Approximate Bayesian Inference via Sparse grid Quadrature Evaluation for Hierarchical Models

Joshua Hewitt and Jennifer A. Hoeting
Colorado State University

Abstract:
We combine conditioning techniques with sparse grid quadrature rules to develop a computationally efficient method to approximate marginal, but not necessarily univariate, posterior quantities, yielding approximate Bayesian inference via Sparse grid Quadrature Evaluation (BISQuE) for hierarchical models. BISQuE reformulates posterior quantities as weighted integrals of conditional quantities, such as densities and expectations. Sparse grid quadrature rules allow computationally efficient approximation of high dimensional integrals, which appear in hierarchical models with many hyperparameters. BISQuE reduces computational effort relative to standard, Markov chain Monte Carlo methods by at least two orders of magnitude on several applied and illustrative models. We also briefly discuss using BISQuE to apply Integrated Nested Laplace Approximations (INLA) to models with more hyperparameters than is currently practical.

Keywords: Approximate Bayesian inference, computational statistics, hierarchical models, parallel computing, sparse grid quadrature

1 Introduction

Computationally efficient posterior approximation remains a key challenge in applied Bayesian analyses, especially for hierarchical models. Hierarchical Bayesian models allow
flexible modeling of complex data, but make posterior inference challenging because simple, conjugate distributions are typically unavailable. Posterior densities, expectations, and other quantities involve computing integrals that often require numerical approximation. The required approximations can be computationally expensive or challenging since many hierarchical models include many unknown parameters, thus integrals are defined over high dimensional state spaces. Sampling-based approaches, like Markov chain Monte Carlo (MCMC) methods, are widely used because they are generally reliable and relatively simple to implement (Gelfand and Smith, 1990). However, MCMC approximations can be computationally expensive for many models. Full conditional posterior distributions required by a Gibbs sampler can be difficult to sample efficiently or lead to highly correlated Monte Carlo samplers. As a result, if \( n \) dependent samples are drawn via MCMC methods, the stochastic approximation error rate can often be higher than the error \( O_p\left( n^{-1/2} \right) \) for direct Monte Carlo approximations. Alternate approaches for Bayesian approximation are available via a range of stochastic and deterministic methods, including Laplace and Integrated Nested Laplace approximations (Rue, Martino and Chopin, 2009; Tierney and Kadane, 1986), classical quadrature-based approximations (Naylor and Smith, 1982), Variational Bayes (Attias, 2000), and Approximate Bayesian Computing (Rubin, 1984; Tavare, Balding, Griffiths and Donnelly, 1997). Generally, each method is motivated by computational issues and structures found in different classes of models, so no method is necessarily well-suited for all hierarchical models. In particular, technical limitations of Integrated Nested Laplace approximations (INLA) and classical quadrature motivate us to develop a strategy to yield approximate Bayesian Inference via Sparse grid Quadrature Evaluation (BISQuE) for a wider range of hierarchical models.

INLA approximates marginal posterior distributions by using a discrete numerical integration grid of hyperparameters to average over Laplace approximations of conditional posterior densities. The method is developed for models that link observations to latent Gaussian variables through link functions, similar to generalized linear models. The INLA
approximation enables fast inference for a wide range of scientifically relevant models. However, it can sometimes be difficult to reformulate models to have the latent Gaussian structure required by the INLA framework. Additionally, the numerical integration in INLA can become computationally infeasible for models with many hyperparameters. The latter issue is a limitation shared by classical quadrature-based approximations for posterior quantities.

Classical quadrature methods can approximate marginal posterior distributions and expectations for general Bayesian models, but like INLA, the models must have relatively small dimension (Naylor and Smith, 1982). Quadrature methods approximate an integral by evaluating its integrand at deterministic nodes and weighting the results. Nodes and weights are chosen using known information about the shape of the integrand. However, classical quadrature methods have limited practical use for approximate Bayesian inference. Classical quadrature methods integrate over all unknown parameters—not just hyperparameters—and the size of the integration grids suffer from the curse of dimensionality, growing exponentially as parameters are added to models.

More recent quadrature literature formalized theory and methods that yield sparse integration grids, thereby mitigating the curse of dimensionality for quadrature approximations of high dimensional integrals (Gerstner and Griebel, 1998; Novak and Ritter, 1996,9). In statistics, sparse grid quadrature methods have been used to approximate likelihoods that involve high dimensional integrals, as can arise from econometric models (Heiss and Winschel, 2008). Sparse grid quadrature has also been used to approximate posterior expectations, densities, and integration constants for non-linear inverse problems with normal errors (Emery and Johnson, 2012; Schillings and Schwab, 2013), estimate Kullback-Leibler information gains to solve Bayesian experimental design problems (Long, Scavino, Tempone and Wang, 2013), and to accelerate computations for specific non-linear Kalman filters (Arasaratnam and Haykin, 2009; Jia, Xin and Cheng, 2012). By comparison, we consider approximate Bayesian posterior inference more generally.

We propose reformulating Bayesian posterior quantities, such as densities and expec-
tations, so that they can be efficiently approximated by combining conditioning techniques with sparse grid quadrature methods. Our reformulation lets us apply sparse grid quadrature methods to hierarchical Bayesian models with non-Gaussian structures and potentially many hyperparameters. The resulting computational approach greatly reduces computation time as compared to MCMC approaches for many models, including fully non-Gaussian models. Our framework is very flexible and can be applied to other contexts. For example, it can also potentially be combined with INLA to allow fast inference for latent Gaussian models with many hyperparameters.

