

A Comparative Review of Dimension Reduction Methods in Approximate Bayesian Computation

M. G. B. Blum, M. A. Nunes, D. Prangle and S. A. Sisson

Abstract. Approximate Bayesian computation (ABC) methods make use of comparisons between simulated and observed summary statistics to overcome the problem of computationally intractable likelihood functions. As the practical implementation of ABC requires computations based on vectors of summary statistics, rather than full data sets, a central question is how to derive low-dimensional summary statistics from the observed data with minimal loss of information. In this article we provide a comprehensive review and comparison of the performance of the principal methods of dimension reduction proposed in the ABC literature. The methods are split into three nonmutually exclusive classes consisting of best subset selection methods, projection techniques and regularization. In addition, we introduce two new methods of dimension reduction. The first is a best subset selection method based on Akaike and Bayesian information criteria, and the second uses ridge regression as a regularization procedure. We illustrate the performance of these dimension reduction techniques through the analysis of three challenging models and data sets.

Key words and phrases: Approximate Bayesian computation, dimension reduction, likelihood-free inference, regularization, variable selection.

1. INTRODUCTION

Bayesian inference is typically focused on the posterior distribution $p(\theta|y_{\text{obs}}) \propto p(y_{\text{obs}}|\theta)p(\theta)$ of a parameter vector $\theta \in \Theta \subseteq \mathbb{R}^q$, $q \geq 1$, representing the updating of one's prior beliefs, $p(\theta)$, through the likelihood (model) function, $p(y_{\text{obs}}|\theta)$, having observed data $y_{\text{obs}} \in \mathcal{Y}$. The term *approximate Bayesian computation* (ABC) refers to a family of models and algorithms that aim to draw samples from an approximate

posterior distribution when the likelihood, $p(y_{\text{obs}}|\theta)$, is unavailable or computationally intractable, but where it is feasible to quickly generate data from the model, $y \sim p(\cdot|\theta)$. ABC is rapidly becoming a popular tool for the analysis of complex statistical models in an increasing number and breadth of research areas. See, for example, Lopes and Beaumont (2010), Bertorelle, Benazzo and Mona (2010), Beaumont (2010), Csilléry et al. (2010) and Sisson and Fan (2011) for a partial overview of the application of ABC methods.

ABC introduces two principal approximations to the posterior distribution. First, the posterior distribution of the full data set, $p(\theta|y_{\text{obs}})$, is approximated by $p(\theta|s_{\text{obs}}) \propto p(s_{\text{obs}}|\theta)p(\theta)$, where $s_{\text{obs}} = S(y_{\text{obs}})$ is a vector of summary statistics of lower dimension than the data y_{obs} . In this manner, $p(\theta|s_{\text{obs}}) \approx p(\theta|y_{\text{obs}})$ is a good approximation if s_{obs} is highly informative for the model parameters, and $p(\theta|s_{\text{obs}}) = p(\theta|y_{\text{obs}})$ if s_{obs} is sufficient. As $p(s_{\text{obs}}|\theta)$ is also likely to be computationally intractable if $p(y_{\text{obs}}|\theta)$ is computationally

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intractable, a second approximation is constructed as $p_{\text{ABC}}(\theta|s_{\text{obs}}) = \int p(\theta, s|s_{\text{obs}}) ds$, with

$$(1) \quad p(\theta, s|s_{\text{obs}}) \propto K_{\epsilon}(\|s - s_{\text{obs}}\|)p(s|\theta)p(\theta),$$

where $K_{\epsilon}(\|u\|) = K(\|u\|/\epsilon)/\epsilon$ is a standard smoothing kernel with scale parameter $\epsilon > 0$. As a result of (1), approximating the target $p(\theta|s_{\text{obs}})$ by $p_{\text{ABC}}(\theta|s_{\text{obs}})$ can be shown to be a good approximation if the kernel scale parameter, ϵ , is small enough, following standard kernel density estimation arguments (e.g., Blum, 2010a).

In combination, both approximations allow for practical methods of sampling from $p_{\text{ABC}}(\theta|s_{\text{obs}})$ that avoid explicit evaluation of the intractable likelihood function, $p(y_{\text{obs}}|\theta)$. A simple rejection-sampling algorithm to achieve this was proposed by Pritchard et al. (1999) (see also Marjoram et al., 2003), which produces draws from $p(\theta, s|s_{\text{obs}})$. In general terms, an importance-sampling version of this algorithm proceeds as follows:

- (1) Draw a candidate parameter vector from the prior, $\theta' \sim p(\theta)$;
- (2) Draw summary statistics from the model $s' \sim p(s|\theta')$;
- (3) Assign to (θ', s') a weight, w' , that is proportional to $K_{\epsilon}(\|s' - s_{\text{obs}}\|)$.

Here, the sampling distribution for (θ', s') is the prior predictive distribution, $p(s|\theta)p(\theta)$, and the target distribution is $p(\theta, s|s_{\text{obs}})$. Using equation (1), it is then straightforward to compute the importance weight for the pair (θ', s') . The weight is proportional to $p(\theta', s'|s_{\text{obs}})/[p(s'|\theta')p(\theta')] = K_{\epsilon}(\|s' - s_{\text{obs}}\|)$, which is free of intractable likelihood terms, $p(s'|\theta')$. The manner by which the intractable likelihoods cancel between sampling and target distributions forms the basis for the majority of ABC algorithms.

Clearly, both ABC approximations to the posterior distribution help to avoid the computational intractability of the original problem. The first approximation allows the kernel weighting of the second approximation, $K_{\epsilon}(\|s - s_{\text{obs}}\|)$, to be performed on a lower dimension than that of the original data, y_{obs} . Kernel smoothing is known to suffer from the curse of dimensionality (e.g., Blum, 2010a), and so keeping $\dim(s) \leq \dim(y)$ as small as possible helps to improve algorithmic efficiency. The second approximation (1) allows the sampler weights (or acceptance probabilities, if one considers rejection-based samplers, such as Markov chain Monte Carlo) to be free of intractable likelihood terms.

In practice, however, there is typically a trade-off between the two approximations: if the dimension of s is large so that the first approximation, $p(\theta|s_{\text{obs}}) \approx p(\theta|y_{\text{obs}})$, is good, the second approximation may then be poor due to the inefficiency of kernel smoothing in large dimensions. Conversely, if the dimension of s is small while the second approximation (1) will be good (with a small kernel scale parameter, ϵ), any loss of information in the mapping $s_{\text{obs}} = S(y_{\text{obs}})$ means that the first approximation may be poor. Naturally, a low-dimensional and near-sufficient statistic, s , would provide a near-optimal and balanced choice.

For a given set of summary statistics, much work has been done on deriving more efficient sampling algorithms to reduce the effect of the second approximation by allowing a smaller value for the kernel scale parameter, ϵ , which in turn improves the approximation $p_{\text{ABC}}(\theta|s_{\text{obs}}) \approx p(\theta|s_{\text{obs}})$. The greater the algorithmic efficiency, the smaller the scale parameter that can be achieved for a given computational burden. These algorithms include Markov chain Monte Carlo (Marjoram et al., 2003; Bortot, Coles and Sisson, 2007) and sequential Monte Carlo techniques (Sisson, Fan and Tanaka, 2007; Toni et al., 2009; Beaumont et al., 2009; Drovandi and Pettitt, 2011; Peters, Fan and Sisson, 2012; Del Moral, Doucet and Jasra, 2012). By contrast, the regression-based methods described in Section 2.1 do not aim at reducing the scale parameter ϵ but rather explicitly account for the imperfect match between observed and simulated summary statistics (Beaumont, Zhang and Balding, 2002; Blum and François, 2010).

Achieving a good trade-off between the two approximations revolves around the identification of a set of summary statistics, s , which are both low-dimensional and highly informative for θ . A number of methods, primarily based on dimension reduction ideas, have been proposed to achieve this (Joyce and Marjoram, 2008; Wegmann, Leuenberger and Excoffier, 2009; Nunes and Balding, 2010; Blum and François, 2010; Blum, 2010b; Fearnhead and Prangle, 2012). The choice of summary statistics is one of the most important aspects of a statistical analysis using ABC methods (along with the choice of algorithm). Poor specification of s can have a large and detrimental impact on both ABC model approximations.

In this article we provide the first detailed review and comparison of the performance of the current methods of dimension reduction for summary statistics within the ABC framework. We characterize these methods

into three nonmutually exclusive classes: (i) best subset selection, (ii) projection techniques and (iii) regularization approaches. As part of this analysis, we introduce two additional novel techniques for dimension reduction within ABC. The first adopts the ideas of Akaike and Bayesian information criteria to the ABC framework, whereas the second makes use of ridge regression as a regularization procedure for ABC. The dimension reduction methods are compared through the analysis of three challenging models and data sets. These involve the analysis of a coalescent model with recombination (Joyce and Marjoram, 2008), an evaluation of the evolutionary fitness cost of mutation in drug-resistant tuberculosis (Luciani et al., 2009) and an assessment of the number and size-distribution of particle inclusions in the production of clean steels (Bortot, Coles and Sisson, 2007).

The layout of this article is as follows: in Section 2 we classify and review the existing methods of summary statistic dimension reduction in ABC, and in Section 3 we outline our two additional novel methods. A comparative analysis of the performance of each of these methods is provided in Section 4. We conclude with a discussion.

2. CLASSIFICATION OF ABC DIMENSION REDUCTION METHODS

In a typical ABC analysis, an initial collection of statistics $s^\top = (s_1, \dots, s_p)$ is chosen by the modeler, the elements of which have the potential to be informative for the model parameters, $\theta^\top = (\theta_1, \dots, \theta_q)$. Choice of these initial statistics is highly problem specific, and the number of candidate statistics, p , often considerably outnumbers the number of model parameters, q , that is, $p \gg q$ (e.g., Bortot, Coles and Sisson, 2007; Allingham, King and Mengersen, 2009; Luciani et al., 2009). For example, Bortot, Coles and Sisson (2007) and Allingham, King and Mengersen (2009) use the ordered observations $S(y) = (s_{(1)}, \dots, s_{(p)})$ so that there is no loss of information at this stage. The analysis then proceeds by either using all p statistics in full or by attempting to reduce their dimension while minimizing information loss. Note that the most suitable set of summary statistics for an analysis may be data set dependent, as the information content of summary statistics may vary within the parameter space, Θ (an exception is when sufficient statistics are known). As such, any analysis should also consider establishing potentially different summary statistics when re-implementing any model with a different data set.

