducting an ABC inference as the likelihood takes too much time to compute. But there is no generic answer to the question since in the ultimate case when there exists a sufficient statistic of fixed dimension size does not matter (and of course ABC is unlikely to be needed).

Do we get any computational benefits by reducing a very big dataset when doing inference using ABC methods?

In most settings, ABC proceeds through a set of summary statistics that are of a much smaller dimension than the data. In that sense they are independent of the size of the data, except that to simulate values of the summaries, most models require simulations of the entire dataset first. Unless a proxy model is used as in synthetic likelihood.
...the rejection criterion in ABC is related to how well we approximate the full likelihood of the dataset which is typically captured in some low-dimensional summary statistics vector.

You have to realise that the rejection is relative to the distribution of the distances between the observed and the simulated summaries [simulated under the prior predictive], rather than absolute. In other words, there is no predetermined value for the tolerance. This comes in addition to the assessment being based on an insufficient statistics rather than the full data. This means that, for a given computing budget, the true likelihood of an accepted parameter may be quite low.

5 Further reading

There are many reviews and retrospective on the Markov Chain Monte Carlo methods, not only in statistics, but also in physics, econometrics and several other fields, most of which provide different perspectives on the topic. For instance, Dunson and Johndrow (2020) recently wrote a celebration of Hastings’ 1970 paper in Biometrika, where they cover adaptive Metropolis (Haario et al., 1999; Roberts and Rosenthal, 2005), the importance of gradient based versions toward universal algorithms (Neal, 2003; Roberts and Tweedie, 1995), discussing the advantages of HMC over Langevin versions. They also recall the significant step represented by Green’s (1995) reversible jump algorithm for multimodal and multidimensional targets, as well as tempering (Miasojedow et al., 2013; Woodard et al., 2009). They further cover intractable likelihood cases within MCMC (rather than ABC), with the use of auxiliary variables (Friel and Pettitt, 2008; Møller et al., 2006) and pseudo-marginal MCMC (Andrieu and Roberts, 2009; Andrieu and Vihola, 2016). They naturally insist upon the need to handle huge datasets, high-dimension parameter spaces, and other scalability issues, with links to unadjusted Langevin schemes (Bardenet et al., 2014; Durmus and Moulines, 2017; Welling and Teh, 2011). Similarly, Dunson and Johndrow (2020) discuss recent developments towards parallel MCMC and see non-reversible schemes such as PDMP as highly promising, with a concluding section on the challenges of automating and robustifying much further the said procedures, if only to reach a wider range of applications. Other directions that are clearly still relevant after decades of development include convergence assessment, e.g. the comparison and aggregation of various approximation schemes, since this is a fairly common request from users, recycling schemes, like Rao-Blackwellisation (Casella and Robert, 1996; Gelfand and Smith, 1990) and other post-processing improvements that address the massive waste of simulation in most method, the potential for mutual gains between machine-learning tools and MCMC refinements, as well as the theoretical difficulties presented by approximations such as synthetic likelihood (Wood, 2010), indirect inference (Drovandi et al., 2011) and incompatible conditionals (Clarté et al., 2019; Jacob et al., 2017; Plummer, 2015).

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