Pre-processing for approximate Bayesian computation in image analysis

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Abstract

The existing algorithms for approximate Bayesian computation (ABC) assume that it is feasible to simulate pseudo-data from the model at each iteration. However, the computational cost of these simulations can be prohibitive for high dimensional data. An important example is the Potts model, which is commonly used in image analysis. The dimension of the state vector in this model is equal to the size of the data, which can be millions of pixels. We introduce a preparatory computation step before model fitting to improve the scalability of ABC. The output of this pre-computation can be reused across multiple datasets. We illustrate this method by estimating the smoothing parameter for satellite images, demonstrating that the pre-computation step can reduce the average runtime required for model fitting from 46 hours to only 21 minutes.

1 Introduction

For many important problems, the computational cost of approximate Bayesian computation (ABC) is dominated by simulation of pseudo-data. This is particularly the case for the Potts model, for which an ABC algorithm was developed by [Grelaud et al. 2009]. The latent state vector of this model has the same dimension as the observed data, which in image analysis can often be millions of pixels. These latent states are highly correlated, requiring algorithms such as [Swendsen and Wang 1987] to simulate efficiently from the generative model. In his comparison of sequential Monte Carlo (SMC-ABC) with a particle MCMC algorithm, [Everitt 2012] found in both cases that the computational requirements were dominated by simulation of this state vector.

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Adaptive ABC algorithms have been developed to reduce the number of iterations required through more efficient exploration of the posterior. Various particle-based methods have been proposed by Sisson et al. [2007], Beaumont et al. [2009], Toni et al. [2009]; and Drovandi and Pettitt [2011]. The SMC-ABC algorithm of Del Moral et al. [2012] adapts both the ABC tolerance $\epsilon$ and the Metropolis-Hastings (MH) proposal bandwidth $\sigma_{\text{MH}}^2$. This algorithm also has the advantage that the computational cost of the importance weights is linear in the number of particles.

Beaumont et al. [2002] post-processed the ABC output by fitting a local linear regression. By modelling the relationship between the simulated parameter values and the corresponding summary statistics, they improved the estimate of the posterior density even with large values of the ABC tolerance. Blum and François [2010] took a similar approach, except that they used a nonlinear, heteroskedastic regression. They then performed a second ABC run, using the estimate of the posterior to draw parameter values.

In this paper, we propose a pre-processing step to calculate the expectation and variance of the summary statistic for fixed values of the parameter. This enables our ABC algorithm to map directly from the proposed parameter value to an approximate summary statistic. The output of the pre-processing can be reused for multiple datasets that share the same parameter space.

The rest of the paper is organised as follows. The ABC rejection sampler and SMC-ABC are reviewed in section 2. Our proposed method is described in section 3. In section 4, we illustrate how the method can be applied to the hidden Potts model. Section 5 contains results from a simulation study as well as real imaging data from the Landsat 7 satellite. The article concludes with a discussion.

2 Approximate Bayesian Computation

The ABC rejection sampler introduced by Pritchard et al. [1999] draws values of the parameter from its prior distribution $\pi(\theta)$, then simulates pseudo-data $\mathbf{x}$ from the model. One or more summary statistics $\rho(\mathbf{x})$ are calculated from the pseudo-data and compared to the values of those statistics in the observed data, $\rho(\mathbf{y})$. If the difference between the statistics is within the ABC tolerance threshold, then the proposed parameter is accepted.

The simulation of pseudo-data from the generative model is the most computationally intensive step in this process. The ABC rejection sampler works best when prior information about the distribution of the parameter is available. The acceptance rate under a sparse or uninformative prior can be extremely low, requiring many pseudo-datasets to be generated for each parameter value that is accepted. The ABC tolerance is a tunable parameter, since a large tolerance means a higher acceptance rate but also increases the error in the estimate of the posterior distribution. If the summary statistic is sufficient for the parameter, then the distribution of the samples approaches the true posterior as $\epsilon$ approaches zero. However, the number of samples that are rejected also in-
Algorithm 1 ABC rejection sampler

1: for all iterations $t \in 1 \ldots T$ do
2: Draw independent proposal $\theta' \sim \pi(\theta)$
3: Generate $x \sim f(\cdot|\theta')$
4: if $|\rho(x) - \rho(y)| < \epsilon$ then
5:    set $\theta_t \leftarrow \theta'$
6: else
7:    set $\theta_t \leftarrow \theta_{t-1}$
8: end if
9: end for

Increases, to the point that almost none are accepted. Adaptive ABC methods have been developed to address this inefficiency.