We briefly review quadrature and sparse grid methods (Section 2), then introduce the Bayesian Inference via Sparse grid Quadrature Evaluation (BISQuE) strategy to yield approximate inference for hierarchical Bayesian models (Section 3). Our method reduces the computational effort required to approximate posterior densities, means, and variances in examples where traditional MCMC methods are relatively slow (Section 4). We conclude with discussions of extensions and other directions for future work (Section 5).

2 Quadrature and Sparse grid methods

Let \( f(x) \) be a map from a \( d \)-dimensional space \( S \) onto the real line \( \mathbb{R} \), and \( w(x) \) be a weight function with the same support. The integral

\[
I(f) = \int_S f(x)w(x)dx
\]

may be approximated via the weighted sum

\[
\hat{I}(f) = \sum_{\ell=1}^{k_i} f(x^{(i,\ell)})w^{(i,\ell)}
\]

for some choice of summation length \( k_i \in \mathbb{N} \), nodes \( \mathcal{A}^i = \{x^{(i,\ell)} : \ell = 1, \ldots, k_i\} \subset S \), and weights \( \mathcal{W}^i = \{w^{(i,\ell)} : \ell = 1, \ldots, k_i\} \subset \mathbb{R}^{k_i} \). We will use the index \( i \) shortly. The approxi-
information (2) is called a quadrature rule if the integration domain $S$, weight function $w$, and desired approximation accuracy or computational cost are used with specific procedures to specify $k_i, A_i, \text{and } W_i$ (Givens and Hoeting, 2013, Section 5.3). The number of nodes and weights $k_i$ balances the approximation error in (2) with the approximation’s computational cost. Large $k_i$ can yield more accurate approximation (or even exact evaluation) of (1), but at potentially high computational cost. In practice, sequences of increasingly accurate quadrature rules defined by $(k_1, A_1, W_1), (k_2, A_2, W_2), \ldots$ such that $k_1 < k_2 < \ldots$ can be used to estimate and control approximation error (Laurie, 1985). Quadrature rules can yield highly accurate approximations for integrals $I(f)$ of smooth functions $f$ defined on $S$, but computational efficiency is difficult to achieve if $S$ has high dimension.

For multidimensional $S$, product rules are the simplest quadrature rules to construct, but these suffer from the curse of dimensionality. Product rules are formed by iteratively applying univariate quadrature rules along each dimension of $S$ to approximate (1); they are aptly named because their nodes $A_i$ are a Cartesian product of nodes from the underlying univariate quadrature rules (cf. Novak and Ritter, 1996). To be precise, let $S$ be the product space $S = S_1 \times \cdots S_d$ of one-dimensional, $\sigma$-finite measure spaces $S_1, \ldots, S_d$, and let the weight function $w(x)$ be the product $w(x) = \prod_{i=1}^d w_i(x_i)$ of weight functions $w_1(x_1), \ldots, w_d(x_d)$ that are respectively defined on $S_1, \ldots, S_d$. If the target integral (1) is well defined, then Fubini’s theorem implies (1) may be evaluated as an iterated integral. Iterated integration allows approximation by applying univariate quadrature rules along each dimension of $S$. Define $U_1^{i_1}, \ldots, U_d^{i_d}$ to be univariate quadrature rules that respectively approximate integrals on $S_1, \ldots, S_d$ with $k_{i_1}, \ldots, k_{i_d}$ nodes $A_1^{i_1}, \ldots, A_d^{i_d}$ and weights $W_1^{i_1}, \ldots, W_d^{i_d}$. The product rule that approximates (1) is defined via

$$
(U_1^{i_1} \otimes \cdots \otimes U_d^{i_d})(f) = \sum_{\ell_1=1}^{k_{i_1}} \cdots \sum_{\ell_d=1}^{k_{i_d}} f(x_1^{(i_1,\ell_1)}, \ldots, x_d^{(i_d,\ell_d)}) w_1^{(i_1,\ell_1)} \cdots w_d^{(i_d,\ell_d)}. 
$$

The product rule (3) is a special case of the general approximation form (2) because the
nested sum in (3) may be re-expressed as a single sum over an enumeration of the quadrature nodes \((x_{1}^{(i_{1},\ell_{1})}, \ldots, x_{d}^{(i_{d},\ell_{d})}) \in A_{1}^{i_{1}} \times \cdots \times A_{d}^{i_{d}}\) that uses aggregated weights \(w_{1}^{(i_{1},\ell_{1})} \cdots w_{d}^{(i_{d},\ell_{d})}\).

The product rule (3) requires evaluation of \(f\) at \(|A_{1}^{i_{1}} \times \cdots \times A_{d}^{i_{d}}| = k_{i_{1}} \cdots k_{i_{d}}\) nodes. The number of quadrature nodes grows exponentially as \(d \uparrow \infty\) if \(f\) is explored equally in all dimensions, i.e., if \(k_{i_{1}} = \cdots = k_{i_{d}}\). The curse of dimensionality for product rules can be partially mitigated by exploring \(f\) unequally in different dimensions, but this approach is only practical if \(f\) is extremely smooth in some dimensions.

