On optimality of kernels for approximate Bayesian computation using sequential Monte Carlo

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Abstract

Sequential Monte Carlo (SMC) approaches have become work horses in approximate Bayesian computation (ABC). Here we discuss how to construct the perturbation kernels that are required in ABC SMC approaches, in order to construct a set of distributions that start out from a suitably defined prior and converge towards the unknown posterior. We derive optimality criteria for different kernels, which are based on the Kullback-Leibler divergence between a distribution and the distribution of the perturbed particles. We will show that for many complicated posterior distributions locally adapted kernels tend to show the best performance. In cases where it is possible to estimate the Fisher information we can construct particularly efficient perturbation kernels. We find that the added moderate cost of adapting kernel functions is easily regained in terms of the higher acceptance rate. We demonstrate the computational efficiency gains in a range of toy-examples which illustrate some of the challenges faced in real-world applications of ABC, before turning to a demanding parameter inference problem for a dynamical system, which highlights the huge increases in efficiency that can be gained from choice of optimal models. We conclude with a general discussion of rational choice of perturbation kernels in ABC SMC settings.

1 Introduction

Statistical practice and theory tend to reflect scientific fashions (Stigler, 1986). Today mathematical models in physics, engineering, biology, but also the social and engineering sciences are becoming increasingly complex. This, together with the deluge of data being produced in many fields, poses severe challenges to statistical inference (Efron, 2010). In particular evaluation of the likelihood (Cox, 2006)

\[ L(\theta) = f(x|\theta), \]

where \( x \) are realizations of the data, and \( \theta \) is the (potentially vector-valued) parameter characterizing the data-generating process, is often turning out to be impractical. Approximate Bayesian Computation (ABC) methods (Beaumont & Zhang, 2002; Marin et al., 2011) were first conceived to allow (Bayesian) statistical inference in situations where the evaluation of the likelihood is too complicated or numerically too demanding (Pritchard et al., 1999; Tanaka, 2006; Lopes & Beaumont, 2010). Rather than evaluating the likelihood directly, ABC-based approaches use systematic comparisons between real and simulated data in order to arrive at approximations of the true (but unobtainable) posterior distribution,

\[ p(\theta|x) \propto f(x|\theta)\pi(\theta), \]
where $\pi(\theta)$ denotes the prior distribution of $\theta$.

Simulating from $f(x|\theta)$ is generally straightforward, even if obtaining a reliable numerical/functional representation of the model is not possible. We then compare the simulated data, $y$, with the real data, $x$, and accept only those simulations where some distance measure, $\Delta(x, y)$, between the two falls below a specified threshold, $\epsilon$. If the data are too intricate or complicated it is common to replace a comparison of the real and simulated data, by a comparison of suitable summary statistics. This results in a often appreciable reduction of the dimension but is fraught with problems if the summary statistics are not sufficient. Given that sufficiency (Cox, 2006) is a rare quality indeed (Lehmann & Casella, 1993), and probably not given for any real-world problem of scientific interest, this problem is now attracting a lot of attention (Robert & Cornuet, 2011; Didelot et al., 2011; Fearnhead & Prangle, 2010). Here, however, we shall focus on the data directly; we thus seek to determine approximate posteriors of the form,

$$p(\theta|x) \approx p_\epsilon(\theta|x) \propto \int f(y|\theta) \mathbb{1}(\Delta(x, y) \leq \epsilon) \pi(\theta) dy,$$

where $y$ is the data simulated from the model $f(\cdot|\theta)$ for a given parameter, $\theta$, drawn from the appropriate prior distribution, and $x$ is the observed data.

The simple ABC scheme outlined above suffers from the same shortcomings as other rejection samplers: most of the samples are drawn from regions of parameter space, which cannot give rise to simulation outputs that resemble the data. Therefore a number of computational schemes have been proposed that makes ABC inference more efficient. These come in loosely three flavours: regression-adjusted ABC (Tallmon, 2004; Fagundes et al., 2007; Blum & François, 2009), Markov chain Monte Carlo ABC schemes (Marjoram & Molitor, 2003; Ratmann et al., 2007), and ABC implementing some variant of sequential importance sampling (SIS) or sequential Monte Carlo (SMC) (Sisson et al., 2007; Toni et al., 2009; Beaumont et al., 2009; Del Moral et al., 2008). Of these the first and last forms have received the greatest attention and it is an ABC scheme based on sequential importance sampling that we will focus on as it offers greater flexibility and applicability and appears to be enjoying greater popularity in applications.

We focus on the implementation of Toni et al. (2009), which like other related SIS and SMC methods works by constructing a series of intermediate distributions that start out from a suitably specified prior distribution and increasingly resemble the (unknown) approximate posterior distribution. These intermediate distributions are defined by

$$p_\epsilon(\theta) \propto \int f(y|\theta) \mathbb{1}(\Delta(x, y) \leq \epsilon_i) \pi(\theta) dy,$$

for $1 \leq t \leq T$ and $\epsilon_1 \geq \epsilon_2 \geq \ldots \geq \epsilon_T = \epsilon$. Each intermediate distribution is described by a sample of $N$ parameter vectors, $\theta^{(i,t)}$, $1 \leq i \leq N$ and their corresponding weights, $\omega^{(i,t)}$, which together we refer to as particles $(\theta^{(i,t)}, \omega^{(i,t)})$. Successive distributions are constructed by perturbing parameters through some kernel function, $\tilde{\theta} \sim K_t(\cdot|\theta)$, generating simulated data, $y \sim f(\cdot|\tilde{\theta})$ and, upon acceptance, calculating the corresponding new weights. Below we will develop this framework in more detail.

While this sequential ABC approach is computationally much more efficient than simple ABC rejection schemes, the overall computational burden does not only depend on the complexity of the model and the amount of data at hand, but also on details of the chosen sequential scheme. In particular the $\epsilon$-schedule, $\{\epsilon_1, \ldots, \epsilon_T\}$, and the choice of perturbation kernels, $K_t(\cdot|\cdot)$ exert considerable influence on the algorithmic complexity. As in all Monte Carlo settings (Gilks & Richardson, 1996; Robert, 2004) problems tend to arise as the dimension of the parameter space increases and balancing convergence with the necessary maintenance of exhaustive exploration of the parameter space becomes harder.
The construction of suitable kernel functions has been a longstanding problem in the context of conventional Markov chain Monte Carlo analysis (Givens, 1996; Douc et al. 2007; Cappé et al. 2008; Cornebise et al. 2008; Cappé et al. 2009; Girolami & Calderhead, 2011). In the SMC setting the first strategies to adapt the proposal kernel were early as (Pitt & Shephard, 1999), with further appealing but ad-hoc methods proposed in Van Der Merwe et al. (2001); but it is still far from being solved. Some recent and more theoretically based approaches including Cornebise et al. (2008, 2011); but especially in an ABC context formal and informal understanding of kernel choice remain areas of pressing concern.