Methods of summary statistics dimension reduction for ABC can be broadly classified into three nonmutually exclusive classes. The first class of methods follows a *best subset selection* approach. Here, candidate subsets are evaluated and ranked according to various information-based criteria, such as measures of sufficiency (Joyce and Marjoram, 2008) or the entropy of the posterior distribution (Nunes and Balding, 2010). In this article we contribute additional criteria for this process derived from Akaike and Bayesian information criteria arguments. From these criteria, the highest ranking subset (or, alternatively, a subset consisting of those summary statistics which demonstrate clear importance) is then chosen for the final analysis.

The second class of methods can be considered as *projection techniques*. Here, the dimension of (s_1, \dots, s_p) is reduced by considering linear or nonlinear combinations of the summary statistics. These methods make use of a regression layer within the ABC framework, whereby the response variable, θ , is regressed by the (possibly transformed) predictor variables, s (Beaumont, Zhang and Balding, 2002; Blum and François, 2010). These projection methods include partial least squares regression (Wegmann, Leuenberger and Excoffier, 2009), feed-forward neural networks (Blum and François, 2010) and regression guided by minimum expected posterior loss considerations (Fearhead and Prangle, 2012).

In this article we introduce a third class of methods for dimension reduction in ABC, based on *regularization techniques*. Using ridge regression, we also make use of the regression layer between the parameter θ and the summary statistics, s . However, rather than explicitly considering a selection of summary statistics, we propose to approach this implicitly, by shrinking the regression coefficients toward zero so that uninformative summary statistics have the weakest contribution in the regression equation.

In the remainder of this section we discuss each of these methods in more detail. We first describe the ideas behind ABC regression adjustment strategies (Beaumont, Zhang and Balding, 2002; Blum and François, 2010), as many of the dimension reduction techniques build on this framework.

2.1 Regression Adjustment in ABC

Standard ABC methods suffer from the curse of dimensionality in that the rate of convergence of posterior expectations with respect to $p_{\text{ABC}}(\theta|s_{\text{obs}})$ (such as the Nadaraya–Watson estimator of the posterior mean)

decreases dramatically as the dimension of the summary statistics, p , increases (Blum, 2010a). ABC regression adjustment (Beaumont, Zhang and Balding, 2002) aims to avoid this by explicitly modeling the discrepancy between s and s_{obs} . When describing regression adjustment methods, for notational simplicity and clarity of exposition, we assume that the parameter of interest, θ , is univariate (i.e., $q = 1$). Regression adjustment methods may be readily applied to multivariate θ , by using a different regression equation for each parameter, $\theta_1, \dots, \theta_q$, separately.

The simplest model for this is a homoscedastic regression in the region of s_{obs} , so that

$$\theta^i = m(s^i) + e^i,$$

where $(\theta^i, s^i) \sim p(s|\theta)p(\theta)$ are $i = 1, \dots, n$ draws from the prior predictive distribution, $m(s^i) = \mathbb{E}[\theta|s = s^i]$ is the mean function, and the e^i are zero-mean random variates with common variance. To estimate the conditional mean $m(\cdot)$, Beaumont, Zhang and Balding (2002) assumed a linear model

$$(2) \quad m(s^i) = \alpha + \beta^\top s^i$$

in the neighborhood of s_{obs} . An estimate of the mean function, $\hat{m}(\cdot)$, is obtained by minimizing the weighted least squares criterion $\sum_{i=1}^n w^i \|m(s^i) - \theta^i\|^2$, where $w^i = K_\epsilon(\|s^i - s_{\text{obs}}\|)$. A weighted sample from the posterior distribution, $p_{\text{ABC}}(\theta|s_{\text{obs}})$, is then obtained by the adjustment

$$(3) \quad \theta^{*i} = \hat{m}(s_{\text{obs}}) + (\theta^i - \hat{m}(s^i))$$

for $i = 1, \dots, n$. In the above, the kernel scale parameter ϵ controls the bias-variance trade-off: increasing ϵ reduces variance by increasing the effective sample size—the number of accepted simulations when using a uniform kernel K —but increases bias arising from departures from a linear mean function $m(\cdot)$ and homoscedastic error structure (Blum, 2010a).

Blum and François (2010) proposed the more flexible, heteroscedastic model

$$(4) \quad \theta^i = m(s^i) + \sigma(s^i)e^i,$$

where $\sigma^2(s^i) = \mathbb{V}[\theta|s = s^i]$ denotes the conditional variance. This variance is estimated using a second regression model for the log of the squared residuals, that is, $\log(\theta^i - \hat{m}(s^i))^2 = \log \sigma^2(s^i) + \eta^i$, where the η^i are independent, zero-mean variates with common variance. The equivalent adjustment to (3) is then given by

$$(5) \quad \theta^{*i} = \hat{m}(s_{\text{obs}}) + [\theta^i - \hat{m}(s^i)] \frac{\hat{\sigma}(s_{\text{obs}})}{\hat{\sigma}(s^i)},$$

where $\hat{\sigma}(s)$ denotes the estimate of $\sigma(s)$. The kernel scale parameter, ϵ , plays the same role as for the homoscedastic model, except with more flexibility on deviations from homoscedasticity. Nott et al. (2013) have demonstrated that regression adjustment ABC algorithms produce samples, $\{\theta^{*i}\}$, for which first- and second-order moment summaries approximate adjusted expectation and variance for a Bayes linear analysis. We do not describe here an alternative regression adjustment method where the summary statistics are rather considered as the dependent variables and the parameters as the independent variables of the regression (Leuenberger and Wegmann, 2010).

2.2 Best Subset Selection Methods

Best subset selection methods are conceptually simple, but are cumbersome to manage for large numbers of potential summary statistics, $s = (s_1, \dots, s_p)$. Exhaustive enumeration of the $2^p - 1$ possible combinations of summary statistics is practically infeasible beyond a moderate value of p . This is especially true of Markov chain Monte Carlo or sequential Monte Carlo based analyses, which require one sampler implementation per combination. As a result, stochastic or deterministic (greedy) search procedures, such as forward or backward selection, are required to implement them.

2.2.1 A sufficiency criterion. The first principled approach to dimension reduction in ABC was the ϵ -sufficiency concept proposed by Joyce and Marjoram (2008), which was used to determine whether to include an additional summary statistic, s_k , to a model already containing statistics s_1, \dots, s_{k-1} . Here, noting that the difference between the log likelihoods of $p(s_1, \dots, s_k|\theta)$ and $p(s_1, \dots, s_{k-1}|\theta)$ is $\log p(s_k|s_1, \dots, s_{k-1}, \theta)$, Joyce and Marjoram (2008) defined the set of statistics s_1, \dots, s_{k-1} to be ϵ -sufficient relative to s_k if

$$(6) \quad \begin{aligned} \delta_k &= \sup_{\theta} \log p(s_k|s_1, \dots, s_{k-1}, \theta) \\ &\quad - \inf_{\theta} \log p(s_k|s_1, \dots, s_{k-1}, \theta) \\ &\leq \epsilon. \end{aligned}$$

Accordingly, if an estimate of δ_k (i.e., the “score” of s_k relative to s_1, \dots, s_{k-1}) is greater than ϵ , then there is enough additional information content in s_k to justify including it in the model. In practice, Joyce and Marjoram (2008) implement a conceptually equivalent assessment, whereby s_k is added to the model if the ratio of posteriors

$$R_k(\theta) = \frac{p_{\text{ABC}}(\theta|s_1, \dots, s_{k-1}, s_k)}{p_{\text{ABC}}(\theta|s_1, \dots, s_{k-1})}$$

differs from one by more than some threshold value $T(\theta)$ for any value of θ . As such, a statistic s_k will be added to the model if the resulting posterior changes sufficiently at any point. The threshold, $T(\theta)$, is user-specified, with one particular choice described in Section 5 of [Joyce and Marjoram \(2008\)](#).

This procedure can be implemented within any step-wise search algorithm, each of which have various pros and cons. Following the definition (6), the resulting optimal subset of summary statistics is then ε -sufficient relative to each one of the remaining summary statistics. Here ε intuitively represents an acceptable error in determining whether s_k contains further useful information in addition to s_1, \dots, s_k . This quantity is also user-specified, and so the final optimal choice of summary statistics will depend on the chosen value.

Sensitivity to the choice of ε aside, this approach may be criticized in that it assumes that every change to the posterior obtained by adding a statistic, s_k , is beneficial. It is conceivable that attempting to include a completely noninformative statistic, where the observed statistic is unlikely to have been generated under the model, will result in a sufficiently modified posterior as measured by ε , but one which is more biased away from the true posterior $p(\theta|y_{\text{obs}})$ than without including s_k . A toy example illustrating this was given by [Sisson and Fan \(2011\)](#).

A further criticism is that the amount of computation required to evaluate $R_k(\theta)$ for all θ , and on multiple occasions, is considerable, especially for large q . In practice, [Joyce and Marjoram \(2008\)](#) considered θ to be univariate, and approximated continuous θ over a discrete grid in order to keep computational overheads to acceptable levels. As such, this method appears largely restricted to dimension reduction for univariate parameters ($q = 1$).

2.2.2 An entropy criterion. [Nunes and Balding \(2010\)](#) propose the entropy of a distribution as a heuristic to measure the informativeness of candidate combinations of summary statistics. Since entropy measures information and a lack of randomness ([Shannon, 1948](#)), the authors propose minimizing the entropy of the approximate posterior, $p_{\text{ABC}}(\theta|s_{\text{obs}})$, over subsets of the summary statistics, s , as a proxy for determining maximal information about a parameter of interest. High entropy results from a diffuse posterior sample, whereas low entropy is obtained from a posterior which is more precise in nature.