By comparison, sparse grid quadrature rules are computationally efficient approximations for integrals on multidimensional \(S\). Novak and Ritter (1996,9) use the Smolyak (1963) formula to combine univariate quadrature rules \(U_{1}^{i_{1}}, \ldots, U_{d}^{i_{d}}\) in a computationally efficient approximation (2) of (1). The Smolyak formula specifies a linear combination \(A(q,d)\) of product rules (3) that approximates (1) via

\[
A(q,d)(f) = \sum_{q-d+1 \leq |\mathbf{i}| \leq q} (-1)^{q-|\mathbf{i}|} \left( \frac{d - 1}{q - |\mathbf{i}|} \right) (U_{1}^{i_{1}} \otimes \cdots \otimes U_{d}^{i_{d}})(f),
\]

in which \(q \geq d\) and \(|\mathbf{i}| = i_{1} + \cdots + i_{d}\). The Smolyak rule (4) is also a special case of the general approximation form (2) because, as with (3), the underlying quadrature nodes and weights may be enumerated and aggregated. The constant \(q \in \mathbb{N}\) is called the rule’s level and most directly controls the accuracy and computational cost of the approximation in applications. The Smolyak rule (4) is called a sparse grid quadrature rule if each of the \(j = 1, \ldots, d\) univariate quadrature rules have nested nodes in the sense that \(A_{j}^{1} \subset A_{j}^{2} \subset \cdots\). The rule (4) requires evaluation of \(f\) at the nodes

\[
A(q,d) = \bigcup_{q-d+1 \leq |\mathbf{i}| \leq q} A_{1}^{i_{1}} \times \cdots \times A_{d}^{i_{d}}.
\]

Adopting the convention that \(A_{j}^{0} = x_{j}^{0}\) for some base point \(x_{j}^{0} \in S_{j}\), nesting implies \(A(q,d)\) is a sparse subset of the nodes used by the product rule \((U_{1}^{q} \otimes \cdots \otimes U_{d}^{q})(f)\).
The sparse grid quadrature rule (4) mitigates the curse of dimensionality by creating sparse integration grids relative to product rules, but requires $f$ to satisfy stricter smoothness properties in exchange. Novak and Ritter (1999) present growth rates, bounds, and approximations for the number of quadrature nodes $k = |A(q,d)|$ under different scenarios. Novak and Ritter (1996) also show that the approximation error’s order of convergence is

$$|I(f) - A(q,d)(f)| = O\left(k^{-r}(\log k)^{(d-1)(r/d)}\right)$$

if $f$ has a bounded mixed derivative $f^{(r,...,r)}$. Even more precisely, Novak and Ritter (1999) show that $I(f) = A(q,d)(f)$ if $f$ is a polynomial with bounded total degree, i.e., that the approximation (4) is exact for the integral (1). In practice, the sparse grid quadrature rule (4) is most computationally efficient for functions $f$ that behave approximately as polynomials with relatively low total degree. In statistical contexts, this is similar to saying that the rule (4) is most useful for polynomial surfaces $f$ that are mainly driven by main effects and low order interaction terms. We will satisfy this requirement for computational efficiency in our application by appealing, in part, to the Bayesian central limit theorem to claim that many posterior surfaces and other quantities can be well approximated by the product of a Gaussian weight function $w(\mathbf{x})$ with a relatively low-order correction term $f$.

3 Posterior inference via weighted mixtures

We combine conditioning techniques with sparse grid quadrature rules to develop specialized, computationally efficient formulas like (4) that approximate Bayesian posterior inference for marginal quantities. For example, when used to approximate marginal posterior densities, our method will yield a weighted mixture of full conditional posterior distributions. Below, we briefly motivate the Bayesian Inference via Sparse grid Quadrature Evaluation (BISQuE) approximation strategy by arguing that it can be computationally inefficient to use sparse grid quadrature rules to directly approximate posterior quantities (Section 3.1). First, our
motivation simultaneously highlights the general strategy used to apply sparse grid quadrature rules to Bayesian models as well as key technical issues addressed by BISQuE. Then, the remainder of Section 3 defines the family of posterior quantities to which BISQuE applies (Section 3.2), the BISQuE approximation (Section 3.3), and a nested integration technique that is useful for applying BISQuE to models that lack closed form expressions of posterior densities (Section 3.4).

### 3.1 Motivation for BISQuE

Consider a generic hierarchical Bayesian model. Let $X \in \Omega_0$ be a sample of continuous, discrete, or mixed random variables from an arbitrary process. Define a conditional probability model for $X$ such that

$$X|\theta_1, \theta_2 \sim f(X|\theta_1, \theta_2)$$

$$(\theta_1, \theta_2) \sim f(\theta_1, \theta_2)$$

for parameters $\theta_1 \in \Omega_1$ and $\theta_2 \in \Omega_2$. Many Bayesian models can be written like (5). For example, many hierarchical Bayesian models add conditional independence assumptions and hierarchical structure to (5) so that

$$f(X|\theta_1, \theta_2) = f(X|\theta_1)$$

$$f(\theta_1, \theta_2) = f(\theta_1|\theta_2)f(\theta_2).$$

Non-hierarchical models also fit within our framework (5). For example, Bayesian formulations of some linear regression models specify prior independence between regression coefficients $\theta_1$ and variance components $\theta_2$, thus define $f(\theta_1, \theta_2) = f(\theta_1)f(\theta_2)$.

The marginal posterior density $f(\theta_1|X)$ is often of interest in posterior inference. The
density may be computed by integrating \( \theta_2 \) out of the joint posterior density

\[
f(\theta_1 | X) = \int f(\theta_1, \theta_2 | X) d\theta_2.
\]

Sparse grid quadrature rules (4) yield weighted-sum approximations (2) of (6) by introducing a weight function \( w(\theta_1, \theta_2, X) \) and proceeding via

\[
f(\theta_1 | X) \approx \sum_{\ell=1}^{k_i} \frac{f\left(\theta_1, \theta_2^{(i,\ell)} \bigg| X\right)}{w\left(\theta_1, \theta_2^{(i,\ell)}, X\right)} w^{(i,\ell, \theta_1)},
\]

in which quadrature nodes \( \theta_2^{(i,\ell)} \) and weights \( w^{(i,\ell, \theta_1)} \) are determined by applying the Smolyak formula (4) to a collection of univariate quadrature rules that are appropriate for the support of \( \theta_2 \). For fixed \( \theta_1 \in \Omega_1 \), the Gaussian approximation to \( f(\theta_1, \theta_2 | X) \) will often be a sensible default choice for the weight function \( w(\theta_1, \theta_2, X) \) since the weight ratio \( f/w \) in (7) accounts for deviations from normality in \( f(\theta_1, \theta_2 | X) \).