Especially for models which are computationally expensive to simulate, such as dynamical systems, the likelihood/posterior surfaces (Gutenkunst et al. 2007; Secrier et al. 2009; Erguler & Stumpf, 2011) suggest that the choice of the kernel will have huge influence on the efficiency with which parameter spaces are explored and posterior estimates obtained. Here we will discuss a range of kernel functions, characterize their performance, and put forward some analytic results as to their optimality. In the next section we discuss the ABC scheme in some detail before describing criteria for optimally choosing the perturbation kernels and outlining different classes of perturbation kernels. We then examine the performance of these kernels in applications to a range of illustrative problems and, compare their algorithmic complexities. We will show that for many problems with complex posterior parameter distributions the choice of suitable kernels can vastly improve the computational cost of ABC SMC inferences.

2 The ABC SMC algorithm

The general scheme of ABC inference is as follows:

- sample a parameter vector \( \theta \) (also called particle) from the prior distribution \( \pi(\theta) \),
- simulate a dataset \( y \) according to the generative model \( f(y|\theta) \),
- compare the simulated dataset with the experimental data \( x \): if \( \Delta(x, y) \leq \epsilon \), accept the particle.

The \( N \) accepted particles form a sample from the posterior distribution

\[
p_\epsilon(\theta|x) \propto \int \mathbf{1}(\Delta(x, y) \leq \epsilon) f(y|\theta) \pi(\theta) dy
\]

which is an approximation of the posterior distribution \( p(\theta|x) \).

Over the past few years many improvements of these algorithms have been proposed. In particular, Marjoram & Molitor (2003) introduced a method based on Markov chain Monte Carlo, which consists in constructing a Markov chain whose stationary distribution is \( p(\theta|x) \). To do so, at each time \( t \), a particle \( \theta \) is simulated from the previous particle \( \theta^{(t-1)} \) according to a perturbation kernel \( K(\cdot|\theta^{(t-1)}) \) (or from the prior distribution for \( t = 0 \)); the simulated data \( y \sim f(\cdot|\theta) \) is compared with the experimental data; and \( \theta^{(t)} \) is set to be equal to \( \theta \) with a Metropolis Hasting acceptance rate if \( \Delta(y, x) \leq \epsilon \) and to \( \theta^{(t-1)} \) otherwise. This algorithm is guaranteed to converge, however it is very difficult to assess when the Markov chain reaches the stationary regime; furthermore the chain may get trapped in local modes.

SIS and SMC samplers have then been introduced in the ABC framework by several authors (Sisson et al. 2007; Toni et al. 2009; Beaumont et al. 2009; Del Moral et al. 2008). These methods aim to sample sequentially from a sequences of distributions, which increasingly resemble the target posterior: they are constructed by estimating intermediate distributions \( p_{\epsilon_t}(\theta|x) \) for a decreasing sequence of \( \{\epsilon_t\}_{1 \leq t \leq T} \). The scheme of the algorithm is as follows: first, the ABC algorithm described above is used to construct a sample from \( p_{\epsilon_1}(\theta|x) \) with a sufficiently large value of \( \epsilon_1 \) such that many particles
are accepted. The ABC algorithm is then used again with \( \epsilon = \epsilon_2 \); but instead of sampling parameters from the prior, they are sampled from the set of accepted particles at the previous stage and perturbed according to a suitable perturbation kernel. This way a sample from \( p_{\epsilon_2}(\theta|x) \) is built, and so on until for \( t = T \) our target posterior has been arrived at. In this article, we focus on the implementation of \cite{Tonietal2009} described in Algorithm 1: from a decreasing sequence of \( \{\epsilon_t\}_{1 \leq t \leq T} \) and a set of perturbation kernels \( \{K_t(\cdot|\cdot)\}_{1 \leq t \leq T} \) (see also \cite{ToniuStumpf2009}), the algorithm generates a weighted sample of particles from \( p_{\epsilon_T}(\theta|x) \). In the following we will refer to this implementation as the ABC SMC algorithm according to \cite{Tonietal2009}. The ABC Population Monte Carlo (PMC) algorithm proposed by \cite{Beaumonteal2009} is similar to the ABC SMC algorithm, except that a specific perturbation kernel is used. It is, however, worth distinguishing between these algorithms and the one of \cite{DelMoraletal2008} and \cite{DrovandiPettitt2011} based on the SMC sampler of \cite{DelMoralDoucet2006}. When using SMC samplers, both a forward and a backward kernel need to be defined, which reduces the algorithmic complexity from \( O(N^2) \) to \( O(N) \) where \( N \) is the number of particles. However, as we will argue later, in many applications of interest, the most computationally expensive part of an ABC algorithm is the simulation of the data which is usually much larger compared to \( O(N^2) \). We will therefore not discuss kernel choice in the context of these approaches, although here, too, the choice of kernel will impact the numerical efficiency.

**Algorithm 1** ABC SMC algorithm

1. **input:** a decreasing sequence of \( \{\epsilon_t\}_{1 \leq t \leq T} \) such that \( \epsilon_T = \epsilon \), a data \( x \), a sequence of \( \{K_t(\cdot|\cdot)\}_{1 \leq t \leq T} \)
2. **output:** a weighted sample of particles from \( p_{\epsilon_T}(\theta|x) \)
3. **for** all \( 1 \leq t \leq T \) **do**
4.   **repeat**
5.     **if** \( t=1 \) **then**
6.         **sample** \( \tilde{\theta} \) from \( \pi(\theta) \)
7.     **else**
8.         **sample** \( \theta \) from the previous population \( \{\theta(i,t-1)\}_{1 \leq i \leq N} \) with weights \( \{\omega(i,t-1)\}_{1 \leq i \leq N} \)
9.         **sample** \( \tilde{\theta} \) from \( K_t(\cdot|\theta) \) and such that \( \pi(\tilde{\theta}) > 0 \)
10. **end if**
11. **sample** \( y \) from \( f(\cdot|\tilde{\theta}) \)
12. **if** \( \Delta(y, x) \leq \epsilon_t \) **then**
13.     \( \theta(i,t) \leftarrow \tilde{\theta} \)
14.     \( i \leftarrow i + 1 \)
15. **end if**
16. **until** \( i = N + 1 \)
17. **calculate** the weights: for all \( 1 \leq i \leq N \)
18. **if** \( t \neq 1 \) **then**
19.     \( \omega(i,t) \leftarrow \frac{\pi(\theta(i,t))}{\sum_{j=1}^{\pi} \omega(j,t-1) K_t(\theta(i,t)|\theta(j,t-1))} \)
20. **else** \( \omega(i,1) \leftarrow 1 \)
21. **end if**
22. **normalize** the weights
23. **end for**
3 Properties of optimal kernels