2.1 Sequential Monte Carlo

The SMC-ABC algorithm of [Del Moral et al. 2012] involves four major stages: initialisation, adaptation, resampling, and mutation.

Initialisation The algorithm is initialised by drawing a population of $N$ parameter values from the prior. These values, known as particles, are each associated with $M$ replicates of the summary statistics calculated from pseudo-data. The generation of multiple sets of pseudo-data $x_{i,m,t}$ for each particle increases the computational cost relative to other ABC methods, but it better handles the situation where there is sizeable variability in the value of the summary statistic for a given parameter. This is the case for the hidden Potts model, as we explain in section 4.

Adaptation At each iteration, the particles are assigned importance weights using a backward Markov kernel:

$$w_{i,t} \propto w_{i,t-1} \frac{\sum_{m=1}^{M} I(\delta(x_{i,m,t-1}) < \epsilon_t)}{\sum_{m=1}^{M} I(\delta(x_{i,m,t-1}) < \epsilon_{t-1})}$$

where $I(\cdot)$ is the indicator function and $\delta(x)$ is the absolute distance between the sufficient statistics of the pseudo-data and the observed data, $|\rho(x) - \rho(y)|$. These weights are normalised so that $\sum_{i=1}^{N} w_{i,t} = 1$. The computational cost of updating the weights is linear in the number of replicates of the summary statistics, $N \times M$. Also note that the weights only depend on $\{x_{\cdot,t-1}\}$, which means that the pseudo-data is not updated for particles with zero weight. These weights gradually degenerate over successive iterations, which is measured by the effective sample size [ESS; Liu 2001, pp. 34–36]:

$$ESS_t = \left( \sum_{i=1}^{N} w_{i,t}^2 \right)^{-1}$$

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Algorithm 2 SMC-ABC

**Initialisation:**
1: \( t \leftarrow 0, \epsilon_0 \leftarrow \infty \)
2: Draw \( \theta_{i,0} \sim \pi(\theta) \, \forall i \in 1 \ldots N \)
3: Generate \( x_{i,m,0} \sim f(\cdot|\theta_{i,0}) \, \forall i \in 1 \ldots N, \forall m \in 1 \ldots M \)
4: \( w_{i,0} \leftarrow \frac{1}{N} \forall i \in 1 \ldots N \)
5: repeat
6: \( t \leftarrow t + 1 \)

**Adaptation:**
7: Update \( \epsilon_t \) by solving equation (3)
8: Update \( w_{i,t} \forall i \in 1 \ldots N \) according to equation (1)
9: if \( ESS_t < N_{\text{min}} \) then
10: Resample \( \theta_{i,t} \forall i \in 1 \ldots N \)
11: \( w_{i,t} \leftarrow \frac{1}{N} \forall i \in 1 \ldots N \)
12: end if

**Resampling:**
13: \( n_{\text{accept}} \leftarrow 0 \)
14: for all \( i \in 1 \ldots N \) do
15: if \( w_{i,t} > 0 \) then
16: Draw \( \theta_{i}^{t} \sim q_t(\cdot|\theta_{i,t-1}) \)
17: Generate \( x_{i,m}^{t} \sim f(\cdot|\theta_{i}^{t}) \forall m \in 1 \ldots M \)
18: Calculate \( \rho_t \) according to equation (4)
19: Draw \( u \sim U(0,1) \)
20: if \( u < \rho_t \) then
21: \( (\theta_{i,t}, x_{i,.t}) \leftarrow (\theta_{i}^{t}, x_{i}^{t}) \)
22: \( n_{\text{accept}} \leftarrow n_{\text{accept}} + 1 \)
23: else
24: \( (\theta_{i,t}, x_{i,.t}) \leftarrow (\theta_{i,t-1}, x_{i,.t-1}) \)
25: end if
26: end if
27: end for
28: until \( \frac{n_{\text{accept}}}{N} < 0.015 \) or \( \epsilon_t = 0 \)
The ABC tolerance $\epsilon_t$ is updated adaptively according to the desired rate $\alpha \in (0, 1)$ of the reduction in the $ESS$