The direct marginal posterior density approximation (7) has two key inefficiencies that the BISQuE approximation completely avoids or minimizes. First, the weight function \( w \) depends on \( \theta_1 \), which implies a separate weight function must be used to approximate \( f(\theta_1 | X) \) at each \( \theta_1 \in \Omega_1 \). Second, the approximation (7) assumes \( f(\theta_1, \theta_2 | X) \) is computable. Oftentimes, the joint posterior density \( f(\theta_1, \theta_2 | X) \) is only known in closed form up to a proportionality constant because the density’s integration constant requires numerical approximation for many Bayesian models. While sparse grid quadrature rules could approximate the integration constant, BISQuE is able to avoid or reduce computational cost of the approximation.

### 3.2 Posterior quantities targeted by BISQuE

We develop BISQuE to approximate marginal posterior quantities \( h(\theta_1; X) \) of hierarchical models (5) that are defined implicitly with respect to a function or random variable
\( h(\theta_1, \theta_2; X) \) via

\[
(8) \quad h(\theta_1; X) = \int h(\theta_1, \theta_2; X) f(\theta_2|X) d\theta_2.
\]

For example, the construction (8) defines the marginal posterior density \( h(\theta_1; X) = f(\theta_1|X) \) when \( h(\theta_1, \theta_2; X) = f(\theta_1|\theta_2, X) \). The posterior marginal density \( f(\theta_2|X) \) and all other marginal posterior quantities may be formed by switching the roles of \( \theta_1 \) and \( \theta_2 \). In comparison to the definition (6) used in the direct sparse grid approximation (7), the BISQuE construction (8) uses conditioning to express the joint posterior density in conditional form, as \( f(\theta_1, \theta_2|X) = f(\theta_1|\theta_2, X)f(\theta_2|X) \). The construction (8) allows us to develop sparse grid quadrature rules with weight functions \( w(\theta_2, X) \) that only depend on \( \theta_2 \) (Section 3.3), thus addresses the first technical issue described in Section 3.1.

The BISQuE construction (8) allows one set of quadrature nodes and weights to be reused to approximate many posterior quantities. For example, (8) defines the posterior mean \( h(\theta_1; X) = E[g(\theta_1)|X] \) when \( h(\theta_1, \theta_2; X) = E[g(\theta_1)|\theta_2, X] \). Again, the approach relies on conditioning as

\[
E[g(\theta_1)|X] = E_{\theta_2|X}\{E[g(\theta_1)|\theta_2, X]\}
= \int E[g(\theta_1)|\theta_2, X] f(\theta_2|X) d\theta_2.
\]

Posterior predictive distributions, variances and higher central moments, cumulative distribution functions, and model selection criteria such as the deviance information criteria (DIC, Spiegelhalter, Best, Carlin and van der Linde, 2002) and the Watanabe-Akaike information criterion (WAIC, Watanabe, 2010) can also be expressed through one or more applications of (8). For example, the posterior variance \( \text{Var}(g(\theta_1)|X) \) can be approximated by using the law of total variance to introduce expectations with respect to \( f(\theta_2|X) \) via

\[
(9) \quad \text{Var}(g(\theta_1)|X) = E_{\theta_2|X}\{\text{Var}(g(\theta_1)|\theta_2, X)\} + 
\]

10
\[ E_{\theta_2|X} \left[ (E[g(\theta_1)|\theta_2, X] - E[g(\theta_1)|X])^2 \right], \]

for which

\[ h(\theta_1, \theta_2; X) = \text{Var}(g(\theta_1)|\theta_2, X) + (E[g(\theta_1)|\theta_2, X] - E[g(\theta_1)|X])^2. \]

(10)

Note that here the marginal posterior expectation \( E[g(\theta_1)|X] \) must be approximated before (9). We present expressions for the other quantities in Supplement Section A.

### 3.3 Approximate posterior inference via BISQuE

We modify the integral form (1) to enable the use of sparse grid quadrature rules (4) to approximate marginal posterior quantities (8) of hierarchical Bayesian models (5). While we define marginal posterior quantities by integrating functions over the posterior density \( f(\theta_2|X) \), numerical integration methods often use transformations to increase computational stability and efficiency. Thus, we develop quadrature rules that integrate over \( f(\nu|X) \) where \( \nu = T(\theta_2) \in \mathbb{R}^p \) is defined by a monotone transformation to a real coordinate space \( T: \Omega_2 \rightarrow \mathbb{R}^p \). Consider a transformed density

\[ f(\nu|X) = f(T^{-1}(\nu)|X) \left| J(T^{-1}(\nu)) \right|, \]

where \( |J(T^{-1}(\nu))| \) is the determinant of the Jacobian for the transformation \( T^{-1} \). We propose using sparse grid quadrature rules (4) to derive quadrature nodes and weights that approximate marginal posterior quantities (8) via the BISQuE approximation

\[ h(\theta_1; X) = \int h(\theta_1, T^{-1}(\nu); X) \frac{f(\nu|X)}{w(\nu,X)} w(\nu, X) d\nu \]

\[ \approx \sum_{\ell=1}^{k_i} h\left( \theta_1, \theta_2^{(i,\ell)}; X \right) \hat{w}^{(i,\ell)}, \]
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in which

\[ \tilde{w}^{(i,\ell)} = \frac{f(\nu^{(i,\ell)}|X)}{w(\nu^{(i,\ell)}, X)} w^{(i,\ell)}, \]

\( w(\nu, X) \) is a weight function; and \( w^{(i,\ell)}, \nu^{(i,\ell)}, \) and \( \theta^{(i,\ell)}_2 = T^{-1}(\nu^{(i,\ell)}) \) are respectively quadrature weights, nodes, and back-transformed nodes.