The behaviour of the algorithm depends on its settings: in particular the decreasing sequence of \( \{\epsilon_t\}_{1 \leq t \leq T} \) and the perturbation kernels \( \{K_t(\cdot, \cdot)\}_{1 \leq t \leq T} \). The effect of the sequence of decreasing threshold is easy to understand: if the difference between two successive tolerances \( \epsilon_t \) and \( \epsilon_{t+1} \) is small, the posterior distributions \( p_{\epsilon_t}(\theta|x) \) and \( p_{\epsilon_{t+1}}(\theta|x) \) are similar and a small number of simulations will be required to generate \( N \) draws from the next intermediate distribution, \( p_{\epsilon_{t+1}}(\theta|x) \), by sampling from the weighted population \( \{\theta^{(i,l-1)}, \omega^{(i,l-1)}\}_{1 \leq i \leq N} \). But a slowly decreasing sequence of thresholds \( \{\epsilon_t\}_{1 \leq t \leq T} \) leads to a large number of iterations (large value of \( T \)) in order to obtain \( \epsilon_T = \epsilon \). Similarly, the choice of the perturbation kernels \( \{K_t(\cdot, \cdot)\}_{1 \leq t \leq T} \) exerts considerable influence on the computational complexity of the algorithm. A local perturbation kernel hardly moves the particles and has the advantage to produce new particles which are accepted with high probability if the successive values of \( \epsilon \) are close enough; on the other hand, a widely spread out or permissive perturbation kernel enables exploring the parameter space more fully, but does so at the cost of achieving only low acceptance rates.

In sequential importance sampling, a perturbation kernel \( K_t \) should fulfill several requirements to be computationally efficient. In particular, the joint proposal distribution, corresponding to picking a particle at random and perturbing it to obtain a new particle, should “resemble” in some sense the target joint distribution, corresponding to picking independently two particles. More precisely, the joint proposal distribution of a particle, which samples first a particle \( \theta^{(l-1)} \sim p_{\epsilon_{l-1}}(\cdot|x) \) then a perturbed particle \( \theta^{(l)} \sim K_t(\cdot|\theta^{(l-1)}) \), and accept the couple if and only if \( \Delta(y, x) \leq \epsilon_t \) where \( y \sim f(\cdot|\theta^{(l)}) \), admits for density

\[
q_{\epsilon_{t-1}, \epsilon_t}(\theta^{(l-1)}, \theta^{(l)}) = \frac{p_{\epsilon_{t-1}}(\theta^{(l-1)}|x)K_t(\theta^{(l)}|\theta^{(l-1)}) \int f(y|\theta^{(l)}) \mathbb{I}(\Delta(x, y) \leq \epsilon_t) dy}{\alpha(K_t, \epsilon_{t-1}, \epsilon_t, x)}.
\]

The normalization factor

\[
\alpha(K_t, \epsilon_{t-1}, \epsilon_t, x) = \iiint p_{\epsilon_{t-1}}(\theta^{(l-1)}|x)K_t(\theta^{(l)}|\theta^{(l-1)}) f(y|\theta^{(l)}) \mathbb{I}(\Delta(x, y) \leq \epsilon_t) dy \theta^{(l-1)} d\theta^{(l)}
\]

is the average acceptance probability, that is, the proportion of proposed particles that will not be rejected. This joint proposal distribution should “resemble” in some sense the target product distribution, that of sampling \( \theta^{(l-1)} \) and \( \theta^{(l)} \) independently from, respectively, \( p_{\epsilon_{t-1}}(\cdot|x) \) and \( p_{\epsilon_t}(\cdot|x) \), whose density is

\[
q_{\epsilon_{t-1}, \epsilon_t}^*(\theta^{(l-1)}, \theta^{(l)}|x) = p_{\epsilon_{t-1}}(\theta^{(l-1)}|x)p_{\epsilon_t}(\theta^{(l)}|x).
\]

As argued by several authors, e.g. [Douc et al. (2007); Cappé et al. (2008); Cornebise et al. (2008); Beaumont et al. (2009)], a mathematically convenient formal definition of this “resemblance” is the Kullback-Leibler (KL) divergence between the proposal distribution \( q_{\epsilon_{t-1}, \epsilon_t}(\theta^{(l-1)}, \theta^{(l)}) \) and the target distribution \( q_{\epsilon_{t-1}, \epsilon_t}^*(\theta^{(l-1)}, \theta^{(l)}) \), i.e.

\[
KL(q_{\epsilon_{t-1}, \epsilon_t}; q_{\epsilon_{t-1}, \epsilon_t}^*) = \int \int \int \int q_{\epsilon_{t-1}, \epsilon_t}^*(\theta^{(l-1)}, \theta^{(l)}) \log \frac{q_{\epsilon_{t-1}, \epsilon_t}^*(\theta^{(l-1)}, \theta^{(l)})}{q_{\epsilon_{t-1}, \epsilon_t}(\theta^{(l-1)}, \theta^{(l)})} \theta^{(l-1)} d\theta^{(l)}
\]

which can be separated into three terms

\[
KL(q_{\epsilon_{t-1}, \epsilon_t}; q_{\epsilon_{t-1}, \epsilon_t}^*) = -Q(K_t, \epsilon_{t-1}, \epsilon_t, x) + \log \alpha(K_t, \epsilon_{t-1}, \epsilon_t, x) + C(\epsilon_{t-1}, \epsilon_t, x),
\]

where

\[
Q(K_t, \epsilon_{t-1}, \epsilon_t, x) = \int p_{\epsilon_{t-1}}(\theta^{(l-1)}|x)p_{\epsilon_t}(\theta^{(l)}|x) \log K_t(\theta^{(l)|\theta^{(l-1)}}) \theta^{(l-1)} d\theta^{(l)}
\]

\( C(\epsilon_{t-1}, \epsilon_t, x) \) is the contribution to the cost of generating \( N \) samples. It can be reduced by choosing slowly decreasing sequences of tolerances and kernels that are similar to the target kernel.
can be maximized easily (hence minimizing \(-Q\)) in some convenient cases (see Section 4), \(\alpha(K_t, \epsilon_{t-1}, \epsilon_t, x)\) is the average acceptance probability already defined in (1), which is much harder to minimize, and \(C(\epsilon_{t-1}, \epsilon_t, x)\) does not depend on the kernel \(K_t\) and can therefore be ignored. This provides a rational criterion for choosing optimally adapted perturbation kernels: we want a kernel \(K_t\) that minimizes the quantity \(\text{argmax}_{K_t} Q(K_t, \epsilon_{t-1}, \epsilon_t, x)\),

which admits a simple solution for certain adequately chosen families of kernels. While they restrain themselves to the component-wise Gaussian kernel (see Section 4.1), their approach tends to work well.