$$ESS_t = \alpha ESS_{t-1}$$

This equation must be solved iteratively, e.g. by interval bisection, since $ESS_t$ depends on the weights $w_{i,t}$, which in turn depend on $\epsilon_t$ according to equation (1).

**Resampling** If $ESS_t$ falls below a threshold value $N_{\text{min}}$ then the particles are all resampled. The new population of $N$ particles can either be drawn from a multinomial distribution with weights $\lambda_i = w_{i,t}$ or more complicated schemes can be used. [Del Moral et al] employed the systematic resampling scheme of Kitagawa [1996]. Once the particles have been resampled, all of the importance weights are set to $N^{-1}$ and thus the $ESS$ is equal to $N$.

**Mutation** Finally, the particles with nonzero weight are updated using a random walk proposal $q_t(\theta' | \theta_{t-1})$. The bandwidth $\sigma^2_{\text{MH}}$ can be chosen adaptively using an SMC approximation of the variance of $\theta$ under $\pi_{t-1}(\theta | y)$, as in Beaumont et al. [2009]. The pseudo-data is also updated using $q(x' | \theta')$ and jointly accepted with probability $\min(1, \rho_i)$ according to the MH acceptance ratio:

$$\rho_i = \frac{\sum_{m=1}^{M} I(\delta(x'_{i,m}) < \epsilon_i) \cdot q_t(\theta_{i,t-1} | \theta_i') \cdot \pi(\theta_i')} {\sum_{m=1}^{M} I(\delta(x_{i,m,t-1}) < \epsilon_i) \cdot q_t(\theta_i' | \theta_{i,t-1}) \cdot \pi(\theta_{i,t-1})}$$

A summary of this method is presented in algorithm 2.

### 2.2 Stopping criterion

The accuracy of the ABC rejection sampler improves as the number of iterations increases, since this results in a greater number of accepted proposals for a fixed value of $\epsilon$. Conversely, if the rejection rate is held at a fixed quantile of the sampled parameters, then it enables a smaller value of $\epsilon$ to be used. The same is not true of algorithm 2 since the effective sample size cannot exceed the number of particles. The set of alive particles is filtered at each iteration, therefore it is important to define a suitable stopping criterion. Running SMC-ABC for too many iterations can lead to over-adaptation, resulting in a posterior distribution that is highly concentrated, or even to collapse of the SMC sampler.

In our simulation study of section 5.1 we found that the MH acceptance rate almost never fell below 1.5%, the stopping criterion employed by Del Moral et al. [2012]. In most cases, the use of an adaptive bandwidth for the random walk proposals $\theta_i'$ led to a stabilisation of the acceptance rate. This is illustrated in figure 1a where the acceptance rate oscillates between 0.3 and 0.6. The stopping criterion of 0.015 is indicated by the horizontal line. The large jumps in the plotted acceptance rate correspond to iterations when the particles were resampled. We used the recommended number of $N = 10,000$ particles, $M = 50$ summary statistics per particle, and $\alpha = 0.95$. 

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Figure 1: Problems with convergence of the SMC-ABC algorithm for the hidden Potts model when the stopping criterion is based on the MH acceptance rate.
Figure 1b shows the SMC estimate of the empirical standard deviation at each iteration. This value is calculated in order to derive the MH bandwidth for the mutation step. The variance of the particles increases between iteration 52 and 53, which indicates that the SMC-ABC algorithm has reached the point where reducing $\epsilon$ no longer improves the posterior estimate of $\pi_t(\theta|y)$.