Sparse grid quadrature theory implies the computational efficiency of the approximation (11) relies on several statistical and numerical assumptions. The weight function \( w(\nu, X) \) should approximate the transformed density \( f(\nu|X) \) and have known, computationally efficient, nested quadrature rules. In particular, such quadrature rules have been developed for Gaussian weight functions (Genz and Keister, 1996). Thus, we appeal to Bayesian analogs of the central limit theorem to justify proposing the Gaussian approximation \( f^G(\nu|X) \) at the posterior mode of \( f(\nu|X) \) as a sensible default choice for a weight function for many Bayesian models. This approximation holds if the same size is large, the dimension of the model is fixed, and both the prior and likelihood are twice differentiable near the mode of the posterior distribution (Berger, 1985, pg. 224–225). Sparse grid quadrature rules will also be most efficient if the integrand \( h(\theta_1, T^{-1}(\nu); X)f(\nu|X)/w(\nu, X) \) in (11) can be well-approximated by a low-order polynomial in \( \nu \). This requirement is easier to satisfy if \( w(\nu, X) \) approximates \( f(\nu|X) \) well and \( h(\theta_1, T^{-1}(\nu); X) \) is slowly varying with respect to \( \nu \).

Standardizing the BISQuE approximation (11) weights \( \tilde{w}^{(i,\ell)} \) can address part of the second technical issue described in Section 3.1. For example, in some Bayesian models both the joint \( f(\theta_1, \theta_2|X) \) and marginal \( f(\theta_2|X) \) posterior densities are known only up to a proportionality constant, but the full conditional posterior \( f(\theta_1|\theta_2, X) \) is available in closed form (Section 4). Marginal posterior probabilities and expectations cannot be computed without either approximating the proportionality constant or using numerical approximation techniques that implicitly cancel the constant. We propose using standardized
weights $\tilde{w}_{\star}^{(i,\ell)} = \frac{\tilde{w}^{(i,\ell)}}{\sum_{j=1}^{k_i} \tilde{w}^{(i,j)}}$ that sum to one in order to approximate marginal posterior quantities $h(\theta_1; X)$ like $f(\theta_1 | X)$ by implicitly cancelling the unknown integration constants. The result borrows ideas from importance sampling (Givens and Hoeting, 2013, pg. 181). An alternate definition for posterior quantities,

$$h(\theta_1; X) = \frac{\int h(\theta_1, \theta_2; X)f(\theta_2 | X)d\theta_2}{\int f(\theta_2 | X)d\theta_2},$$

is equivalent to the original construction (8) since $\int f(\theta_2 | X)d\theta_2 = 1$. Plugin BISQuE approximations (11) for the numerator and denominator in (12) yield quadrature approximations with standardized weights via

$$\int h(\theta_1, \theta_2; X)f(\theta_2 | X)d\theta_2 \approx \frac{\sum_{\ell=1}^{k_i} h\left(\theta_1, \theta_2^{(i,\ell)} ; X\right) \tilde{w}^{(i,\ell)}}{\sum_{j=1}^{k_i} \tilde{w}^{(i,j)}} = \sum_{\ell=1}^{k_i} h\left(\theta_1, \theta_2^{(i,\ell)} ; X\right) \tilde{w}^{(i,\ell)} \tilde{w}_{\star}^{(i,\ell)}.$$ 

Standardization also allows approximations of $f(\theta_1 | X)$ to integrate exactly to one. Table 1 summarizes the BISQuE approach outlined in this section as it would be applied when using a Gaussian approximation to the transformed posterior density to approximate posterior quantities (8).

### 3.4 Nested integration strategies for BISQuE

While hierarchical Bayesian models (5) typically have closed form expressions for the likelihood $f(X | \theta_1, \theta_2)$ and prior $f(\theta_1, \theta_2)$, many models do not have closed form expressions for the posterior densities $f(\theta_2 | X)$ and $f(\theta_1 | \theta_2, X)$. Lack of closed form expressions is a concern related to the second technical issue described in Section 3.1. We propose a nested numerical integration scheme to address the concern and allow application of BISQuE to a wider range of models. Recall that for a fixed dataset $X$, the joint posterior density
$f(\theta_1, \theta_2 | X)$ is often only known up to a proportionality constant since

$$f(\theta_1, \theta_2 | X) = \frac{f(\theta_1, \theta_2, X)}{f(X)} \propto f(X| \theta_1, \theta_2) f(\theta_1, \theta_2)$$

and the marginal density $f(X)$ often requires prohibitively expensive numerical approximation.