However, a close study of Equation (2) shows that this approach does not actually minimize the real Kullback-Leibler divergence in the non-asymptotic case, as we would hope to. Eventually minimizing this KL divergence would require two modifications: evaluate \(Q\) Kullback-Leibler divergence in the non-asymptotic case, as we would hope to. Eventually minimizing \(\alpha\) per se would seem unattainable. This KL divergence would require two modifications: evaluate \(Q\) and, since \(\alpha(K_t, 0, 0, x) = 1\) for any \(K_t\), they would ideally want to find the kernel that maximizes \(Q(K_t, 0, 0, x)\). Because it is impossible to solve this problem in the asymptotic case, they revert back to the non-asymptotic case by setting \(\epsilon_t = \epsilon_{t-1}\) for both thresholds, and therefore eventually solve

\[
\text{argmax}_{K_t} Q(K_t, \epsilon_{t-1}, \epsilon_t, x),
\]

where \(Q\) is defined in equation (3). We have shown that this choice corresponds to a trade-off between two desirable properties of the kernel, namely the resemblance of the proposal distribution and the target in the sense of the KL divergence, and a high acceptance rate. And our criterion not only sheds new light on the justification of some existing, proven criteria, but, additionally, refines them.
4 Optimal choice of random walk kernels

Perturbing a parameter \( \theta \) consists of sampling a new particle according to a probability parametrized by \( \theta \) and often centred on \( \theta \). In the ABC SMC algorithm, in addition to sampling from the kernel, we must be able to compute the transition density \( K_t(\theta^{(t)}|\theta^{(t-1)}) \) for any particles \( \theta^{(t)} \) and \( \theta^{(t-1)} \). Then, instead of choosing the perturbation kernel \( K_t \) that maximises equation (3) over all possible kernels, the space of possible kernels is often restrained to a parametric family from which it is easy to sample and perform optimization. Different probability models may be used, with the most common being the uniform and the Gaussian distributions [Sisson et al., 2007; Toni et al., 2009; Liepe et al., 2010]. In the following, we outline different classes of Gaussian perturbation kernels and compare their efficiency in terms of acceptance rates and computational cost.

4.1 Component-wise perturbation kernel

In most cases the particle is moved component-wise: for each component \( 1 \leq j \leq d \) of the parameter vector \( \theta = (\theta_1, \ldots, \theta_d) \), \( \theta_j \) is perturbed independently according to a Gaussian distribution with mean \( \theta_j \) and variance \( \sigma_j \). The parameters \( \{\sigma_j\}_{1 \leq j \leq d} \) may be fixed in advance, but more frequently [Beaumont et al., 2009; McKinley et al., 2009; Toni & Stumpf, 2009b; Jasra et al., 2010; Barnes et al., 2011; Didelot et al., 2011] adaptively set parameter choices \( \{\sigma_j^{(t)}\}_{1 \leq j \leq d} \) are used which depend on the previous population — the scale or variance is then indexed by the population index, \( t \). Considering a kernel of the form

\[
K_t(\theta^{(t)}|\theta^{(t-1)}) = \frac{1}{\sqrt{2\pi \sigma_j^{(t)}}} \exp \left\{ -\frac{(\theta_j^{(t)} - \theta_j^{(t-1)})^2}{2\sigma_j^{(t)}^2} \right\}
\]

and maximizing \( Q(K_t, 0, 0, x) \) — or more precisely \( Q(K_t, \epsilon_{t-1}, \epsilon_{t-1}, x) \) — Beaumont et al. (2009) showed that the optimal value of \( \sigma_j^{(t)} \) is twice the variance of the \( j \)-th component in the previous population:

\[
\sigma_j^{(t)} = 2\text{Var}(\{\theta_j^{(k,t-1)}\}_{1 \leq k \leq N})
\]

Maximizing \( Q(K_t, \epsilon_{t-1}, \epsilon_t, x) \), however, leads to a slightly different choice of \( \sigma_j^{(t)} \) which is

\[
\sigma_j^{(t)} = E_{p_{t-1}(\cdot|x)p_{t}(\cdot)} \left[ (\theta_j^{(t)} - \theta_j^{(t-1)})^2 \right].
\]

This quantity can be computed from the set \( \{\theta_j^{(i,t-1)}, \omega_j^{(i,t-1)}\}_{1 \leq i \leq N} \), where \( y_j^{(i,t-1)} \) is the observation simulated according to \( \theta_j^{(i,t-1)} \), as follows

\[
\sigma_j^{(t)} = \frac{1}{N} \sum_{i=1}^{N} \omega_j^{(i,t-1)} \sum_{k=1}^{N_0} (\tilde{\theta}_j^{(k)} - \tilde{\theta}_j^{(i,t-1)})^2.
\]

We denote by \( \{\tilde{\theta}_j^{(k)}\}_{1 \leq k \leq N_0} \) the set of particles \( \{\theta_j^{(i,t-1)} \text{ s.t. } \Delta(x, y_j^{(i,t-1)}) \leq \epsilon_t, 1 \leq i \leq N\} \) and by \( \{\tilde{\omega}^{(k)}\}_{1 \leq k \leq N_0} \) the associated weights normalized such that \( \sum_{k=1}^{N_0} \tilde{\omega}^{(k)} = 1 \).

Another commonly used component-wise kernel is the uniform kernel, which consists of perturbing the \( j \)-th component of particle \( \theta \) to any value in the interval \( [\theta_j - \sigma_j^{(t)}; \theta_j + \sigma_j^{(t)}] \) with density \( 1/2\sigma_j^{(t)} \). A natural choice is to set the parameter \( \sigma_j^{(t)} \) to the scale of the previous population, that is

\[
\sigma_j^{(t)} = \frac{1}{2} \left( \max_{1 \leq k \leq N} \{\theta_j^{(k,t-1)}\} - \min_{1 \leq k \leq N} \{\theta_j^{(k,t-1)}\} \right).
\]

Note that the main difference between the uniform and the component-wise normal kernels concerns their support: finite vs. infinite.
Figure 1: A population of particles and isodensity curves for a uniform kernel (left), a component-wise normal kernel (centre) and a multivariate normal perturbation kernel (right) around one particle (red point).

4.2 Multivariate normal perturbation kernels

Consider a population of two-dimensional parameters that are highly correlated. The perturbation of a particle according to the uniform kernel consists simply in sampling a parameter uniformly in a rectangle whose sides are parallel to the axes (see Figure 1 left). Similarly, the density levels of the component-wise normal kernel are ellipsoids whose principal axes are parallel to the parameter axes (see Figure 1 center). But for highly correlated parameters the use of those two perturbation kernels in the ABC SMC framework leads to a small acceptance rate as they only poorly reflect the structure of the true posterior.

Instead of using a component-wise kernel, it may thus be more efficient to take into account the correlations between the different elements of the parameter vectors, in effect perturbing the particles according to a multivariate normal distribution with a covariance matrix $\Sigma^t$, which depends on the covariance of the previous population. Figure 1 (right) represents a multivariate normal perturbation kernel for a $d$ dimensional square matrix $\Sigma^t$ proportional to the covariance of the previous population.