3 Precomputation of the Summary Statistic

Model fitting with ABC can be decomposed into two separate stages: learning about the summary statistic, given the parameter $(\rho(x)|\theta)$; and choosing parameter values, given the summary statistic $(\theta|\rho(y))$. The first stage is achieved by simulating pseudo-data from the generative model, while the second stage involves either accept/reject in the case of algorithm 1 or SMC for algorithm 2. In the case of latent models there is a third stage, which involves learning about the summary statistic given the data $(\rho(z)|y, \theta)$. ABC for latent models will be discussed further in section 4.2.

Our proposed method splits the computation of these stages into two separate parts, a pre-processing step followed by model fitting. The pre-processing step involves simulating pseudo-data for fixed values of the parameter. The results of these simulations are used to create an approximate mapping function from the parameter to the corresponding summary statistic. This function can then be used during model fitting to evaluate $\hat{\rho}(x)$ given $\theta'$, instead of simulating pseudo-data from the model for every proposed value of the parameter. Since the simulation of pseudo-data is usually the most computationally-intensive step of an ABC algorithm, our method can greatly improve the speed of model fitting. This is particularly the case when fitting the same model to multiple datasets because the output of the pre-processing step can be reused, thus amortising its computational cost.

The degree of complexity required for the mapping function is dependent on the dimensionality of the parameter space, the number of summary statistics, and the properties of the relationship between them. These factors will also influence how much pseudo-data must be simulated in order to achieve sufficiently good fit. The nonlinear, heteroskedastic regression that was applied by Blum and François [2010] would be a good choice in many cases, although simpler mapping functions could also be used.

Essentially we are fitting two models, one for the mapping function $\theta \mapsto \hat{\rho}(x)$ and the other for posterior inference on $\pi(\theta|y)$. The auxiliary model that is employed for the mapping function introduces an additional level of approximation, since it is used as a replacement for the generative model in evaluating the fit between the proposed parameter values and the data.

Precomputation for the ABC Rejection Sampler  The use of an approximate mapping function means that many more parameter values can be proposed and evaluated for the same computational cost. The mapping function could also be used to tune the ABC tolerance based on the variance of the
summary statistic. This would be particularly useful in heteroskedastic models where the amount of variance depends on the parameter value. In some cases, this will enable the ABC rejection sampler to be used for applications where it was previously infeasible due to its inefficiency.

**Precomputation for SMC-ABC** The benefit of using a mapping function in SMC-ABC is that a greater number of particles, and summary statistics per particle, could be used. It is much faster to draw $M$ summary statistics from $f(\hat{\rho}(x)|\theta')$ than to simulate pseudo-data from the model. Our method also reduces the memory requirements for each particle, since the pseudo-data does not need to be generated and stored. This in turn has advantages for massively parallel implementation of SMC-ABC. If each particle requires its own independent copy of the state space, then the scalability of the algorithm is limited by the available memory. The mapping function provides a more compact representation, enabling all of the particles to be updated in parallel.

4 Hidden Potts Model

We illustrate our method using a hidden Potts model. The Potts model is a Markov random field with discrete states $z \in 1 \ldots k$. It is defined in terms of its conditional probabilities:

$$p(z_i|z_{i-\ell}, \beta) = \frac{\exp \{\beta \sum_{\ell} \delta(z_i, z_{i})\}}{\sum_{j=1}^{k} \exp \{\beta \sum_{\ell} \delta(j, z_{i})\}}$$

(5)

where $i \in 1 \ldots n$ are the nodes in the image lattice, also known as pixels, $\beta$ is a scale parameter known as the inverse temperature, $i \sim \ell$ are the neighbouring pixels of $i$, and $\delta(u, v)$ is the Kronecker delta function. In this paper we use the first-order neighbourhood, so $i \sim \ell$ are the four pixels immediately adjacent to an internal node of the lattice. Pixels on the image boundary have less than four neighbours.