The densities $f(\theta_2 | X)$ and $f(\theta_1 | \theta_2, X)$ may be derived (and ultimately approximated) indirectly, by factoring the joint density $f(\theta_1, \theta_2, X)$ into components $g_1(\theta_1, \theta_2; X)$ and $g_2(\theta_2; X)$ such that

$$f(\theta_1, \theta_2, X) = g_1(\theta_1, \theta_2; X)g_2(\theta_2; X). \quad (14)$$

The factored joint density (14) implies

$$f(\theta_2 | X) = \int f(\theta_1, \theta_2 | X) d\theta_1 \frac{g_2(\theta_2; X)C_1(\theta_2)}{f(X)} \quad (15)$$

and

$$f(\theta_1 | \theta_2, X) = \frac{f(\theta_1, \theta_2 | X)}{f(\theta_2 | X)} = \frac{g_1(\theta_1, \theta_2; X)C_1(\theta_2)}{f(\theta_2 | X)} \quad (16)$$

for which the integration constant $C_1(\theta_2)$ must be approximated numerically and is specified via

$$C_1(\theta_2) = \int g_1(\theta_1, \theta_2; X) d\theta_1. \quad (17)$$

The alternate expressions (15) and (16) allow BISQuE to approximate posterior inference for models that lack closed form expressions for the densities $f(\theta_2 | X)$ and $f(\theta_1 | \theta_2, X)$. Standardized BISQuE weights $\tilde{w}_{s}^{(i,\ell)}$ implicitly cancel the unknown factor $f(X)$, and standard quadrature techniques can efficiently approximate the integration constant (17) when
the parameter vector $\theta_1$ has small dimension. The parameters $\theta_1$ and $\theta_2$ can often be defined or repartitioned to satisfy this requirement because the hierarchical model (5) places few restrictions on the parameters; we use this flexibility in Section 4. The added computational cost that the nested integration (17) adds to the BISQuE approximation is minimized as the integration constant (17) only needs to be approximated relatively few times, specifically, at the quadrature nodes and when developing the weight function—e.g., the Gaussian approximation at the posterior mode.

4 Examples

We demonstrate the benefits of the BISQuE approximation (11) on data that are typically analyzed with standard, Gibbs sampling techniques for approximate Bayesian posterior inference. We approximate posterior inference for a fully non-Gaussian capture-recapture model (Section 4.1), a spatial Gaussian process model (Section 4.2), and a more complex, applied spatial Gaussian process model for climate teleconnection (Section 4.3). Posterior distributions in the first and third examples respectively require integration over 8 and 5-dimensional parameter vectors $\theta_2$. Posterior approximations for the second and third examples have computational complexity that is $O(MN^3)$ in the number of spatial observations $N$ and $M$ points at which the posterior distribution is explored, thus computational strategies like BISQuE that reduce the number of points required for posterior approximation can be extremely beneficial.

We compare posterior inference and computational effort between standard Gibbs sampling techniques and BISQuE. Computational effort is measured indirectly with respect to computation time. All computations are conducted on a modest workstation with eight logical processors. We use parallelization to compute the $k_i$ mixture components of the BISQuE approximation and to draw posterior predictive samples via composition sampling in the spatial examples (cf. Banerjee, Carlin and Gelfand, 2015, pg. 126). For each posterior quan-
tity, the level $q$ for the underlying sparse grid quadrature rule (4) is chosen to be the smallest value (i.e., the simplest approximation) such that the posterior density approximations have converged. The number of Gibbs steps used in each approximation is similarly chosen. The BISQuE approximation also requires specification of univariate quadrature rules, for which we choose nested Gauss-Hermite rules (Genz and Keister, 1996).

## 4.1 Fur seals

### 4.1.1 Data and model

Givens and Hoeting (2013, example 7.7) analyze data from a capture-recapture study conducted in New Zealand. The study’s research goal was to estimate the total number of pups in a fur seal colony $N \in \mathbb{N}$. Researchers visited the colony $I = 7$ times throughout the course of a single season. In each visit, the researchers captured and marked all of the fur seal pups present, noting the total number of pups captured in each visit $c = (c_1, \ldots, c_I) \in \mathbb{N}^I$ in addition to the number of newly captured pups $m_1, \ldots, m_I \in \mathbb{N}$. The data are analyzed using a Bayesian model for capture-recapture data (18), and posterior distributions are approximated with a Gibbs sampler. Gibbs sampling is particularly inefficient for this model as one pair of hyperparameters has high posterior correlation and are only weakly identified by the data. By comparison, the BISQuE strategy (11) approximates posterior quantities for this model with substantially less computational effort.

The model (18) assumes the total population size $N$ remains fixed during the time period of the study (i.e., the model assumes a closed population). Let $r = \sum_{i=1}^I m_i$ be the total number of pups captured during the study. Givens and Hoeting (2013) introduce a vector $\alpha = (\alpha_1, \ldots, \alpha_I) \in [0, 1]^I$ with capture probabilities for each census attempt and discuss
modeling the data with the hierarchical model

\[
    f(c, r| N, \alpha) \propto \frac{N!}{(N - r)!} \prod_{i=1}^{I} \alpha_i^{c_i} (1 - \alpha_i)^{N-c_i}
\]

\[
    f(N) \propto 1/N
\]

\[
    f(\alpha_i| \theta_1, \theta_2) \sim \text{Beta}(\theta_1, \theta_2) \text{ for } i = 1, \ldots, I
\]

\[
    f(\theta_1, \theta_2) \propto \exp\{-(\theta_1 + \theta_2)/1000\},
\]

in which \((\theta_1, \theta_2)\) are hyperparameters for the capture probabilities. We use the Beta distribution’s mean–sample size parameterization to increase the identifiability of the hyperparameters. Specifically, let \(U_1 = \text{logit}(\theta_1/(\theta_1 + \theta_2))\) and \(U_2 = \log(\theta_1 + \theta_2)\) and fix \(U_2 = 5.5\).