We observe that fewer particle proposals are likely to be rejected with this perturbation kernel than with the uniform or component-wise normal one.

The multivariate normal perturbation kernel relies on the covariance matrix $\Sigma^t$ which depends on the previous population. As before, it is possible to calculate the optimal covariance matrix $\Sigma^t$ using the Kullback-Leibler divergence minimization approach. Maximizing equation (3) for $K_t(\theta^t|\theta^{t-1}) = (2\pi)^{-d/2} (\det \Sigma^t)^{-1} \exp \left\{ -\frac{1}{2} (\theta^t - \theta^{t-1})^T (\Sigma^t)^{-1} (\theta^{t+1} - \theta^t) \right\}$ with respect to $\Sigma^t$ leads to maximizing the real-valued function

$$g(M) = \log \det (M) - E_{p_{t-1}(|x)p_{t}(|x)} \left[ (\theta^t - \theta^{t-1})^T M (\theta^t - \theta^{t-1}) \right] ,$$

with respect to the symmetric $d \times d$ matrix $M$, and defining $\Sigma^t = M^{-1}$. We denote by $v^T$ the transpose of vector $v$. Taking the partial derivatives of the function $g : \mathbb{R}^{d \times d} \rightarrow \mathbb{R}$, we obtain, for all $1 \leq i, j \leq d$,

$$\frac{\partial g(M)}{\partial M_{ij}} = (M^{-1})_{ij} - \frac{\partial}{\partial M_{ij}} E_{p_{t-1}(|x)p_{t}(|x)} \left[ \text{Tr} \left( (\theta^t - \theta^{t-1})^T M (\theta^t - \theta^{t-1}) \right) \right]$$

$$= (M^{-1})_{ij} - \frac{\partial}{\partial M_{ij}} \text{Tr} (MC) = (M^{-1})_{ij} - C_{ji} = (M^{-1})_{ij} - C_{ij} .$$
where \( \text{Tr}(M) \) denotes the trace of the matrix \( M \), and the symmetric matrix \( C \) is equal to

\[
C = E_{p_{t-1}} \left( |x| p_t(\cdot | x) \right) \left( (\theta^{(t)} - \theta^{(t-1)}) (\theta^{(t)} - \theta^{(t-1)})^T \right). 
\]

Therefore the covariance matrix \( \Sigma^{(t)} \) of the optimal kernel in the multivariate Gaussian family is the matrix \( C \) defined above. Similarly to the component-wise case, if \( \epsilon_t = \epsilon_{t-1} \) then the optimal covariance matrix is equal to \( 2 \text{Cov}(\{\theta^{(k,t)}\}_{1 \leq k \leq N}) \). In the general case, however, an optimal choice of the covariance matrix \( \Sigma^{(t)} \) for the multivariate normal perturbation kernel is then

\[
\Sigma^{(t)} = \sum_{i=1}^{N} \sum_{k=1}^{N_0} \omega^{(i,t-1)} \omega^{(k)} (\tilde{\theta}^{(k)} - \theta^{(i,t-1)}) (\tilde{\theta}^{(k)} - \theta^{(i,t-1)})^T. 
\]

where \( \{\tilde{\theta}^{(k)}\}_{1 \leq k \leq N_0} \) and \( \{\omega^{(k)}\}_{1 \leq k \leq N_0} \) are defined as previously. In the following, if nothing else is specified, the multivariate normal kernel refers to the kernel with this choice of covariance matrix. It is worth noting that Beaumont et al. (2009) restrained their optimality criteria to cases where either only a single parameter is to be estimated or where the covariance matrix is diagonal. Our scheme generalises their criterion to a much broader class of kernels.

4.3 Local perturbation kernels

Let us now consider one of the canonical examples of a posterior distribution which poses challenges to simple kernels: the so-called banana shape distribution in two dimensions. In this case the components of the parameters are highly correlated but the multivariate normal and the component-wise normal kernels discussed above behave similarly (see Figure 2 left). Indeed, the covariance matrix based on all the previous particles is nearly diagonal. It yields only limited information about the local correlation among the individual components of the parameter vectors. In such cases it is interesting to consider the use of a local covariance matrix which differs between particles. In the following we discuss three local perturbation kernels for which the particle \( \theta \) is perturbed according to a multivariate normal kernel whose covariance matrix \( \Sigma^{(t)}_{\theta} \) is a function of \( \theta \).

4.3.1 The multivariate normal kernel with \( M \) nearest neighbours

The multivariate normal kernel with \( M \) neighbours follows this principle: for each particle \( \theta \in \{\theta^{(l,t)} \mid 1 \leq l \leq N\} \), the \( M \)-nearest neighbours of \( \theta \) are selected, and the perturbed particle is sampled according to a multivariate normal distribution of mean \( \theta \) and of covariance \( \Sigma^{(t)}_{\theta,M} \) estimated from the \( M \) neighbouring particles.

The main drawback of this perturbation kernel is that the parameter \( M \) typically needs to be fixed in advance before any of the intricacies of the posterior are known. Figures 2 (centre) and 2 (right) illustrate the effect of the parameter \( M \) on the perturbation kernel. Using too small a value may lead to a lack of exploration of parameter space, while too large a value of \( M \) would offer little or no advantage compared to the standard multivariate normal kernel. Ideally, a mixture of multivariate normal kernels with different values of \( M \) should be used; however, in practice, this solution is computationally too expensive.

4.3.2 The multivariate normal kernel with optimal local covariance matrix

The theoretical calculation of the optimal covariance matrix above (see Section 4.2) may be adapted to identify an optimal local covariance matrix. Considering that the covariance matrix \( \Sigma^{(t)}_{\theta} \) depends
on the particle $\theta$, and following the same steps as before, it is easy to show that the covariance matrix $\Sigma^{(t)}_{\theta^{(t-1)}}$ for a particle $\theta^{(t-1)} \sim p_{\epsilon t-1}(\cdot|x)$ maximizing equation (3) is such that

$$E_{p_{\epsilon t-1}(\cdot|x)} \left[ \Sigma^{(t)}_{\theta^{(t-1)}} - E_{p_{\epsilon t}(\cdot|x)} \left( (\theta^{(t)} - \theta^{(t-1)})(\theta^{(t)} - \theta^{(t-1)})^T \right) \right] = 0 .$$

In particular, the set of covariance matrices such that, for all $t$ and each particle $\theta^{(j,t-1)}$, $1 \leq j \leq N$,

$$\Sigma^{(t)}_{\theta^{(j,t-1)}} = E_{p_{\epsilon t}(\cdot|x)} \left[ (\theta^{(t)} - \theta^{(j,t-1)})(\theta^{(t)} - \theta^{(j,t-1)})^T \right]$$

satisfies the above condition. The multivariate normal perturbation kernel whose covariance matrix is equal to $\Sigma^{(t)}_{\theta^{(t-1)}}$ as defined above will be referred to as the multivariate normal kernel with OLCM (where OLCM stands for optimal local covariance matrix). We now have a different covariance matrix $\Sigma^{(t)}_{\theta^{(t-1)}}$ for each particle $\theta^{(j,t-1)}$ of the previous population.