The inverse temperature parameter governs the strength of spatial association. A value of zero corresponds with spatial independence, while values greater than zero increase the probability of adjacent neighbours having the same state. The full conditional distribution of the inverse temperature is given by

$$p(\beta|z) = C(\beta)^{-1} \pi(\beta) \exp \{\beta S(z)\}$$

(6)

where $C(\beta)$ is an intractable normalising constant. It involves a sum over all $k^n$ possible combinations of the labels $z \in \mathcal{Z}$:

$$C(\beta) = \sum_{z \in \mathcal{Z}} \exp \{\beta S(z)\}$$

(7)

A sufficient statistic is available for this model since it belongs to the exponential family, as noted by Grelaud et al. [2009]. If $\mathcal{E}$ is the set of all unique
Figure 2: Distribution of the sufficient statistic of the Potts model for increasing values of the inverse temperature hyperparameter $\beta$, the number of pixels $n$, and the number of unique labels $k$. The expectation and standard deviation of $S(z)$ were calculated exactly, using a brute force method.
neighbour pairs, or edges in the image lattice, then the sufficient statistic is

$$S(z) = \sum_{i \sim \ell \in \mathcal{E}} \delta(z_i, z_\ell)$$  \hspace{1cm} (8)$$

Thus, this statistic represents the total number of like neighbor pairs in the image. As $\beta$ approaches infinity, all of the pixels in the image are almost surely assigned the same label, thus the expectation of $S(z)$ approaches the total number of edges $|\mathcal{E}|$ asymptotically, while the variance approaches zero. When $\beta = 0$, the probability of any pair of neighbours being assigned the same label follows an independent Bernoulli distribution with $p = k^{-1}$, thus $S(z)$ follows a Binomial distribution with expectation $|\mathcal{E}|/k$ and variance $|\mathcal{E}| \times k^{-1} \times (1 - k^{-1})$. The distribution of $S(z)$ changes smoothly between these two extremes, as illustrated by figure 2, but its computation is intractable for nontrivial images. The expectations and variances in figure 2 were calculated for $k$ up to 4 unique labels and $n$ up to 12 pixels, much less than required for any practical application.

The maximum variance of $S(z)|\beta$, which corresponds to the steepest gradient in the expectation, occurs at the critical temperature. This is the point at which the Potts model transitions from a disordered to an ordered state. The phase transition behaviour has analogies in physical systems, such as the Curie temperature in ferromagnetic materials. When $\beta > \beta_{\text{crit}}$, the values of the labels begin to exhibit long-range dependence and coalesce into clusters of similar values. Potts [1952] showed that this critical point can be calculated exactly for a two-dimensional regular lattice by $\beta_{\text{crit}} = \log\{1 + \sqrt{k}\}$, so $\beta_{\text{crit}} \approx 0.881$ for $k = 2$ and $\beta_{\text{crit}} \approx 1.099$ for $k = 4$. The nonlinearity and heteroskedasticity evident in figure 2 will need to be accounted for in our choice of mapping function $f(S(z)|\beta)$.

4.1 Precomputation of $S(z)$

Since it is impossible to sample from $\beta | z$ directly, we use ABC methods. This requires simulating pseudo-data from the Gibbs distribution $z_i | z_{-i}, \beta$ defined by equation (5). It is difficult to simulate from this distribution because neighbouring pixels are highly correlated with each other, particularly for $\beta > \beta_{\text{crit}}$. We use the algorithm of Swendsen and Wang [1987], which updates clusters of pixels simultaneously. Nevertheless, simulating pseudo-data remains computationally expensive, which is why we approximate $S(z)|\beta$ offline using a pre-processing step.

To fit the mapping function for the Potts model, we use 61 values of $\beta$, evenly spaced between 0 and 3. We choose to space these values evenly because we use a uniform prior for $\beta$, even though the distribution of $S(z)|\beta$ is far from uniform, as figure 2 shows. We perform 1000 iterations of Swendsen-Wang for each value of $\beta$, discarding the first 500 as burn-in. The remaining 500 iterations are used to compute the expectation and variance of the sufficient statistic. It should be noted that this operation is embarrassingly parallel, since the computation for each value of $\beta$ is completely independent. The results of this pre-processing step are stored in a matrix, which can then be used to fit the same model to multiple
Estimate of the expectation $E\{S(\mathbf{z})|\beta\}$

Estimate of the standard deviation $\sigma\{S(\mathbf{z})|\beta\}$

Figure 3: Approximation of the expectation and standard deviation of the sufficient statistic for the Potts model with $n = 125 \times 125$ and $k = 3$. 
datasets. During model fitting, these pre-computed values are interpolated to estimate $E[S(z)|\beta']$ and $\text{Var}\{S(z)|\beta'\}$, then the conditional distribution of the sufficient statistic is approximated by a Gaussian with these parameters.