[Nunes and Balding \(2010\)](#) estimate entropy using the unbiased k th nearest neighbor estimator of

[Singh et al. \(2003\)](#). For a weighted posterior sample, $(w^1, \theta^1), \dots, (w^n, \theta^n)$, where $\sum_i w^i = 1$, this estimator can be written as

$$(7) \quad \hat{E} = \log \left[\frac{\pi^{q/2}}{\Gamma(q/2+1)} \right] - \psi(k) + \log n + q \sum_{i=1}^n w^i \log \hat{C}_i^{-1}(k/(n-1)),$$

where $q = \dim(\theta)$, $\psi(x) = \Gamma'(x)/\Gamma(x)$ denotes the digamma function, and where $\hat{C}_i(\cdot)$ denotes the empirical distribution function of the Euclidean distance from θ^i to the remainder of the weighted posterior sample, that is, of the weighted samples $\{(\tilde{w}^j, \|\theta^i - \theta^j\|)\}_{j \neq i}$, where $\tilde{w}^j = w^j / \sum_{j \neq i} w^j$. Following [Singh et al. \(2003\)](#), the original work of [Nunes and Balding \(2010\)](#) used $k = 4$ and was based on an equally weighted posterior sample (i.e., with $w^i = 1/n, i = 1, \dots, n$), so that $\hat{C}_i^{-1}(k/(n-1))$ denotes the Euclidean distance from θ^i to its k th closest neighbor in the posterior sample $\{\theta^1, \dots, \theta^{i-1}, \theta^{i+1}, \dots, \theta^n\}$.

While minimum entropy could in itself be used to evaluate the informativeness of a vector of summary statistics for θ (although see the criticism of entropy below), [Nunes and Balding \(2010\)](#) propose a second stage to their analysis, which aims to assess the performance of a candidate set of summary statistics using a measure of posterior error. For example, when the true parameter vector, θ_{true} , is known, the authors suggest the root sum of squared errors (RSSE), given by

$$(8) \quad \text{RSSE} = \left(\sum_{i=1}^n w^i \|\theta^i - \theta_{\text{true}}\|^2 \right)^{1/2},$$

where the measure $\|\theta^i - \theta_{\text{true}}\|$ compares the components of θ on a suitable scale (and so some component-wise standardization may be required). Naturally, the true parameter value, θ_{true} , is unknown in practice. However, if the simulated summary statistics from the samples (θ^i, s^i) are treated as observed data, it is clear that $\theta_{\text{true}} = \theta^i$ for the posterior $p_{\text{ABC}}(\theta|s^i)$. As such, the RSSE can be easily computed with a leave-one-out technique.

As the subset of summary statistics that minimizes (8) will likely vary over observed data sets, s^i , [Nunes and Balding \(2010\)](#) propose minimizing the average RSSE over some number of simulated data sets which are close to the observed, s_{obs} . To avoid circularity, [Nunes and Balding \(2010\)](#) define these ‘‘close’’ data sets to be the $j = 1, \dots, n^*$ simulated data sets, $\{s^j\}$, that minimize $\|s_{\text{ME}}^j - s_{\text{ME}}\|$, where s_{ME}^j and s_{ME} are the

vectors of minimum entropy summary statistics computed via (7) from s^j and the observed summary statistics, s_{obs} , respectively. That is, the quantity

$$(9) \quad \overline{\text{RSSE}} = \frac{1}{n^*} \sum_{j=1}^{n^*} \text{RSSE}_j$$

is minimized (over subsets of summary statistics), where RSSE_j corresponds to (8) using the simulated data set s^j .

This approach is intuitive and is attractive because the second stage directly measures error in the posterior with respect to a known truth, θ_{true} , which is not typically considered in other ABC dimension reduction approaches, albeit at the extra computational expense of a two-stage procedure. A weakness of the first stage, however, is the assumption that addition of an informative statistic will reduce the entropy of the resulting posterior distribution. An example of when this does not occur is when the posterior distribution is diffuse with respect to the prior—for instance, if an overly precise prior is located in the distributional tails of the posterior (e.g., [Jeremiah et al., 2011](#)). In this case, attempting to include an informative additional statistic, s_k , can result in a distribution that is more diffuse than with s_k excluded. As such, the entropic approach is therefore mostly suited to models with relatively diffuse prior distributions. Another potential criticism of the first stage is that minimizing the entropy does not necessarily provide the *minimal* subset of sufficient statistics. This provides an argument for considering the mutual information between θ and s , rather than the entropy ([Barnes et al., 2012](#); see also [Filippi, Barnes and Stumpf, 2012](#)). However, it is clear that the overall approach of [Nunes and Balding \(2010\)](#) could easily be implemented with alternative first-stage selection criteria.

2.2.3 AIC and BIC criteria. Information criteria based on Akaike and Bayesian information are natural best subset selection techniques for summary statistic dimension reduction in ABC analyses. We introduce and develop these criteria in Section 3.1.

2.3 Projection Techniques

Selecting a best subset of summary statistics from $s = (s_1, \dots, s_p)$ suffers from the problem that it may require several statistics to provide the same information content as a single, highly informative statistic that was not specified in the initial set, s . To avoid this, projection techniques aim to combine the elements of s through linear or nonlinear transformations, in order to

construct a potentially much lower-dimensional set of highly informative statistics.

One of the main advantages of projection techniques is that, unlike best subset selection methods, they scale well with increasing numbers of summary statistics. They can handle large numbers of possibly uninformative summary statistics, in addition to accounting for high levels of interdependence and multicollinearity. A minor disadvantage of projection techniques is that the final sets of projected summary statistics typically (but not universally) lack interpretability. In addition, most projection methods require the specification of a hyperparameter that governs the number of projections to perform.

2.3.1 Partial least squares regression. Partial least squares regression seeks the orthogonal linear combinations of the explanatory variables which have high variance and high correlation with the response variable (e.g., [Boulesteix and Strimmer, 2007](#); [Vinzi et al., 2010](#); [Abdi and Williams, 2010](#)). [Wegmann, Leuenberger and Excoffier \(2009\)](#) proposed the use of partial least squares regression for dimension reduction in ABC, where the explanatory variables are the suitably (e.g., Box–Cox) transformed summary statistics, s , and the response variables is the parameter vector, θ .

The output of a partial least squares analysis is the set of k orthogonal components of the regression design matrix

$$(10) \quad X = \begin{pmatrix} 1 & s_1^1 & \cdots & s_p^1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & s_1^n & \cdots & s_p^n \end{pmatrix}$$

that are optimally correlated (in a specific sense) with θ . Here, s_j^i denotes the j th component of the i th simulated summary statistic, s^i . To choose the appropriate number of orthogonal components, [Wegmann, Leuenberger and Excoffier \(2009\)](#) examine the root mean square error of θ for each value of k , as estimated by a leave-one-out cross-validation strategy. For a fixed number of components, k , this corresponds to

$$(11) \quad \text{RMSE}_k = \left(\frac{1}{n} \sum_{i=1}^n \|\hat{m}_k^{-i}(s^i) - \theta^i\|^2 \right)^{1/2},$$

where $\hat{m}_k^{-i}(s)$ denotes the mean response of the partial least squares regression, estimated without the i th simulated summary statistic, s^i (e.g., [Mevik and Cedervik, 2004](#)). The optimal number of components is then chosen by inspection of the RMSE_k values, based on minimum gradient change arguments (e.g., [Mevik and Wehrens, 2007](#)).

A potential disadvantage of partial least squares regression, as performed by [Wegmann, Leuenberger and Excoffier \(2009\)](#), is that it aims to infer a global linear relationship between θ and s based on draws from the prior predictive distribution, $p(s|\theta)p(\theta)$. This may differ from the relationship observed in the region around $s = s_{\text{obs}}$, and as such may produce unsuitable orthogonal components as a result. A workaround for this would be to follow [Fearnhead and Prangle \(2012\)](#) (see Section 2.3.3) and elicit the relationship between θ and s based on samples from a truncated prior $(\theta^i, s^i) \sim p(s|\theta)p(\theta)I(\theta \in \Theta^R)$, where $\Theta^R \subset \Theta$ restricts the samples, θ^i , to regions of significant posterior density. One simple way to identify such a region is through a pilot ABC analysis ([Fearnhead and Prangle, 2012](#)).

2.3.2 Neural networks. In the regression setting, feed-forward neural networks can be considered as a nonlinear generalization of the partial least squares regression technique described above. Blum and François (2010) proposed the neural network as a machine learning approach to dimension reduction by estimating the conditional mean and variance functions, $m(\cdot)$ and $\sigma^2(\cdot)$ in the nonlinear, heteroscedastic regression adjustment model (4)—see Section 2.1.

The neural network reduces the dimension of the summary statistics to $H < p$, using H hidden units in the network, z_1, \dots, z_H , defined as

$$(12) \quad z_j = h\left(\sum_{k=1}^p \omega_{jk}^{(1)} s_k + \omega_{j0}^{(1)}\right)$$

for $j = 1, \dots, H$. The $\omega_{jk}^{(1)}$ terms are the weights of the first layer of the neural network, and $h(\cdot)$ is a nonlinear function, typically the logistic function. The reduced and nonlinearly transformed summary statistics of the hidden units, z_j , are then combined through the regression function of the neural network

$$(13) \quad m(s) = g\left(\sum_{j=1}^H \omega_j^{(2)} z_j + \omega_0^{(2)}\right),$$

where $\omega_j^{(2)}$ denotes the weights of the second layer of the neural network and $g(\cdot)$ is a link function. A similar neural network is used to model $\log \sigma^2(s)$ (e.g., [Nix and Weigend, 1995](#)), with the possibility of allowing for a different number of hidden units to estimate heteroscedasticity in the regression adjustment compared to that in the mean function $m(s)$.

Rather than dynamically determining the number of hidden units H , [Blum and François \(2010\)](#) propose to specify a fixed value, such as $H = q$ where $q = \dim(\theta)$

is the number of parameters to infer. The weights of the neural network are then obtained by minimizing the regularized least-squares criterion

$$\sum_{i=1}^n w^i \|m(s^i) - \theta^i\|^2 + \lambda \|\omega\|^2,$$

where ω is the vector of all weights in the neural network model for $m(s)$, $w^i = K_\epsilon(\|s^i - s_{\text{obs}}\|)$ is the weight of the sample $(\theta^i, s^i) \sim p(s|\theta)p(\theta)$, and $\lambda > 0$ denotes the regularization parameter (termed the weight-decay parameter for neural networks). The idea of regularization is to shrink the weights toward zero so that only informative summary statistics contribute in the models (12) and (13) for $m(s)$. Following the estimation of $m(s)$, a similar regularization criterion is used to estimate $\log \sigma^2(s)$. Both mean and variance functions can then be used in the regression adjustment of equation (5).