### 4.1.2 Posterior inference and results

Givens and Hoeting (2013) use standard Gibbs-sampling approaches to draw posterior samples for model parameters. The full conditional posterior distributions \(f(N| c, r, \alpha, \theta_1, \theta_2)\) and \(f(\alpha| c, r, N, \theta_1, \theta_2)\) are conjugate and easy to sample. Posterior samples for \(U_1\) are drawn using Metropolis steps. The sampler is run for 100,000 iterations, taking 298 seconds to complete; posterior inference uses the final 50,000 samples.

We use the BISQuE strategy to approximate the posterior marginal densities \(f(N| c, r), f(\alpha_i| c, r),\) and \(f(U_1| c, r)\). Table 2 connects this example’s notation to that used with BISQuE. When used as the BISQuE conditioning variable \(\theta_2\), we map parameters to the real line by using log transforms with \(N-r\) and logit transforms with the capture probabilities \(\alpha\).

We also rely on the Gaussian approximation to the negative binomial distribution in order to justify using \(N\) as a conditioning variable \(\theta_2\) in BISQuE. Almost all conditional and marginal posterior densities required for BISQuE are computable in closed form up to a proportionality constant; refer to Givens and Hoeting (2013, eqs. 7.16, 7.17) and Supplement Section C.1 for details. The posterior for \(f(U_1| c, r)\) requires approximation via nested integration strategies (Section 3.4).
Posterior inference via BISQuE is effectively identical to posterior inference via Gibbs sampling, but is computed with substantially less effort. Gibbs sampling takes 298 seconds to complete on our test machine, whereas the BISQuE approximations require a total of 5 seconds (Table 2), and posterior densities are nearly identical (Figures 1 to 2).

4.2 Spatial

4.2.1 Simulated data and model

We work with data simulated from a geostatistical spatial model. Gibbs sampling is computationally expensive for such models because it involves decomposing spatially-structured covariance matrices in $\mathbb{R}^{N \times N}$ at each Gibbs iteration, where $N$ is the number of observations. Let $\{X(s)\}_{s \in \mathcal{D}}$ be a random field, whose stochasticity is defined by a mean-zero Gaussian process on a continuous spatial domain $\mathcal{D} \subset \mathbb{R}^2$. Let the covariance $\text{Cov}(X(s), X(t))$ between random variates $X(s), X(t)$ be specified by the isotropic Matérn covariance function, defined via

$$\kappa(s, t; \sigma^2, \rho, \nu) = \frac{\sigma^2}{2^{\nu-1} \Gamma(\nu)} (\|s - t\| / \rho)^\nu K_\nu (\|s - t\| / \rho),$$

in which $\|\cdot\|$ is the Euclidean norm, $K_\nu$ is the modified Bessel function of the second kind with order $\nu > 0$, which governs the smoothness of the process; $\sigma^2 > 0$ is a scaling parameter; and $\rho > 0$ is a range parameter. Gaussian processes imply the vector of observations $X = (X(s_1), \ldots, X(s_N))^T \in \mathbb{R}^N$ at locations $\mathcal{S} = \{s_1, \ldots, s_N\} \subset \mathcal{D}$ is normally distributed $X \sim \mathcal{N}(0, \Sigma)$. The covariance matrix $\Sigma \in \mathbb{R}^{N \times N}$ is spatially-structured, with entries $\Sigma_{ij} = \kappa(s_i, s_j; \sigma^2, \rho, \nu)$. The Gaussian process assumption allows estimation of the field $\{X(s)\}_{s \in \mathcal{D}}$ at unobserved locations $\mathcal{S}_0 = \{s_{01}, \ldots, s_{0M}\} \subset \mathcal{D}$ via kriging, which uses conditional normal distributions for the unobserved responses. Standard Bayesian hierarchical modeling techniques for spatial data (e.g., Banerjee et al., 2015, Chapter 6) use conjugate
or weakly informative priors for the covariance parameters, specified via

\[ \sigma^2 \sim \text{Inverse-Gamma}(a, b), \]
\[ \rho \sim \text{Uniform}(L_0, U_0), \]
\[ \nu \sim \text{Uniform}(L_1, U_1). \]

We simulate one dataset with \( N = 300 \) locations, sampled uniformly from the unit square \( \mathcal{D} = [0, 1]^2 \) and with covariance parameters \((\sigma^2, \rho, \nu) = (1, .3, .5)\). We then estimate the covariance parameters as well as the field \( \{X(s)\}_{s \in \mathcal{D}} \) at \( M = 400 \) unobserved, gridded locations \( \mathcal{S}_0 \subset \mathcal{D} \). The priors are specified via \((a, b, L_0, U_0, L_1, U_1) = (2, 1, 0, 1, 0, 1)\).

### 4.2.2 Posterior inference and results

Standard techniques approximate posterior distributions with a Gibbs sampler and composition sampling (e.g., Banerjee et al., 2015, Chapter 6). Conjugate distributions are used to sample the scale \( \sigma^2 \) and unobserved field values \( X_0 = (X(s_{01}), \ldots, X(s_{0M})) \in \mathbb{R}^M \), but Metropolis steps are used for the range \( \rho \) and smoothness \( \nu \) parameters. The Gibbs sampler is used to draw 60,000 posterior samples for the covariance parameters, taking 2,043 seconds to complete; posterior inference uses the final 30,000 iterations. After drawing posterior samples for the covariance parameters, composition sampling is used to draw samples for the unobserved field values \( X_0 \) in parallel, taking 608 seconds to complete (Banerjee et al., 2015, pg. 126).