Figure 3 shows the estimated mapping function using linear interpolation between the observed values of the mean and standard deviation for a regular lattice with $n = 125 \times 125$ pixels and $k = 3$, which corresponds to the simulation study in section 5.1. We have also plotted 1000 points that were computed using Swendsen-Wang, but for values drawn from $\beta \sim \mathcal{N}(\beta_{\text{crit}}, (\beta_{\text{crit}}/2)^2)$. These values are more concentrated in the neighbourhood of the critical temperature to illustrate the heteroskedastic behaviour in that region. The value of $\beta_{\text{crit}}$ is indicated by the vertical line. The mapping function provides a very good fit for the distribution of the expected values, but there is a larger approximation error in the estimate of the standard deviation. This is particularly evident at the critical point, where the variance of the sufficient statistic is much larger than estimated. Nevertheless, this simple function appears to be adequate for our purposes, as demonstrated in section 5.

4.2 Additive Gaussian noise

In the hidden Potts model, the observed data $y$ are independently distributed conditional on the latent labels $z$. Under the assumption of additive Gaussian noise, the observation process is characterised by

$$y_i|z_i = j \overset{iid}{\sim} \mathcal{N}(\mu_j, \sigma^2_j)$$  \hspace{1cm} (9)

Since each unique label value corresponds to the mean and variance of a Normal distribution, this model can be viewed as a spatially-correlated generalisation of the mixture of Gaussians.

When the parameters of these mixture components are unknown, they must be estimated as part of the model fitting procedure. This can be problematic for SMC-ABC because the value of the sufficient statistic depends on both the current likelihood of the data as well as the distribution of the particles, while the particles in turn depend on the current value of $S(z)$:

$$p(\beta|y) = p(\beta|z)p(z|y)$$  \hspace{1cm} (10)

where the intractable posterior $p(\beta|z)$ is estimated using ABC methods.

The posterior distribution of the latent labels can be decomposed into the observation equation and the spatial model:

$$p(z_i|y_i) = p(y_i|z_i, \mu, \sigma^2)p(\mu)p(\sigma^2)p(z_i|z_{i-\ell}, \beta)p(\beta)$$  \hspace{1cm} (11)

where

$$p(y_i|z_i, \mu, \sigma^2) = \frac{\phi\left(y_i|\mu_{z_i}, \sigma^2_{z_i}\right)}{\sum_{j=1}^{k}\phi\left(y_i|\mu_j, \sigma^2_j\right)}$$  \hspace{1cm} (12)

and $p(z_i|z_{i-\ell}, \beta)$ is given by equation (5). This is the third stage of ABC estimation for latent models that was mentioned in section 5.
Figure 4: Change in the value of the sufficient statistic according to the current distribution of $\pi_t(\beta|z)$. 
One approach to overcoming this circular dependency would be to include the noise parameters $\mu_j, \sigma_j^2$ in the state vector for each SMC particle. Updating these parameters would require generating latent labels from equation (11), which would severely limit the scalability of the algorithm. Simulating from the distribution of $z|\mathbf{y}$ is even more difficult than drawing pseudo-data from $x|\beta$ [Hurn, 1997, Higdon, 1998]. It is simply infeasible to do this for each particle individually.

An alternative is to use a single copy of the latent state vector to calculate $S(z)$ at each SMC iteration, as well as the sufficient statistics of the Gaussian components $\bar{y}_j|z$ and $s_j^2|z$. This is the approach that we have implemented in this paper. Values of $\beta$ are drawn at random from $\pi_t(\beta|z)$ according to the importance weights of the particles, then $z$ is updated using multiple iterations of chequerboard sampling [Winkler, 2003, chap. 8]. Figure 4 illustrates how the value of $S(z)$ changes between SMC iterations. As the distribution of the particles becomes more precise, the variance in the sufficient statistic narrows accordingly.