2.3.3 Minimum expected posterior loss. [Fearnhead and Prangle \(2012\)](#) proposed a decision-theoretic dimension reduction method with a slightly different aim to previous dimension reduction approaches. Here, rather than constructing appropriate summary statistics to ensure that $p_{\text{ABC}}(\theta|s_{\text{obs}}) \approx p(\theta|y_{\text{obs}})$ is a good approximation, $p_{\text{ABC}}(\theta|s_{\text{obs}})$ is alternatively required to be a good approximation in terms of the accuracy of specified functions of the model parameters. In particular, assuming that interest is in point estimates of the model parameters, if θ_{true} denotes the true parameter value and $\hat{\theta}$ an estimate, then [Fearnhead and Prangle \(2012\)](#) propose to choose those summary statistics that minimize the quadratic loss

$$L(\theta_{\text{true}}, \hat{\theta}) = (\theta_{\text{true}} - \hat{\theta})^\top A (\theta_{\text{true}} - \hat{\theta})$$

for some $p \times p$ positive-definite matrix A . This loss is minimized for $s_{\text{obs}} = E_{p(\theta|y_{\text{obs}})}(\theta)$, the true posterior mean.

To estimate $E_{p(\theta|y)}(\theta)$, [Fearnhead and Prangle \(2012\)](#) propose least squares regression models for the $k = 1, \dots, q$ model parameters, $(\theta_1, \dots, \theta_q)$, given by

$$(14) \quad \theta_k^i = E_{p(\theta|y)}(\theta_k) + \eta_k^i = \alpha_k + \beta_k^\top f(s^i) + \eta_k^i,$$

where $(\theta^i, s^i) \sim p(s|\theta)p(\theta)$ are draws from the prior predictive distribution, α_k and β_k are unknown regression parameters to be estimated, and η_k^i denotes a zero-mean noise process. Here $f(s)$ is a vector of potentially nonlinear transformations of the data (i.e., of the original summary statistics). For example, in one application, [Fearnhead and Prangle \(2012\)](#) use the polynomial basis functions $f(s) = (s, s^2, s^3, s^4)$, that is,

a vector of length $4p$, where $p = \dim(s)$ is the number of elements in s , consisting of the first four powers of each element of s . The choice of $f(s)$ can be based on standard diagnostics of regression fit, such as BIC. If the prior $\pi(\theta)$ is diffuse with respect to the posterior, then one may estimate the regression model (14) based on samples from a truncated prior $(\theta^i, s^i) \sim p(s|\theta)p(\theta)I(\theta \in \Theta^R)$, where $\Theta^R \subset \Theta$ restricts the samples, θ^i , to regions of significant posterior density (e.g., via a pilot ABC analysis). Clearly, more sophisticated alternatives to least squares regression may be used.

After fitting equation (14), the new, single summary statistic for the parameter θ_k is $\hat{\beta}_k^\top f(s)$, where $\hat{\beta}_k$ denotes the least squares estimate of β_k . The resulting q -dimensional vector of new summary statistics is then used in a standard ABC analysis. Fearnhead and Prangle (2012) show that these new statistics can lead to posterior inferences that considerably outperform inferences based on the original statistics, s . Nott, Fan and Sisson (2012) demonstrate that these summary statistics can be viewed as Bayes linear estimates of the posterior mean.

2.4 Regularization Approaches

Regularization approaches aim to reduce overfitting in a model by penalizing model complexity. A simple example where overfitting can occur in ABC is the standard regression adjustment (Beaumont, Zhang and Balding, 2002; Section 2.1), where there is a risk of over adjusting the parameters, θ^i , in the direction of uninformative summary statistics via (3). Regularization is used as part of the estimation of the neural network weights in the projection technique proposed by Blum and François (2010) (see Section 2.3.2). As such, the regression adjustment of Beaumont, Zhang and Balding (2002) is a procedure that could greatly benefit from the inclusion of regularization techniques. We introduce the ridge regression adjustment to ABC in Section 3.2.

2.5 Other Methods

There are a number of alternative approaches to dimension reduction for ABC, including methods that aim to circumvent the dimensionality issue, that we do not include in our comparative analysis (Section 4). Drovandi, Pettitt and Faddy (2011) proposed to adopt ideas from indirect inference (e.g., Heggland and Frigessi, 2004) as a means to identify summary statistics for an ABC analysis. This involves specification of a model $\tilde{p}(\cdot|\tilde{\theta})$ which is similar to $p(\cdot|\theta)$, but which

is computationally tractable. The idea is that estimates of $\tilde{\theta}$ under $\tilde{p}(\cdot|\tilde{\theta})$, such as maximum likelihood estimates or posterior means, are likely to be informative about θ if $p(\cdot|\theta)$ and $\tilde{p}(\cdot|\tilde{\theta})$ are sufficiently similar. This approach can be considered similar in spirit to that of Fearnhead and Prangle (2012) which uses estimated posterior means under a pilot ABC analysis (see Section 2.3.3). Blum (2010b) proposed a Bayesian criterion related to the BIC (see Section 3.1) as a best subset selection procedure. The idea is to implement a Bayesian analysis of the standard regression adjustment model (3). The criterion, called the *evidence* approximation, seeks the best subset of summary statistics to regress the parameter θ . In comparison to the BIC, the evidence criterion is attractive because it contains no approximation in its derivation. However, the downside is that its computation requires the tuning of the Bayesian linear regression hyperparameters. Additionally, Aeschbacher, Beaumont and Futschik (2012) proposed to use boosting for choosing summary statistics and Jung and Marjoram (2011) developed a genetic algorithm that weights the summary statistics so that individual statistics do not contribute equally to the comparisons between observations and simulations. The aim is that the uninformative summary statistics should ideally have negligible weights.

Finally, a number of recent ABC modeling approaches have attempted to find ways of accurately handling the full vector of initial statistics, s [or the full data set, $s = S(y) = y$], thereby avoiding the need to perform dimension reduction. Bonassi, You and West (2011) propose fitting a $(p + q)$ -dimensional mixture of Gaussian distributions to the sample $(\theta^i, s^i) \sim p(s|\theta)p(\theta)$, $i = 1, \dots, n$, and then finding the distribution of $\theta|s_{\text{obs}}$ by conditioning on observing $s = s_{\text{obs}}$. This approach potentially requires a large number of mixture components to accurately model the joint density when $(p + q)$ is large. Fan, Nott and Sisson (2012) suggest using an approximation to $p(s|\theta)$ by approximating each marginal likelihood function, $p(s_i|\theta)$, using a mixture of experts model, where the weights, mean and variance of each mixture component is allowed to depend on θ , and then inducing dependence between these marginals using a mixture of multivariate Gaussian distributions. This approach requires continuous summary statistics for the mixture regression and is practically useful for moderate p (i.e., hundreds of summary statistics). Writing $y = (y_1, \dots, y_p)$, Barthelmé and Chopin (2011) propose to factorize the likelihood as $p(y|\theta) =$

$\prod_i p(y_i|y_{1:i-1}, \theta)$ and construct an ABC approximation of each component in turn [i.e., $p_{\text{ABC}}(y_i|y_{1:i-1}) = \int K_\epsilon(\|y_i - y_{\text{obs},i}\|) p(y_i|y_{1:i-1}, \theta) dy_i$] with computation performed using an expectation-propagation algorithm (Minka, 2001). This approach, while potentially fast and accurate, assumes that conditional simulation of $y_i \sim p(y_i|y_{1:i-1}, \theta)$ is available for $i = 1, \dots, n$, and so is not suitable for all models and analyses. Last, Jasra et al. (2012) exploit the structure of hidden Markov models to perform an iterative sequence of ABC analyses, each using only a single data point in each analysis, and Nakagome, Fukumizu and Mano (2012) propose a novel approach to post-processing ABC importance sampling output whose convergence rate is claimed to avoid the curse of dimensionality.

3. NEW DIMENSION REDUCTION METHODS

In this section we introduce two new dimension reduction criteria for ABC methods. The first is a best subset selection procedure deriving from AIC and BIC criteria, constructed under implementation of the local linear model of equation (2) (Beaumont, Zhang and Balding, 2002). A similar idea was proposed and tested for a Gaussian model by Sedki and Pudlo (2012). The second is a modification to the fitting of (2) by considering ridge regression instead of least squares regression. Both of these methods are now implemented in the freely available R package `abc` (Csilléry, François and Blum, 2012).

3.1 AIC and BIC Criteria

Akaike information criterion (AIC) and Bayesian information criterion (BIC) provide a measure of the relative goodness of fit of a statistical model. Each can be expressed as the sum of the maximized log-likelihood that measures the fit of the model to the data, and a penalty for model complexity (Akaike, 1974; Schwarz, 1978). While evaluation of $\log p(y_{\text{obs}}|\hat{\theta}_{\text{mle}})$ or $\log p(s_{\text{obs}}|\hat{\theta}_{\text{mle}})$ is unavailable in the ABC framework and determination of the maximum likelihood estimator, $\hat{\theta}_{\text{mle}}$, is challenging, a simple and tractable likelihood function is available though the local-linear regression model of equation (2) (Section 2.1).

Specifically, we consider the local linear regression model equation (2) of Beaumont, Zhang and Balding (2002) for each parameter $\theta_1, \dots, \theta_q$ and assume independent Gaussian errors, $e^j \sim N(0, \sigma_j^2)$, for $j = 1, \dots, q$. Then the AIC becomes

$$(15) \quad \text{AIC} = \tilde{n} \log \prod_{j=1}^q \hat{\sigma}_j^2 + 2d,$$

where $d = q(p + 1)$ is the number of estimated regression parameters and \tilde{n} is the *effective* number of simulations used in the local-linear regression model, which we define as $\tilde{n} = \sum_{i=1}^n I(w^i > 0)$ when the kernel K_ϵ has compact support. Alternative definitions of the effective number of simulations, such as $c \sum_{i=1}^n w^i$ for some $c > 0$, can be on an arbitrary scale, since the least squares regression solution is insensitive to the scale of the weights. For any fixed value of c , the value of $c \sum_{i=1}^n w^i$ will decrease as $p = \dim(s)$ increases so that it will artificially favor larger numbers of (even uninformative) summary statistics. Our definition of \tilde{n} guarantees that the AIC scores are comparable for different subsets of summary statistics. A downside is that this definition of \tilde{n} is only suitable for kernels, K_ϵ , with a compact support.