Figure 2: A population of particles and isodensity curves of a multivariate normal perturbation kernel with respectively a covariance based on the whole population (left), on the 50 nearest neighbours (centre) and on the 200 nearest neighbours (right) around one particle (red point). The nearest neighbours are represented by yellow points.

Figure 3: The eigenvectors of $I^{-1}(\theta)$ (red arrows) of size proportional to the eigenvalues for a particle $\theta$ (red point).
4.3.3 Perturbation kernel based on the Fisher information

The final perturbation kernel considered here uses information from the generative model via the Fisher Information Matrix (Rao, 1945; MacKay, 2003; Cox, 2006). The Fisher Information Matrix (FIM) defined as

\[ I(\theta) = -E_X \left[ \frac{\partial^2}{\partial \theta^2} \log f(X|\theta) \right] \]

measures the amount of information that the observable random variable \( X \) carries about the parameter \( \theta \). As previously mentioned the ABC algorithm is mainly used when the likelihood function \( f(\cdot|\theta) \) is not known, and so the Fisher Information Matrix can not be computed exactly. Nevertheless, Komorowski et al. (2011) have developed a method that evaluates the FIM for deterministic and stochastic dynamical systems represented by ordinary differential equations (ODEs) and stochastic differential equations (SDEs) using the linear noise approximation, which can be applied in such cases on the fly as the ABC SMC procedure progresses.

In the Laplace expansion, the eigenvectors and eigenvalues of the inverse of the FIM \( I(\theta) \) map out ellipsoidal levels of equal density around the parameter \( \theta \). The eigenvectors of \( I^{-1}(\theta) \) (scaled such that their lengths are proportional to their corresponding eigenvalues) are represented for two different values of \( \theta \) in Figure 3. The directions of the eigenvectors and the relative size of their eigenvalues are both relevant for perturbing the parameter \( \theta \) efficiently. However, in Figure 4 we observe that the determinant of \( I^{-1}(\theta) \) varies exponentially with \( \theta \) over 5 orders of magnitude. The determinant of \( I(\theta) \) is of course a measure of the amount of information available around \( \theta \); its value is very small for some parameters \( \theta \) and this leads to a perturbation kernel with too large a covariance. On the other hand, if the determinant of \( I(\theta) \) is large, additional information may be gained by moving only in the direct vicinity of \( \theta \), and a perturbation kernel based on the inverse of the FIM explores only the immediate neighbourhood of the parameter. We therefore consider two versions of the multivariate normal perturbation kernel based on the FIM: the first consists of normalizing the matrix such that its determinant is equal to the determinant of the covariance matrix of the previous population

\[ \Sigma_{\theta}^{(t)} = \left( \frac{\det(\Sigma_{\theta}^{(t)})}{\det(I^{-1}(\theta))} \right)^{1/d} I^{-1}(\theta), \]

where \( \Sigma^{(t)} \) is the matrix defined equation (10), and the second consists of normalizing the matrix such that its determinant is equal to the determinant of the covariance matrix \( \Sigma_{\theta,M}^{(t)} \) based on the \( M \) nearest neighbours of the particle defined according to

\[ \Sigma_{\theta,M}^{(t)} = \left( \frac{\det(\Sigma_{\theta,M}^{(t)})}{\det(I^{-1}(\theta))} \right)^{1/d} I^{-1}(\theta). \]

The parameter \( M \) may, for instance, be equal to 20% of the previous population.
Figure 4: Logarithm of the determinant of $I^{-1}(\theta)$ rescaled to be in $[0, 1]$ for each particle $\theta$. The maximum value of $I^{-1}(\theta)$ over the population is equal to 85745 and the minimum one is equal to 0.14.

5 Numerical results

We first apply the ABC SMC algorithm with different kernels to three illustrative examples, which exhibit certain pathological features that highlight differences between the perturbation kernels considered here.

5.1 Ellipsoid shape

We begin with a toy example where the prior distribution of the two dimensional parameter is a uniform distribution on the square $[-50, 50] \times [-50, 50]$ and the likelihood function is given by

$$x \sim \mathcal{N} \left( (\theta_1 - 2\theta_2)^2 + (\theta_2 - 4)^2, 1 \right).$$

It is assumed that $x = 0$ is observed. The posterior density is then

$$p(\theta|x) \propto \phi(0; (\theta_1 - 2\theta_2)^2 + (\theta_2 - 4)^2, 1) \mathbb{I}_{[-50,50] \times [-50,50]}(\theta)$$

where $\phi(x; \mu, \sigma^2)$ is the one dimensional normal density with mean $\mu$ and variance $\sigma^2$, and is represented in Figure 5. The ABC SMC algorithm is used to estimate $p_\epsilon(\theta|x)$ for $N = 800$ particles, $\epsilon = 1$ and the decreasing sequence of $(\epsilon_t)_{1 \leq t \leq T}$ equal to $(160, 120, 80, 60, 40, 30, 20, 15, 10, 8, 6, 4, 3, 2, 1)$. We compare 5 different perturbation kernels: the uniform kernel, the component-wise normal kernel, the multivariate normal kernel with the covariance matrix computed from the whole previous population, the multivariate normal kernel whose covariance matrix is computed according to the $M$ nearest neighbours of each particle, with $M = 50$, and the multivariate normal kernel with OLCM.
Figure 5: Scatter plot and marginal posterior distribution for an ellipsoid posterior. Top left and bottom right: the marginal posterior distributions; Top right and bottom left: each population of particles for all the values of $\epsilon$ in the parameter space.

Figure 6 shows that the acceptance rate differs significantly between kernels. The uniform kernel has the same acceptance rate as the component-wise normal kernel. Given the shape of the posterior distribution, it is easy to understand that a multivariate normal kernel results in a larger acceptance rate than other kernels. Since the two components of the parameters are strongly correlated using an estimate of the covariance from the previous population instead of an estimation of only the component-wise variances makes a marked difference on the acceptance rates. Both the multivariate normal kernel based on the 50 nearest neighbours and the one based on the OLCM result in acceptance rates over two times higher than component-wise kernels.
Figure 6: Ellipsoid Shape. Average of the acceptance rate over 10 independent runs for 5 different kernels: the uniform kernel (green), the component-wise normal kernel (blue), the multivariate normal kernel (black), the multivariate normal kernel with 50 neighbours (red), the multivariate normal kernel with OLCM (cyan).

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5.2 Ring shape

Figure 7: Scatter plot and marginal posterior distribution for a ring-shaped posterior. Top left and bottom right: the marginal posterior distributions; Top right and bottom left: each population of particles for all the values of $\epsilon$ in the parameter space.