5 Illustration

For comparison, we have implemented both the SMC-ABC algorithm of Del Moral et al. as well as our own method for SMC-ABC with a pre-computed mapping function. An R source package containing this implementation is provided in Online Resource 1. The computational engine is implemented in C++ using RcppArmadillo [Eddelbuettel and Sanderson, 2014] with OpenMP for parallelism.

We fit the model to each image using $N = 10,000$ SMC particles with $M = 50$ summary statistics per particle. We used $\alpha = 0.95$ and resampled the particles using residual resampling [Douc et al., 2005]. The algorithm terminated when the weighted empirical variance of the particles fell below a threshold of 0.012. As explained in section 2.2, we found that the usual stopping criterion based on the Metropolis-Hastings acceptance rate was unsuitable for this application.

The elapsed times were recorded on 2.66GHz Intel Xeon processors. We used 8 parallel cores for fitting the model to each image and the precomputation was performed on a dual-CPU computer with 16 parallel cores. Memory usage varied depending on the number of pixels and the degree of parallelism. Approximate memory requirements for each computation are reported below.

5.1 Simulation Study

Since the inverse temperature cannot be directly observed, we have used a simulation study to evaluate the accuracy of our method where the true value of $\beta$ is known. Following a similar methodology to that introduced by [Cook et al., 2006], we first simulated 20 values of $\beta$ from the prior, then generated 20 images from the model that corresponded to those parameter values. Each image had $125 \times 125$ pixels with $k = 3$ unique labels. We used a uniform prior on the
Figure 5: Distribution of CPU times (left) and elapsed (wall clock) times for model fitting with pseudo-data in comparison to precomputed $S(z)$. 
Figure 6: Results for the simulation study of 20 images. The $x$ axis is the true value of $\beta$ and the $y$ axis shows the posterior samples from $\pi_t(\beta|z)$.
Figure 7: Distribution of posterior sampling error for $\beta$, comparing 10,000 particles with pseudo-data to 50,000 particles using pre-computation.
interval $[0, 1.005]$ for $\beta$ and natural conjugate priors $\pi(\mu_j) \sim \mathcal{N}(0, 100^2)$ and $\pi(\sigma^2_j) \sim \mathcal{IG}(1, 0.01)$ for the additive Gaussian noise.

Precomputation of the mapping function took under 6 minutes for 61 values of $\beta$, using a thousand iterations of Swendsen-Wang for each. The mapping function is illustrated in figure 3. Total CPU time for all 16 parallel threads was 1 hour 17 minutes, indicating about 70% utilisation of the available capacity. Memory usage was less than 1.3GB. Since the same mapping function was reused for all 20 images, this 6 minutes could be amortised across the entire corpus. Thus, the cost of precomputation was almost negligible.

Across the 20 simulated images, our algorithm took an average of 21 minutes per image for between 39 and 70 SMC iterations. Using pseudo-data to compute the sufficient statistic took an average of 46.5 hours for 44 to 85 SMC iterations. Figure 4 illustrates that this two orders of magnitude difference in the distribution is consistent for both elapsed (wall clock) time and CPU time. This shows that the gain in performance is due to computational efficiency, not because of any increase in parallelism.

Figure 6 shows that both versions of the SMC-ABC algorithm produced erroneous estimates of $\beta$ for some of the images, with a large difference between the posterior distribution of the particles and the true value of the inverse temperature. This is most likely due to problems with simultaneously estimating the sufficient statistic $S(z|y)$ as well as $\pi_t(\beta|z)$, as explained in section 4.2. We also ran our algorithm with 50,000 particles and this did seem to show an improvement in the accuracy of the posterior estimate. The violin plot in figure 7 is a comparison of the error in the posterior estimate between 10,000 particles with pseudo-data on the left and 50,000 particles with pre-computation on the right. The distribution of the errors appears to be equivalent. Even with a much larger number of particles, our algorithm was still considerably faster with an average runtime of 1.7 hours.