In equation (15), $\hat{\sigma}_j^2$ is defined as the weighted mean of squared residuals for the regression of θ_j and is given by

$$\hat{\sigma}_j^2 = \frac{\sum_{i=1}^n w^i [\theta_j^i - \hat{m}_j(s^i)]^2}{\sum_{i=1}^n w^i},$$

where θ_j^i is the j th component of θ^i and $\hat{m}_j(s)$ denotes the estimate of the mean function $m_j(s) = \mathbb{E}[\theta_j|s]$. For small sample sizes, the corrected AIC, the so-called AICc, is given by replacing d in (15) by $d(d + 1)/(\tilde{n} - d - 1)$ (Hurvich and Tsai, 1989). In the same manner the BIC can be defined as

$$(16) \quad \text{BIC} = \tilde{n} \log \prod_{j=1}^q \hat{\sigma}_j^2 + d \log \tilde{n}.$$

Alternative penalty terms involving the hat matrix of the regression could also be used in the above (e.g., Hurvich, Simonoff and Tsai, 1998; Irizarry, 2001; Konishi, Ando and Imoto, 2004).

It is instructive to note that in using the linear regression adjustment (3), the above information criteria may be expressed as

$$\text{xIC} = \tilde{n} \log \prod_{j=1}^q \text{Var}(\theta_j^*) + \text{penalty term},$$

where θ_j^* is the j th element of the regression adjusted vector $\theta^* = (\theta_1^*, \dots, \theta_q^*)$. As such, up to the penalty terms, both AIC and BIC seek the combination of summary statistics that minimizes the product of the marginal variances of the adjusted posterior sample. Similarly to the entropy criterion of Nunes and Balding (2010) (see Section 2.2.2), these information criterion will select those summary statistics that maximize the

precision of the posterior distribution, $p_{\text{ABC}}(\theta|s_{\text{obs}})$. However, unlike Nunes and Balding (2010), this precision is traded off by a penalty for model complexity.

A rationale for the construction of AIC and BIC in this manner is that the summary statistics that should be included within an ABC analysis are those which are good predictors of θ . However, an obvious requirement for AIC or BIC to identify an informative statistic is that the statistic varies (with θ) within the local range of the regression model. If a statistic is informative outside of this range, but uninformative within it, it will not be identified as informative under these criteria.

3.2 Regularization via Ridge Regression

As described in Section 2.1, the local-linear regression adjustment of Beaumont, Zhang and Balding (2002) fits the linear model

$$\theta^i = \alpha + \beta^\top s^i + e^i$$

based on the prior predictive samples $(\theta^i, s^i) \sim p(s|\theta)p(\theta)$ and with regression weights given by $w^i = K_\epsilon(\|s^i - s_{\text{obs}}\|)$. (As before, we describe the case where θ is univariate for notational simplicity and clarity of exposition, but the approach outlined below can be readily implemented for each component of a multivariate θ .) However, in fitting the model by minimizing the weighted least squares criteria, $\sum_{i=1}^n w^i \|\alpha - \beta^\top s^i - \theta^i\|^2$, there is a risk of over-adjustment by adjusting the parameter values via (3) in the direction of uninformative summary statistics.

To avoid this, implicit dimension reduction within the regression framework can be performed by alternatively minimizing the regularized weighted sum of squares (Hoerl and Kennard, 1970)

$$(17) \quad \sum_{i=1}^n w^i \|\theta^i - (\alpha + \beta^\top s^i)\|^2 + \lambda \|\beta\|^2$$

with regularization parameter $\lambda > 0$. As with the regularization component within the neural network model of Blum and François (2010) (Section 2.3.2), with ridge regression the risk of over-adjustment is reduced because the regression coefficients, β , are shrunk toward zero by imposing a penalty on their magnitudes. Note that while we consider ridge regression here, a number of alternative regularization procedures could be implemented, such as the Lasso method.

An additional advantage of ridge regression is that standard least squares estimates, $(\hat{\alpha}_{\text{LS}}, \hat{\beta}_{\text{LS}})^\top = (X^\top \cdot WX)^{-1} X^\top W\Theta$, are not guaranteed to have a unique solution. Here X is a $n \times (p + 1)$ design matrix given

in equation (10), $\Theta = (\theta^1, \dots, \theta^n)$ is the $n \times 1$ column vector of sampled θ^i , and $W = \text{diag}(w^1, \dots, w^n)$ is an $n \times n$ diagonal matrix of weights. The lack of a unique solution can arise through multicollinearity of the summary statistics, which can result in singularity of the matrix $X^\top WX$. In contrast, minimization of the regularized weighted sum of squares (17) always has a unique solution, provided that $\lambda > 0$. This solution is given by $(\hat{\alpha}_{\text{ridge}}, \hat{\beta}_{\text{ridge}})^\top = (X^\top WX + \lambda I_p)^{-1} X^\top W\Theta$, where I_p denotes the $p \times p$ identity matrix. There are several approaches for dealing with the regularization parameter λ , including cross-validation and generalized cross-validation to identify an optimal value of λ (Golub, Heath and Wahba, 1979), as well as averaging the regularized estimates $(\hat{\alpha}_{\text{ridge}}, \hat{\beta}_{\text{ridge}})^\top$ obtained for different values of λ (Taniguchi and Tresp, 1997).

4. A COMPARATIVE ANALYSIS

We now provide a comparative analysis of the previously described methods of dimension reduction within the context of three previously studied analyses in the ABC literature. Specifically, this includes the analysis of a coalescent model with recombination (Joyce and Marjoram, 2008), an evaluation of the evolutionary fitness cost of mutation in drug-resistant tuberculosis (Luciani et al., 2009) and an assessment of the number and size-distribution of particle inclusions in the production of clean steels (Bortot, Coles and Sisson, 2007).

Each analysis is based on $n = 1,000,000$ simulations where the parameter θ is drawn from the prior distribution $p(\theta)$. The performance of each method is measured through the $\overline{\text{RSSE}}$ criterion (9) following Nunes and Balding (2010), based on the same randomly selected subset of $n^* = 100$ samples $(\theta^i, s^i) = (\theta_{\text{true}}, s_{\text{obs}})$ as ‘‘observed’’ data sets. When evaluating the RSSE error measure of equation (8), we give a weight $w^i = 1$ for the accepted simulations and a weight of 0 otherwise. As the value of the RSSE (8) depends on the scale of each parameter, we standardize the parameters in each example by dividing the parameter values by the standard deviation obtained from the $n = 1,000,000$ simulations (with the exception of the first example, where the parameters are on similar scales). For comparative ease, and to provide a performance baseline for each example, all $\overline{\text{RSSE}}$ results are presented as relative to the $\overline{\text{RSSE}}$ obtained when using the maximal vector of summary statistics and no regression adjustment. In this manner, a relative $\overline{\text{RSSE}}$

of $x/-x$ denotes an $x\%$ worsening/improvement over the baseline score.

Within each ABC analysis, we use Euclidean distance within an Epanechnikov kernel $K_\epsilon(\|s - s_{\text{obs}}\|)$. The Euclidean distances are computed after standardizing the summary statistics with a robust estimate of the standard deviation (the mean absolute deviation). The kernel scale parameter, ϵ , is determined as the value at which exactly 1% of the simulations, (θ^i, s^i) , have nonzero weight. This yields exactly $\tilde{n} = 10,000$ simulations that form the final sample from each posterior. To perform the method of Fearnhead and Prangle (2012), a randomly chosen 10% of the n simulations were used to fit the regression model that determines the choice of summary statistics, with the remaining 90% used for the ABC analysis. The final ABC sample size $\tilde{n} = 10,000$ was kept equal to the other methods by slightly adjusting the scale parameter, ϵ . In addition, for the method of Fearnhead and Prangle (2012), following exploratory analyses, the regression model (14) was fitted using $f(s) = (s, s^2, s^3, s^4)$ for examples 1 and 2 (as described in Section 2.3.3) and using $f(s) = (\log s, [\log s]^2, [\log s]^3, [\log s]^4)$ for example 3, always resulting in $4 \times p$ independent variables in the regression model of equation (14).

When using neural networks or ridge regression to estimate the conditional mean and variance, $m(s)$ and $\sigma^2(s)$, we take the pointwise median of the estimated functions obtained with the regularization parameters $\lambda = 10^{-3}, 10^{-2}$ and 10^{-1} . These values of λ assume that the summary statistics and the parameters have been standardized before fitting the regression function (Ripley, 1994). However, because the optimization procedure for neural networks (the R function `nnet`) only finds local optima, in this case we take the pointwise median of ten estimated functions, with each optimization initialized from a different random starting point, and randomly choosing the regularization parameter with equal probability from the above values (see Taniguchi and Tresp, 1997).

4.1 Example 1: A Coalescent Analysis

This model was previously considered by Joyce and Marjoram (2008) and Nunes and Balding (2010), each while proposing their respective ABC dimension reduction strategies (see Sections 2.2.1 and 2.2.2). The analysis focuses on joint estimation of the scaled mutation rate, $\tilde{\theta}$, and the scaled recombination rate, ρ , in a coalescent model with recombination (Nordborg,

2007). Under this model, 5001 base pair DNA sequences for 50 individuals are generated from the coalescent model, with recombination, under the infinite-sites mutation model, using the software `ms` (Hudson, 2002). The initial summary statistics, $s = (s_1, \dots, s_6)$, are the number of segregating sites (s_1), the pairwise mean number of nucleotidic differences (s_2), the mean R^2 across pairs separated by $<10\%$ of the simulated genomic regions (s_3), the number of distinct haplotypes (s_4), the frequency of the most common haplotype (s_5) and the number of singleton haplotypes (s_6).