In the second toy example, the prior distribution of the two dimensional parameter is still a uniform distribution on the square $[-50, 50] \times [-50, 50]$ but the likelihood function is 

$$x \sim N(\theta_1^2 + \theta_2^2, 0.5).$$

Again we assume that $x = 0$ is observed; the posterior density is then 

$$p(\theta|x) \propto \phi(0; \theta_1^2 + \theta_2^2, 0.5) \mathbb{1}_{[-50,50] \times [-50,50]}(\theta).$$

As in the previous example we used the ABC SMC algorithm with $N = 800$ particles and the decreasing sequence of thresholds is equal to (160, 120, 80, 60, 40, 30, 20, 15, 10, 8, 6, 4, 3, 2, 1). We compare the same 5 perturbation kernels.

The posterior distribution, represented by Figure 7 has a ring shape centred around 0. In this case, in contrast to the previous example, the multivariate normal perturbation kernel using an estimation of the covariance based on the previous population, as well as the OLCM version of it, have an acceptance rate similar to the component-wise normal perturbation kernel. Indeed, in this example, the correlation between the two parameters, $\theta_1$ and $\theta_2$, at the whole population level is weak. This kind of shape needs a more local perturbation kernel in order to obtain higher acceptance rates. This is the case for the perturbation kernel based on the covariance matrix computed from the 50 nearest neighbours.
Figure 8: Ring Shape. Evolution of the acceptance rate for 10 independent runs and for 5 different kernels: the uniform kernel (green), the gaussian kernel (blue), the multivariate normal kernel (black), the multivariate normal kernel with 50 neighbours (red), the multivariate normal kernel with OLCM (cyan).
5.3 Banana shape

Figure 9: Scatter plot and marginal posterior distribution for a banana-shaped posterior. Top left and bottom right: the marginal posterior distributions; Top right and bottom left: each population of particles for all the values of $\epsilon$ in the parameter space.

In the third toy example, the prior distribution of the two dimensional parameter is still a uniform distribution on the square $[-50, 50] \times [-50, 50]$ but the observation is two dimensional and the likelihood function is

$$
\begin{pmatrix}
    x_1 \\
    x_2
\end{pmatrix}
\sim
\mathcal{N}_2
\left(
\begin{pmatrix}
    \theta_1 \\
    \theta_1 + \theta_2^2
\end{pmatrix}
\cdot
\begin{pmatrix}
    1 & 0 \\
    0 & 0.5
\end{pmatrix}
\right)
$$

It is assumed that $x = (0, 0)$ is observed. The posterior density is then

$$
p(\theta|x) \propto \Phi
\left(\begin{pmatrix}
    0 \\
    0
\end{pmatrix};
\begin{pmatrix}
    \theta_1 \\
    \theta_1 + \theta_2^2
\end{pmatrix}
\cdot
\begin{pmatrix}
    1 & 0 \\
    0 & 0.5
\end{pmatrix}
\right)\mathbb{1}_{[-50,50] \times [-50,50]}(\theta)
$$

where $\Phi(x; v, \Sigma)$ is the multi-dimensional normal density of mean $v$ and covariance $\Sigma$. We use the same ABC SMC settings and again compare the 5 perturbation kernels, as well as two versions of the multivariate normal perturbation kernel where the covariance matrix is proportional to the inverse of the FIM. Here the FIM is exactly computable:

$$
I(\theta) = \begin{pmatrix}
    1.5 & \theta_2 \\
    \theta_2 & 2\theta_2^2
\end{pmatrix}.
$$

When $\theta_2 = 0$, we replace it by a very small value, $10^{-4}$ such that $I(\theta)$ is no longer singular; safeguarding against singular FIMs is straightforward and a sensible precaution when running such algorithms without manual intervention.

The posterior distribution is represented in Figure 9. As in the ring example, the multivariate normal perturbation kernel using the full estimated covariance of the whole previous population has
an acceptance rate similar to the component-wise normal perturbation kernel with adaptive estimation of the variances (see Figure 10). The multivariate normal kernel with OLCM obtains slightly better results. The two versions of the perturbation kernel based on the FIM have significantly different acceptance rates. The most efficient version is the one using the $M$ nearest neighbours, as might be expected. However this kernel, as the multivariate normal kernel based on the $M$ nearest neighbours, can show undesirable dependence on the chosen value of $M$. Figure 10 represents the acceptance rate evolution for this last perturbation kernel with different values of $M$. The acceptance rate diminish considerably as $M$ increases and the kernel becomes less “locally aware”.

Figure 10: Banana Shape. Evolution of the acceptance rate for 10 independent runs; each colour corresponds to a kernel. Left: the uniform kernel (green), the component-wise normal kernel (blue), the multivariate normal kernel (black), the multivariate normal kernel with 50 neighbours (red), the multivariate normal kernel with OLCM (cyan), the multivariate normal kernel based on the FIM version 1 (dashed magenta) and version 2 (dotted magenta); Right: multivariate normal kernels based on the $M$ neighbours for $M \in \{50, 100, 200, 300, 400, 500, 600, 700, 800\}$ (from red to yellow) and the multivariate kernel with an estimated covariance based on the whole population (black).
6 Real Application: The Repressilator Model

Figure 11: Scatter plot and marginal posterior distribution. On the diagonal: the marginal posterior distributions; Other plots: each population of particles for all the values of $\epsilon$ projected into two components of the parameter space.

To analyse the differences between the efficiency of the perturbation kernel in a real application we focus on the repressilator model, a popular model for gene regulatory systems (Elowitz & Leibler, 2000). This model also exemplifies the challenges that are frequently encountered in attempts to reverse engineer the structure and parameters of dynamical systems from data (Toni et al., 2009; Girolami & Calderhead, 2011). There are now several studies that appear to demonstrate that, even for large data-sets, only about a third of parameters of dynamical systems can be inferred with high confidence (or high posterior probability) (Gutenkunst et al., 2007; Rand 2008; Erguler & Stumpf, 2011); there are also signs, however, that judiciously chosen experimental conditions can lead to an increased information content in the data (Casey et al., 2007; Apgar et al., 2008).

The model is described by six ordinary differential equations and a four dimensional parameter
Figure 12: Cumulative number of simulation over the iterations of the algorithm (left) and total of the computational time to generate $N$ accepted particles with different kernels normalized by the required time using the uniform kernel (right) for the following kernels: the Gaussian kernel (blue), the multivariate normal kernel (black), the multivariate normal kernel with 50 neighbours (red), the multivariate normal kernel with OLCM (cyan), the multivariate normal kernel based on the FIM version 1 (dashed magenta) and version 2 (dotted magenta).

For the simulated data, the initial condition are $(m_1, p_1, m_2, p_2, m_3, p_3) = (0, 2, 0, 1, 0, 3)$ and the time points at which we observe the quantities are $(0.0, 0.6, 4.2, 6.2, 8.6, 13.4, 16, 21.4, 27.6, 34.4, 39.8, 40.6, 45.2)$. We assume that only the time series of $m_1$, $m_2$ and $m_3$ (which correspond to mRNA measurements) are observed.