### 5.2 Satellite Remote Sensing

We have also illustrated our method on real data, using a satellite image of Brisbane, Australia. The pixel values correspond to the Normalized Difference Vegetation Index (NDVI), which was calculated according to equation (13):

$$\text{NDVI} = \frac{NIR - VIS}{NIR + VIS}$$

In Landsat 7 images, the visible red ($VIS$) band corresponds to light wavelengths of $(0.63 \ldots 0.69)\mu m$ and the near-infrared ($NIR$) band corresponds to $(0.76 \ldots 0.90)\mu m$ [NASA, 2011].

The image was cropped to a region of interest that was approximately 40km east to west and 20km north to south, containing a total of 978,380 pixels. Precomputation of the mapping function took 50 minutes. Total CPU time for all 16 parallel threads was 10 hours 38 minutes, indicating 81% utilisation of the available capacity. Memory usage was approximately 6.5GB.
We used weakly informative priors $\pi(\beta) \sim U[0, 3]$, $\pi(\mu_j) \sim N(y, 5)$, and $\pi(\sigma^2_j) \sim IG(1, 0.01)$ for the hidden Potts model with $k = 6$ unique labels. Model fitting took 5 hours 36 minutes using our algorithm. CPU time for 8 parallel threads was 39 hours, indicating 88% utilisation. The 95% posterior credible interval for $\beta$ was $[1.243; 1.282]$.

Running the original SMC-ABC algorithm of Del Moral et al. [2012] on this dataset is clearly infeasible, due to the cost of simulating pseudo-data. It takes 89 hours to perform a single SMC iteration on our hardware. We also found that the exchange algorithm of Murray et al. [2006] was unable to scale to data of this dimension, even when using 500 iterations of Gibbs sampling for the auxiliary variable as recommended by Cucala et al. [2009]. It took 97 hours for 10,000 MCMC iterations. Discarding the first 5,000 as burn-in left an effective sample size of only 390 due to auto-correlation of the Markov chain.

We were able to obtain results using path sampling [Gelman and Meng, 1998], which is another algorithm that uses pre-computation to approximate the relationship between $\beta$ and the sufficient statistic. We ran path sampling for 100,000 iterations, which took 2.5 hours. We discarded the first 10,000 iterations as burn-in, which left an effective sample size of 11,526. The 95% highest posterior density (HPD) interval for $\beta$ was $[1.249; 1.251]$, which overlaps with our estimate from SMC-ABC although it has a smaller posterior variance.

6 Discussion

We have demonstrated that the scalability of ABC (and SMC-ABC in particular) can be dramatically improved by replacing the simulation of pseudo-data with a pre-computed mapping function. We observed two orders of magnitude improvement in runtime in our simulation study, from an average of 46.5 hours down to only 21 minutes. Simulating pseudo-data from the generative model is the most computationally intensive step in ABC and can render the algorithm infeasible for high-dimensional data, such as satellite imagery.

This improvement in scalability comes at the cost of adding an extra layer of approximation, since the mapping function introduces another source of error into the algorithm. We showed that it is possible to compensate for the loss of accuracy by increasing the number of SMC particles and that the cost of doing this is relatively small.

Our approach bears some similarities to path sampling, another method that uses a pre-computation step. The main difference is that path sampling is a MCMC algorithm that uses thermodynamic integration to approximate the Metropolis-Hastings ratio. This places restrictions on the form that the mapping function can take, since this integral must be computed at each iteration. Our SMC-ABC method could be adapted for multivariate problems, such as simultaneously estimating $k$ as well as $\beta$. Our method also accounts for the heteroskedasticity in the distribution of $S(z) | \beta$ by sampling multiple values of the sufficient statistic for each particle. Like most MCMC algorithms, path sampling suffers from auto-correlation, which reduces its efficiency in comparison to
Once the mapping function has been computed, it can be reused to fit the same model to multiple datasets. This is an advantage in many applications such as satellite imaging, where there are a large number of images with approximately the same dimensions. In a longitudinal setting it would also be possible to update the mapping function sequentially as each image is processed.

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