We first examine the performance of ABC without using dimension reduction techniques. For different parameter combinations, $\tilde{\theta}, \rho$ and $(\tilde{\theta}, \rho)$, we compute the relative $\overline{\text{RSSSE}}$ obtained with a single optimal summary statistic and the relative $\overline{\text{RSSSE}}$ obtained when using all six population genetic statistics (s_1 – s_6) (Table 1). When estimating $\tilde{\theta}$ only, we find that using only the number of segregating sites (s_1) provides lower relative $\overline{\text{RSSSE}}$ than when including all 6 summary statistics even when performing regression adjustment. For all other parameter combinations, using a single statistic produces substantially worse than the rejection algorithm with all summary statistics. For all inferences [i.e., of $\tilde{\theta}, \rho$ and $(\tilde{\theta}, \rho)$ jointly], regression adjustments generally improve the inference when using all six summary statistics, which is consistent with previous results (Nunes and Balding, 2010). The only exception is when jointly estimating $(\tilde{\theta}, \rho)$, where homoscedastic linear adjustment neither decreases nor increases the error obtained with the pure rejection algorithm.

Next, we investigate the performance of each dimension reduction technique. Table 2 and Figure 1 show the relative $\overline{\text{RSSSE}}$ obtained under each dimension reduction method for each parameter combination and under heteroscedastic regression adjustment. For all three examples, more complete tables that contain the results obtained with no regression adjustment and homoscedastic adjustment can be found in the supplementary information to this article (Blum et al., 2013).

The performance achieved with AIC, AICc or BIC is comparable to (i.e., the same or slightly better than) the result obtained when including all six population genetic statistics. When using the ϵ -sufficiency criterion, we find that the performance is improved for the inference on $\tilde{\theta}$ only. The only best subset selection method for dimension reduction that substantially and uniformly improves the performance of ABC posterior estimates is the entropy-based approach. For the projection techniques, all methods (partial least squares,

TABLE 1

Relative $\overline{RSS\bar{E}}$ for examples 1 and 2. The leftmost column shows the minimal $\overline{RSS\bar{E}}$ when considering only one summary statistic (with no regression adjustment). Rightmost columns show relative $\overline{RSS\bar{E}}$ using all summary statistics under no, homoscedastic and heteroscedastic regression adjustment. All $\overline{RSS\bar{E}}$ are relative to the $\overline{RSS\bar{E}}$ obtained when using no regression adjustment with all summary statistics. The score of the best method in each analysis (row) is emphasised in boldface

		One optimal statistic (no adj.)	All summary statistics		
			No adj.	Homo adj.	Hetero adj.
Example 1	$\tilde{\theta}$	-7 (s_1)	0	-3	-3
	ρ	9 (s_5)	0	-5	-4
	$(\tilde{\theta}, \rho)$	7 (s_1)	0	0	-7
Example 2	α	6	0	-3	-3
	c	-7	0	-5	-5
	ρ	-9	0	-8	-8
	μ	-14	0	-5	-6
	(α, c, ρ, μ)	5	0	-4	-4

neural nets and minimum expected posterior loss) outperform the adjustment method based on all six population genetics statistics, with a large performance advantage for partial least squares when estimating $(\tilde{\theta}, \rho)$ jointly. By contrast, ridge regression provides no improvement over the standard regression adjustment (the “All” column).

Based on these results, a loose performance ranking of the dimension reduction methods can be obtained by computing, for each method, the mean (relative) $\overline{RSS\bar{E}}$ over all parameter combinations $\tilde{\theta}, \rho$ and $(\tilde{\theta}, \rho)$ using the heteroscedastic adjustment. The worst performers were ridge regression and the ε -sufficiency criterion (with a mean relative $\overline{RSS\bar{E}}$ of -3%). These are

TABLE 2

Relative $\overline{RSS\bar{E}}$ for examples 1–3 for different parameter combinations using each method of dimension reduction, and under heteroscedastic regression adjustment. Columns denote no dimension reduction (All), BIC, AIC, AICc, the ε -sufficiency criterion (ε -suff), the two-stage entropy procedure (Ent), partial least squares (PLS), neural networks (NNet), minimum expected posterior loss (Loss) and ridge regression (Ridge). All $\overline{RSS\bar{E}}$ are relative to the $\overline{RSS\bar{E}}$ obtained when using no regression adjustment with all summary statistics. The score of the best method in each analysis (row) is emphasized in boldface

	Best subset selection					Projection techniques			Regularization	
	All	BIC	AIC	AICc	ε -suff	Ent	PLS	NNet ¹	Loss	Ridge ¹
$\tilde{\theta}$	-3	-5	-5	-5	-6	-11	-6	-4	-7	1
ρ	-4	-6	-6	-6	0	-12	-7	-8	-7	-3
$(\tilde{\theta}, \rho)$	-7	-7	-7	-7	-	-24	-16	-7	-6	-6
α	-3	-15	-15	-15	0	-17	-13	-15	-17	-15
c	-5	-15	-15	-15	-8	-15	-8	-12	-9	-9
ρ	-8	-16	-16	-16	-8	-16	1	-12	-9	-10
μ	-6	-18	-18	-18	-8	-13	-10	-13	-12	-12
(α, c, ρ, μ)	-4	-19	-19	-19	-	-13	-10	-9	-12	-11
τ	-49	-47	-47	-48	-19	-52	-22	-20/-42	-75	-48/-48
σ	-45	-46	-47	-46	-15	-50	-15	-21/-37	-56	-43/-43
ξ	-27	-29	-29	-28	-13	-32	-28	-7/-41	-41	-26/ -44
(τ, σ, ξ)	-39	-39	-40	-39	-	-42	-11	-4/-38	-60	-39/-32

¹For the third example, the first value is found by integrating out the regularization parameter, whereas the second one is found by choosing an optimal regularization parameter with cross-validation. In examples 1 and 2, integration over the regularization parameter is performed.

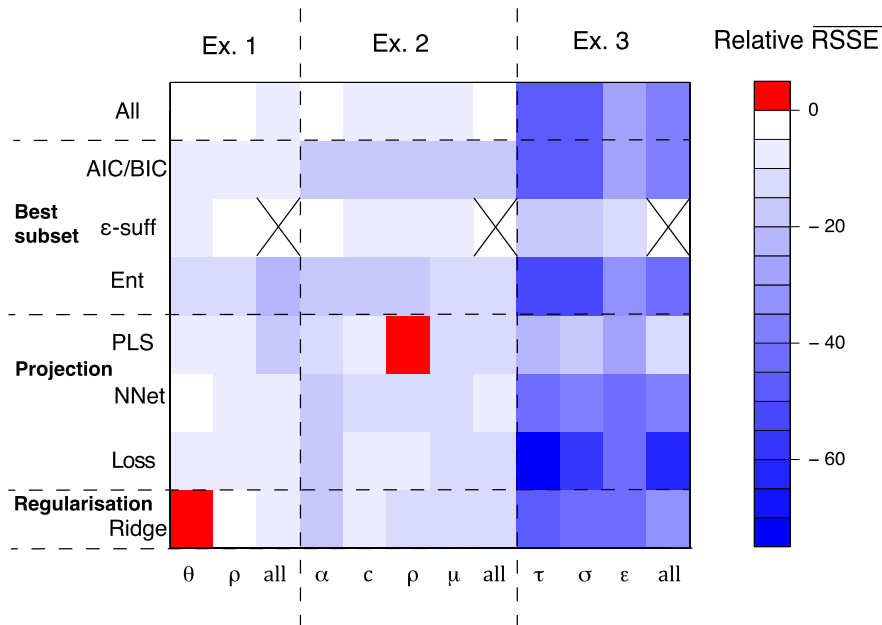


FIG. 1. Relative \overline{RSSE} for the different methods of dimension reduction in the three examples. All \overline{RSSE} are relative to the \overline{RSSE} obtained when using no regression adjustment with all summary statistics. Methods of dimension reduction include no dimension reduction (All), AIC/BIC, the ϵ -sufficiency criterion (ϵ -suff), the two-stage entropy procedure (Ent), partial least squares (PLS), neural networks (NNet), minimum expected posterior loss (Loss) and ridge regression (Ridge). The crosses correspond to situations for which there is no result available.

followed by the standard regression adjustment with all summary statistics (-5%) and the AIC/BIC, neural nets and the posterior loss method (-6%). The best performing methods are partial least squares (-10%) and the two-stage entropy-based procedure (-16%).

4.2 Example 2: The Fitness Cost of Drug Resistant Tuberculosis

We now consider an example of Markov processes for epidemiological modeling. If a pathogen, such as *Mycobacterium tuberculosis*, mutates to gain an evolutionary advantage, such as antibiotic resistance, it is biologically plausible that this mutation will come at a cost to the pathogen's relative fitness. Based on a stochastic model to describe the transmission and evolutionary dynamics of *Mycobacterium tuberculosis*, and based on incidence and genotypic data of the IS6110 marker, Luciani et al. (2009) estimated the posterior distribution of the pathogen's transmission cost and relative fitness. The model contained $q = 4$ free parameters: the transmission rate, α , the transmission cost of drug resistant strains, c , the rate of evolution of resistance, ρ , and the mutation rate of the IS6110 marker, μ .

Luciani et al. (2009) summarized information generated from the stochastic model through $p = 11$ summary statistics. These statistics were expertly elicited

as quantities that were expected to be informative for one or more model parameters, and included the number of distinct genotypes in the sample, gene diversity for sensitive and resistant cases, the proportion of resistant cases and measures of the degree of clustering of genotypes, etc. It is considered likely that there is dependence and potentially replicate information within these statistics.

As before, we examine the relative performance of the statistics without using dimension reduction techniques. Table 1 shows that for the univariate analysis of c , ρ or μ , performing rejection sampling ABC with a single, well-chosen summary statistic can provide an improved performance over a similar analysis using all 11 summary statistics, under any form of regression adjustment. In particular, the proportion of isolates that are drug resistant is the individual statistic which is most informative to estimate c (with a relative \overline{RSSE} of -7%) and ρ (-9%). For the marker mutation rate, μ , the most informative statistic is the number of distinct genotypes, with a relative \overline{RSSE} of -14% . Conversely, an analysis using all summary statistics with a regression adjustment offers the best inferential performance for α alone, or for (α, c, ρ, μ) . These results provide support for recent arguments in favor of "marginal regression adjustments" (Nott et al., 2013), whereby the

univariate marginal distributions of a full multivariate ABC analysis are replaced by separately estimated marginal distributions using only statistics relevant for each parameter. Here, more precisely estimated margins can improve the accuracy of the multivariate posterior sample, beyond the initial analysis.