The ABC SMC algorithm is used to estimate $p(\theta|\{m_1(k), m_2(k), m_3(k)\}_k)$ with $N = 800$ particles and a decreasing sequence of thresholds equal to $(160, 150, 140, 130, 120, 100, 80, 50, 40, 37, 35, 33, 31, 29, 27, 25, 23, 21, 20)$. The posterior distribution is represented in Figure 11 and agrees very well with what is known from previous studies [Toni et al., 2009]. In Figure 12 (left), we compare the cumulative number of sampled data over the algorithm for different perturbation kernels. Using the uniform kernel, up to $6.5 \times 10^6$ simulations are required to obtain an approximation of the posterior distribution whereas only $1.6 \times 10^5$ simulations are required if the second version of the multivariate normal kernel based on the FIM is used. In order to contrast the efficiencies of these kernels further we show the time required to generate a sample of $N$ particles of the posterior $p(x|\cdot)$, where $x = \{m_1(k), m_2(k), m_3(k)\}_k$, as a...
function of $t$ for all kernel scaled by the time required for the uniform kernel in Figure 12 (right). Using the FIM results in a 23-fold speed-up compared to the uniform kernel. The time spent to evaluate the FIM for each parameter is small compared to the time saved by sampling new parameters more efficiently. So even in this simple model, a significant improvement is possible through appropriate choice of perturbation kernel.

7 Conclusion

In contrast to MCMC, where the pivotal role of perturbation kernels for convergence and mixing has been well documented, for ABC SMC approaches there has been comparatively little work. In particular in the ABC context, which often relies on computationally costly simulation routines, poor choice of the perturbation kernel will result in potentially prohibitive computational overheads. We have addressed this lack of suitable kernels here in a rigorous but non-exhaustive fashion by focusing on kernels that are based around uniform or normal/multivariate normal parametric families. Importantly, in all examples we were able to ensure that the different kernels had arrived at essentially identical posterior distributions, and for fixed $\epsilon_t$ schedule we can use the acceptance rate as an objective criterion for the numerical efficiency of different kernels.

For all these models it is relatively straightforward to construct optimality criteria by reference to the KL divergence following Beaumont et al. (2009). In higher-dimensional parameter spaces it is important to take into account the potentially correlated nature of parameters, and, not surprisingly we find that component-wise perturbation of particles tends to perform poorly compared to the other approaches considered here. In more complicated cases, e.g. decidedly non-Gaussian posteriors, multimodal posteriors, or posteriors with ridges, we find that a straightforward multivariate normal kernel is in turn inferior to kernels that are conditioned on the local environment of a particle.

In most applications of interest, the computational cost of simulating the data overtakes the algorithmic complexity $O(N^2)$ of the ABC SMC scheme. We therefore argue that the choice of a kernel with a high acceptance rate enables users to optimize the computational cost. However, when two kernels have the same acceptance rate — which may happen for some shapes of the posterior — it is more appropriate to select the one which is cheaper in term of algorithmic complexity. The following table summarizes the computational cost of implementing the proposed perturbation kernels from a previous population of $N$ particles with dimension $d$ (the number of individual parameters). In the case of the multivariate normal kernel based on the FIM, we denote by $C$ the computational cost of simulating an observation, e.g. by solving the set of ODEs or SDEs which define the generative model.

| Kernel Description                           | Computational Cost |
|---------------------------------------------|--------------------|
| Component-wise normal                       | $O(dN^2)$          |
| Multivariate normal based on the whole previous population | $O(d^3N^2)$        |
| Multivariate normal based on the $M$ nearest neighbours | $O(dN^2 + d^3M^2N)$ |
| Multivariate normal with OLCM               | $O(d^3N^2)$        |
| Multivariate normal based on the FIM (normalized with entire population) | $O(dCN + d^3N^2)$  |

As a general rule of thumb we would recommend the use of multi-variate kernels with OLCM which tends to have the highest acceptance rate in our toy-examples and is relatively easy to implement at acceptable computational cost. Where applicable we would advocate the use of the FIM in order to perturb particles in a rational way, by which we mean, taking large steps in directions where the information is flat, and small steps where the information changes more quickly. This will have the advantage of exploring so-called neutral spaces more efficiently while maintaining the acceptance rate. But here again there is a potential tension between global and local aspects: if we take the global FIM as the basis for the perturbation we may have a very poor representation of the internal
structure of e.g. the posterior (very much as might happen in the Laplace expansion); if, on the other hand, we evaluate the FIM based on the $M$ nearest neighbours of a particle, then we may overly restrict the particles making up the next intermediate distribution. For some probability models, in particular those describing dynamical systems, the FIM has attracted a lot of attention recently (Amari, 2007; Arwini et al., 2008; Secrier et al., 2009; Girolami & Calderhead, 2011; Erguler & Stumpf, 2011; Komorowski et al., 2011), and it appears likely that we will be able to exploit these notions, and those of information geometry more generally, fruitfully in ABC SMC.

The cost of local measures based on $M$ nearest neighbours may seem too high to contemplate the use of such measures. Given the increase in acceptance rate that we have observed this matters very little, however, especially when the computational cost to generate simulated data from a candidate particle is high.

To some, especially those from a background in evolutionary computation, the kernels discussed here may seem restrictive. We may, for example, wish to consider other perturbations to generate new candidate particles, such as recombination etc (Baragona & Battaglia, 2010), as is frequently done in global optimization. In principle it is possible to include this in ABC SMC approaches, as long as the weights for new particles can be calculated (which turns out to be relatively straightforward for recombination and different cross-over schemes). It has to be kept in mind, however, that these perturbations work best in cases where the parameter space is so under-sampled that random combinations of individual parameters are sufficiently likely to end up in a region with a more favourable cost-function than a local, e.g. gradient-based proposal would. While such strategies have been applied in many optimization settings, their use in Bayesian inference is rare, since generally here the optimum (by whichever criterion) parameter value is of less interest than the distribution as a whole. For maximum a posteriori inferences such methods may be fruitfully applied, but here we do not see an obvious advantage (as is also borne out by simulation studies, data not shown).

Kernel choice is one of the obvious means of speeding up ABC SMC inferences. Setting the $\epsilon$ schedule optimally another. The latter is straightforwardly automated by basing the next $\epsilon_{t+1}$ on the acceptance rate obtained during the generation of the intermediate distribution, $p_{\epsilon_t}(\theta|x)$. But again there is a trade-off to be made between convergence and exhaustive exploration of the parameter space. In particular too gentle a decrease in $\epsilon_t$ may result in loss of particle diversity (in a process mimicking drift in population genetics). Here we believe that further investigation of FIMs may hold important clues to how the $\epsilon_t$ are best chosen. This would, for example, resonate with the perspective on $\epsilon$ proposed by Ratmann et al. (2009).

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