The performance results of each dimension reduction method are shown in Table 2 and Figure 1. In contrast with the previous example, here the use of the AIC/BIC criteria can substantially decrease posterior errors. For example, compared to the linear adjustment of all 11 parameters, which produces a mean relative $\overline{\text{RSSE}}$ between -3% and -8% depending on the parameter (Table 2), using the AIC/BIC criteria results in a relative $\overline{\text{RSSE}}$ of between -15% and -19% . The ε -sufficiency criterion produces more equivocal results, however, as the error is sometimes increased with respect to baseline performance (e.g., $+6\%$ when estimating α with homoscedastic adjustment) and sometimes reduced (e.g., -8% for c , ρ and θ with heteroscedastic adjustment). As with the previous example, the entropy criterion provides a clear improvement to the ABC posterior, and this improvement is almost comparable to that produced by AIC/BIC. Finally, the projection and regularization methods mostly all provide comparable and substantive improvements compared to the baseline error, with only partial least squares producing more equivocal results (e.g., $+1\%$ when estimating ρ).

Based on these results, the loose performance ranking of the dimension reduction methods determines the worst performers to be the standard least squares regression adjustment (with a mean relative $\overline{\text{RSSE}}$ of -5%), the ε -sufficiency approach (-6%) and partial least squares (-8%). These are followed by ridge regression (-11%), neural networks and the posterior loss method (-12%). The best performing methods for this analysis are the two-stage entropy-based procedure (-15%) and the AIC/BIC criteria (-17%).

In this example, it is interesting to compare the performance of the standard linear regression adjustment of all 11 summary statistics (mean relative $\overline{\text{RSSE}}$ of -5%) with that of the ridge regression equivalent (mean relative $\overline{\text{RSSE}}$ of -11%). The increase in performance with ridge regression may be attributed to its more robust handling of multicollinearity of the summary statistics than under the standard regression adjustment. To see this, Figure 2 illustrates the relationship between the relative $\overline{\text{RSSE}}$ (again, relative to using all summary statistics and no regression adjustment) and the condition number of the matrix $X^T W X$, for

both the standard regression (top panel) and ridge regression (bottom panel) adjustments based on inference for (α, c, ρ, μ) . The condition number of $X^T W X$ is given by $\kappa = \sqrt{\lambda_{\max}/\lambda_{\min}}$, where λ_{\max} and λ_{\min} are the largest and smallest eigenvalues of $X^T W X$. Extremely large condition numbers are evidence for multicollinearity.

Figure 2 demonstrates that for large values of the condition number (e.g., for $\kappa > 10^8$), the least-squares-based regression adjustment clearly performs very poorly. The region of $\kappa > 10^8$ corresponds to almost 5% of all simulations, and for these cases the relative error is hugely increased (w.r.t. rejection) to anywhere between 5% and 200%. In contrast, for ridge regression, the relative errors corresponding to $\kappa > 10^8$ are not larger than the errors obtained for nonextreme condition numbers. This analysis clearly illustrates that, unlike ridge regression, the standard least squares regression adjustment can perform particularly poorly when there is multicollinearity between the summary statistics.

In terms of the original analysis of Luciani et al. (2009) which used all eleven summary statistics with no regression adjustment (although with a very low value for ϵ), the above results indicate that a more efficient analysis may have been achieved by using a suitable dimension reduction technique.

4.3 Example 3: Quality Control in the Production of Clean Steels

Our final example concerns the statistical modeling of extreme values. In the production of clean steels, the occurrence of microscopic imperfections (termed *inclusions*) is unavoidable. The strength of a clean steel block is largely dependent on the size of the largest inclusion. Bortot, Coles and Sisson (2007) considered an extreme value twist on the standard stereological problem (e.g., Baddeley and Jensen, 2004), whereby inference is required on the size and number of 3-dimensional inclusions, based on data obtained from those inclusions that intersect with a 2-dimensional slice. The model assumes a Poisson point process of inclusion locations with rate parameter $\tau > 0$ and that the distribution of inclusion size exceedances above a measurement threshold of $5\mu\text{m}$ are drawn from a generalized Pareto distribution with scale and shape parameters $\sigma > 0$ and ξ , following standard extreme value theory arguments (e.g., Coles, 2001).

The observed data consist of 112 cross-sectional inclusion diameters measured above $5\mu\text{m}$. The summary

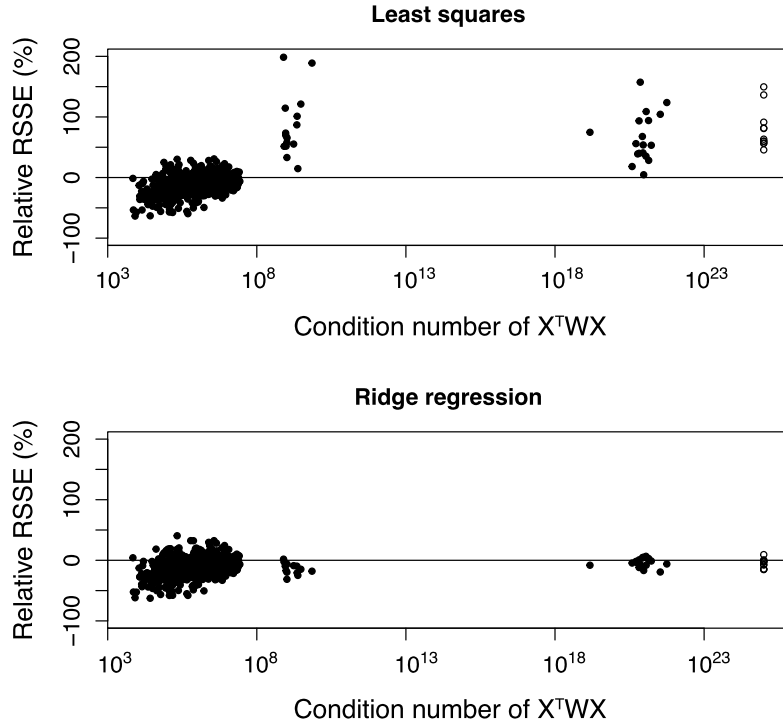


FIG. 2. Scatterplots of relative RSSE versus the condition number of the matrix $X^T W X$ for linear least squares (top) and ridge (bottom) regression adjustments. Points are based on joint inference for (α, c, ρ, μ) in example 2 using 1000 randomly selected vectors of summary statistics, s^i , as “observed” data. When the minimum eigenvalue, λ_{\min} , is zero, the (infinite) condition number is arbitrarily set to be 10^{25} for visual clarity (open circles on the scatterplot).

statistics thereby comprise 112 equally spaced quantiles of the cross-sectional diameters, in addition to the number of inclusions observed, yielding $p = 113$ summary statistics in total. The ordering of the summary statistics creates strong dependences between them, a fact which can be exploited by dimension reduction techniques. Bortot, Coles and Sisson (2007) considered two models based on spherical or ellipsoidal shaped inclusions. Our analysis here focuses on the ellipsoidal model.

By construction, the large number (2^{113}) of possible combinations of summary statistics means that the best subset selection methods are strictly not practicable for this analysis, unless the number of summary statistics is reduced further a priori. In order to facilitate at least some comparison with the other dimension reduction approaches, for the best subset selection methods *only*, we consider six candidate subsets. Each subset consists of the number of observed inclusions in addition to 5, 10, 20, 50, 75 or 112 empirical quantiles of the inclusion size exceedances (the latter corresponds to the complete set of summary statistics). Due to the extreme value nature of this analysis, the parameter estimates are likely to be more sensitive to the precise values of

the larger quantiles. As such, rather than using equally spaced quantiles, we use a scheme which favors quantiles closer to the maximum inclusion and we always include the maximum inclusion.

The relative \overline{RSSE} obtained under each dimension reduction method is shown in Table 2 and Figure 1. In comparison to an analysis using all 113 summary statistics and regression adjustment (the “All” column), the best subset selection approaches do not in general offer any improvement. While the entropy-based method provides a slight improvement, the relative \overline{RSSE} under the ε -sufficiency criterion is substantially worse (along with partial least squares). Of course, these results are limited to the few subsets of statistics considered and it is possible that alternative subsets could perform substantially better. However, it is computationally untenable to evaluate this possibility based on exhaustive enumeration of all subsets.

When using neural networks to perform the regression adjustment based on computing the pointwise median of the $m(s)$ and $\sigma^2(s)$ estimates, obtained using varying regularization parameter values (see the introduction to Section 4), the relative performance is quite poor (left-hand side \overline{RSSE} values in Table 2). The mean

relative $\overline{\text{RSSE}}$ is -13% for neural networks, compared to -40% for heteroscedastic least squares regression. As an alternative approach, rather than averaging over the regularization parameter λ , we rather choose the value of $\lambda \in \{10^{-3}, 10^{-2}, 10^{-1}\}$ that minimizes the leave-one-out error of θ [equation (11)]. This approach considerably improves the performance of the network (right-hand side $\overline{\text{RSSE}}$ values in Table 2) with the mean relative $\overline{\text{RSSE}}$ improving to the same level as for heteroscedastic regression. Adopting the same procedure to determine the regularization parameter within ridge regression, there is also a mean gain in performance from -39% to -42% , although the joint parameter inference on (τ, σ, ξ) actually performs worse under this alternative approach. The variability in these results highlights the importance of making an optimal choice of the regularization parameter for an ABC analysis.

The minimum expected posterior loss approach performs particularly well here. This approach has also been shown to perform well in a similar analysis: that of performing inference using quantiles of a large number of independent draws from the (intractable) g -and- k distribution (Fearnhead and Prangle, 2012).

The loose performance ranking of each of the dimension reduction methods finds that the worst performers are the ε -sufficiency criterion (with a mean relative $\overline{\text{RSSE}}$ of -16%) and partial least squares (-19%). Neural networks and AIC/BIC perform just as well as standard least squares regression (-40%), ridge regression slightly outperforms standard regression (-42%) and the entropy-based approach is a further slight improvement at -44% . The clear winner in this example is the posterior loss approach with a mean relative $\overline{\text{RSSE}}$ of -58% .

5. DISCUSSION

The process of dimension reduction is a critical and influential part of any ABC analysis. In this article

we have provided a comparative review of the major dimension reduction approaches (and introduced two new ones) in order to provide some guidance to the practitioner in choosing the most appropriate technique for their own analysis. A summary of the qualitative features of each dimension reduction method is shown in Table 3, and a comparison of the relative performances of each method for each example is illustrated in Figure 3. As with each individual example, we may compute an overall performance ranking of the dimension reduction methods by averaging the mean relative $\overline{\text{RSSE}}$ values over the examples. Performing worse, on average, than a standard least squares regression adjustment with no dimension reduction (with an overall mean relative $\overline{\text{RSSE}}$ of -17%) is the ε -sufficiency technique (-8%) and partial least squares (-12%). Performing better, on average, than standard least squares regression is ridge regression and neural networks (-19%) and AIC/BIC (-21%). In this study, the top performers, on average, were the entropy-based procedure and the minimum expected posterior loss approach, with an overall mean relative $\overline{\text{RSSE}}$ of -25% . It is worth emphasizing that the potential gains in performing a regression adjustment alone (with all summary statistics and *no* dimension reduction) can be quite substantial. This suggests that regression adjustment should be an integral part of the majority of ABC analyses. Further gains in performance can then be obtained by combining regression adjustment with dimension reduction procedures, although in some cases (such as with the ε -sufficiency technique and partial least squares) performance can sometimes worsen.

While being ranked in the top three, a clear disadvantage of the entropy-based procedure and the AIC/BIC criteria is the quantity of computation required. This primarily occurs as the best subset selection procedures require evaluation of all 2^P potential models. For examples 1 and 2, a greedy algorithm was able to find

TABLE 3
Summary of the main features of the different methods of dimension reduction for ABC

Class	Method	Hyper-parameter	Choice of hyper-parameter	Computational burden
Best subset selection	AIC/BIC	None	–	Substantial/greedy alg.
	ε -suff	$T(\theta)$	User choice	Substantial/greedy alg.
	Ent	None	–	Substantial/greedy alg.
Projection techniques	PLS	Number of PLS components, k	Cross-validation	Weak
	NNet	Regularization parameter, λ	Integration or cross-validation	Moderate (optimization algorithm)
	Loss	Choice of basis functions	BIC	Weak (closed-form solution)
Regularization	Ridge	Regularization parameter, λ	Integration or cross-validation	Weak (closed-form solution)

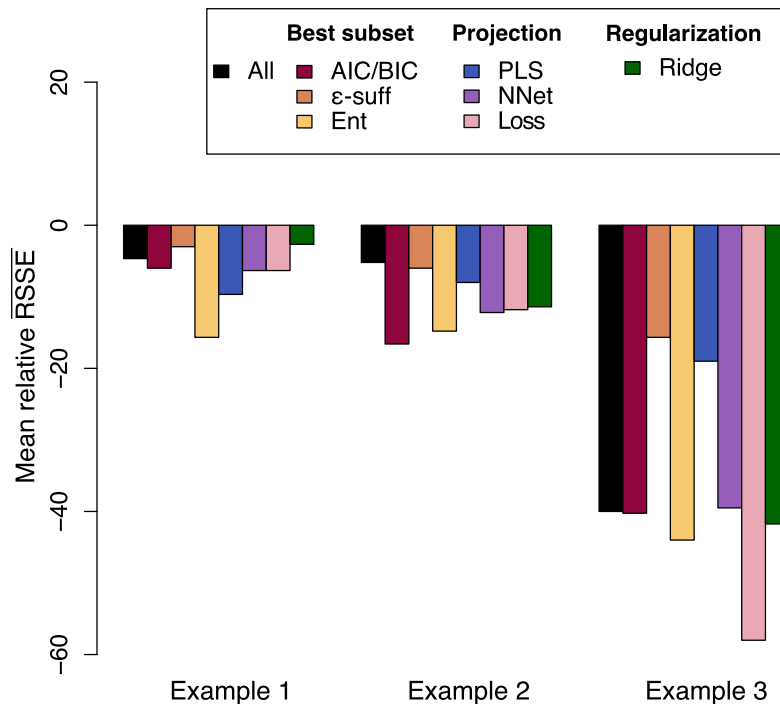


FIG. 3. Mean relative \overline{RSSE} values using each method of dimension reduction and for each example. Methods of dimension reduction include no dimension reduction (All), AIC/BIC, the ϵ -sufficiency criterion (ϵ -suff), the two-stage entropy procedure (Ent), partial least squares (PLS), neural networks (NNet), minimum expected posterior loss (Loss) and ridge regression (Ridge). For examples 1 and 2, the results for ridge regression and neural networks estimate $m(s)$ and $\sigma^2(s)$ have been obtained by taking the pointwise median curve over varying values of the regularization parameter; $\lambda = 10^{-3}, 10^{-2}$ and 10^{-1} (see introduction to Section 4). For example 3, an optimal value of λ was chosen based on a cross-validation procedure (see Section 4.3).

the optimum solution in a reasonable time. This was not possible for example 3. Additionally, in this latter case, for the subsets of summary statistics considered, the performance obtained by implementing computationally expensive methods of dimension reduction was barely an improvement over the computationally cheap, least squares regression adjustment. This raises the important point that the benefits of performing potentially expensive forms of dimension reduction over, say, the simple linear regression adjustment, should be evaluated prior to their full implementation. We also note that the second stage of the entropy-based method (Section 2.2.2) targets minimization of (9), the same error measure used in our comparative analysis. As such, this approach is likely to be numerically favored in our results.

The top ranked (ex aequo) minimum expected posterior loss approach particularly outperforms other dimension reduction methods in the final example (the production of clean steels). In such analyses, with large numbers of summary statistics (here $p = 113$), non-linear methods such as neural networks may become overparametrized, and simpler alternatives, such as

least squares or ridge regression adjustment, can work more effectively. This is naturally explained through the usual bias-variance trade-off: more complex regression models such as neural networks reduce the bias of the estimate of $m(s)$ [and optionally $\sigma^2(s)$], but in doing so the variance of the estimate is increased. This effect can be especially acute for high-dimensional regression (Geman, Bienenstock and Doursat, 1992).

Our analyses indicate that the original least squares, linear regression adjustment (Beaumont, Zhang and Balding, 2002) can sometimes perform quite well, despite its simplicity. However, the presence of multicollinearity between the summary statistics can cause severe performance degradation, compared to not performing the regression adjustment (see Figure 2). In such situations, regularization procedures, such as ridge regression (e.g., example 2 and Figure 2) and projection techniques, can be beneficial.

However, an important issue with regularization procedures, such as neural networks and ridge regression, is the handling of the regularization parameter, λ . The “averaging” procedure that was used in the first two examples proved quite suboptimal in the third, where

a cross-validation procedure to select a single best parameter value produced much improved results. This problem can be particularly critical for neural networks with large numbers of summary statistics, p , as the number of network weights is much larger than p , and, accordingly, massive shrinkage of the weights (i.e., large values of λ) is required to avoid overfitting.

The posterior loss approach produced the superior performance in the third example. In general, a strong performance of this method can be primarily attributed to two factors. First, in the presence of large numbers of highly dependent summary statistics, the extra analysis stage in determining the most appropriate regression model (14) by choosing $f(s)$ through, for example, BIC diagnostics, affords the opportunity to reduce the complexity of the regression in a simple and relatively low-parameterized manner. This was not a primary contributor in example 3, however, as the regression [equation (14)] was directly performed on the full set of 113 statistics. Given the benefits of using regularization methods in this setting, it is possible that a ridge regression model would allow a more robust estimate of the posterior mean (as a summary statistic) as part of this process. Second, the posterior loss approach determines the number of summary statistics to be equal to the number of posterior quantities of interest—in this case, $q = 3$ posterior parameter means. This small number of derived summary statistics naturally allows more precise posterior statements to be made, compared to dimension reduction methods that produce a much larger number of equally informative statistics. Of course, the dimension advantage here is strongly related to the number of parameters ($q = 3$) and summary statistics ($p = 113$) in this example. However, it is not fully clear how any current methods of dimension reduction for ABC would perform for substantially more challenging analyses with considerably higher numbers of parameters and summary statistics. This is because the curse of dimensionality in ABC (Blum, 2010a) has tended to restrict existing applications of ABC methods to problems of moderate parameter dimension, although this may change in the future.

What is very apparent from this study is that there is no single “best” method of dimension reduction for ABC. For example, while the posterior loss and entropy-based methods were the best performers for example 3, AIC and BIC were ranked first in the analysis of example 2, and partial least squares outperformed the posterior loss approach in example 1. A number of factors can affect the most suitable choice for any

given analysis. As discussed above, these can include the number of initial summary statistics, the amount of dependence and multicollinearity within the statistics, the computational overheads of the dimension reduction method, the requirement to suitably determine hyperparameters and sensitivity to potentially large numbers of uninformative statistics.

One important point to understand is that all of the ABC analyses of this review were performed using the rejection algorithm optionally followed by some form of regression adjustment. While alternative, potentially more efficient and accurate methods of ABC posterior simulation exist, such as Markov chain Monte Carlo or sequential Monte Carlo based samplers, the computational cost of separately implementing such an algorithm 2^p times (in the case of best subset selection methods) means that such dimension reduction methods can become rapidly untenable, even for small p . The price of the benefit of using the more computationally practical, fixed large number of samples is that decisions on the dimension reduction of the summary statistics will be made on potentially worse estimates of the posterior than those available under superior sampling algorithms. As such, the final derived summary statistics may in fact not be those which are most appropriate for subsequent use in, for example, Markov chain Monte Carlo or sequential Monte Carlo based algorithms.

However, this price is arguably a necessity. It is practically important to evaluate the performance of any dimension reduction procedure in a given analysis. Here we used a criterion [the RSSE of equation (9)] that is based on a leave-one-out procedure. When using a fixed, large number of samples, evaluation of such a performance diagnostic is entirely practicable, as no further model simulations are required. This idea is also relevant to methods of dimension reduction for model selection (Barnes et al., 2012; Estoup et al., 2012) where a misclassification rate based on a leave-one-out procedure can serve as a comparative criterion.

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SUPPLEMENTARY MATERIAL

Supplement to “A Comparative Review of Dimension Reduction Methods in Approximate Bayes-

ian Computation” (DOI: [10.1214/12-STS406SUPP](https://doi.org/10.1214/12-STS406SUPP); .pdf). The supplement contains for each of the three examples a comprehensive comparison of the errors obtained with the different methods of dimension reduction.

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