We use the BISQuE strategy to approximate the posterior density \( f(X_0|X) \). Sparse grid quadrature techniques are used to directly approximate the marginal posterior densities \( f(\sigma^2|X) \), \( f(\rho|X) \), and \( f(\nu|X) \). Table 2 connects this example’s notation to that used with BISQuE. When used as the BISQuE conditioning variable \( \theta_2 \), we map covariance parameters to the real line by log-transforming the scale parameter \( \sigma^2 \), and logit-transforming the range \( \rho \) and smoothness \( \nu \) parameters. All conditional and marginal posterior densities required for
BISQuE are computable in closed form up to a proportionality constant; refer to Banerjee et al. (2015, eqs. 2.15–16) for details.

Posterior inference via BISQuE and sparse grid quadrature is effectively identical to posterior inference via Gibbs sampling, but is computed with substantially less effort. Drawing posterior covariance parameter samples takes 2,043 seconds and composition sampling takes an additional 608 seconds, whereas the BISQuE and sparse grid quadrature approximations take a total of 238 seconds (Table 2), and posterior inference is nearly identical (Figures 3 to 4).

4.3 Remote effects spatial process models

4.3.1 Data and model

While most spatial data can be modeled with the assumption that distant points are uncorrelated, large-scale atmospheric circulations can induce dependence between fields separated by large distances. The resulting climate phenomena, known as teleconnection, may be modeled using remote effects spatial process (RESP) models, which can improve teleconnection-based predictions of seasonal precipitation (Hewitt, Hoeting, Done and Towler, 2018). The RESP model is given by

\[ Y(s, t) = x^T(s, t)\beta + w(s, t) + \gamma(s, t), \]  

(19)

which uses a stochastic teleconnection term

\[ \gamma(s, t) = \int_{D_z} z(r, t)\alpha(s, r)dr \]  

(20)

to extend standard geostatistical regression models for a process \( \{Y(s, t) : s \in D_Y, t \in T\} \) defined on a continuous spatial domain \( D_Y \) for discrete times \( T \). Regression coefficients \( \beta \) and spatially-correlated variation \( w(s, t) \) are augmented by (20), which uses doubly-indexed
random effects $\alpha(s, r)$ to aggregate the impact of remote covariates $\{z(r, t) : r \in D_Z, t \in T\}$, such as sea surface temperatures, on a distant response, such as the standardized deviation $Y(s, t)$ from mean seasonal precipitation. The authors adopt the climate science convention that mean precipitation is treated as known, and the standardized deviation $Y(s, t)$ is the scientifically interesting response variable to model.

The RESP model uses two isotropic Matérn covariance functions $\kappa(s, s'; \sigma_w^2, \rho_w, \nu_w)$, $\kappa(r, r'; \sigma_\alpha^2, \rho_\alpha, \nu_\alpha)$, and a nugget effect $\sigma_\varepsilon^2$ to define Gaussian processes that model the spatial variation $\{w(s, t) : s \in D_Y\}$ and teleconnection effects $\{\alpha(s, r) : s \in D_Y, r \in D_Z\}$. The Matérn smoothness parameters $\nu_w$ and $\nu_\alpha$ are treated as fixed, and standard priors are used to model the remaining regression coefficients $\beta$ and covariance parameters $\sigma_w^2$, $\rho_w$, $\sigma_\varepsilon^2$, $\sigma_\alpha^2$, and $\rho_\alpha$ (cf. Section 4.2.1).

We follow Hewitt et al. (2018) and use the RESP model to analyze Colorado precipitation data in a statistical downscaling-like scenario. The RESP model regresses standardized deviations $Y(s, t)$ from mean Colorado precipitation observed at 240 locations $s \in D_Y$ onto local surface temperatures $x(s, t)$ and Pacific Ocean sea surface temperatures $z(r, t)$. The model is fit to Winter averages from 1981–2012 and an ordinal response $\tilde{Y}(s, t)$ is predicted for Winter 2013, given the covariate values $x(s, t)$ and $z(r, t)$ for $t = 2013$. The distribution for $\tilde{Y}(s, t)$ is induced by known cut points $c_0(s), \ldots, c_m(s)$ and defined such that $P(\tilde{Y}(s, t) = v_i) = P(c_{i-1}(s) < Y(s, t) < c_i(s))$. In this application, the ordinal response $\tilde{Y}(s, t)$ represents below average $v_1$, about average $v_2$, or $v_3$ above average precipitation.

### 4.3.2 Posterior inference and results

Hewitt et al. (2018) construct a Gibbs sampler that approximates posterior distributions for the RESP model (19). Gibbs sampling is computationally expensive for the RESP model because two spatially-structured covariance matrices must be decomposed at each Gibbs iteration. Let $Y$ denote all observations $Y(s, t)$ from $t = 1981, \ldots, 2012$; $Y_0$ denote all unobserved responses $Y(s, t)$ at $t = 2013$; and $\tilde{Y}_0$ denote all unobserved ordinal responses.
$\tilde{Y}(s,t)$ at $t = 2013$. Conjugate distributions are used to sample the regression parameters $\beta$, scales $\sigma^2_w$ and $\sigma^2_\alpha$, and continuous predictions $Y_0$; and Metropolis steps are used for the ranges $\rho_w$ and $\rho_\alpha$. The Gibbs sampler is used to draw 41,000 posterior samples for the regression and covariance parameters, taking 8,331 seconds to complete; posterior inference discards the first 1,000 iterations as the chain mixes quickly, but requires many iterations to control Monte Carlo integration error. Composition sampling is then used to draw samples for the predicted response $Y_0$ in parallel, taking 755 seconds to complete. The continuous posterior predictive density $f(Y_0 | Y)$ is discretized after sampling to approximate $f(\tilde{Y}_0 | Y)$ by using the empirical quantiles of historical precipitation as cut points $c_0(s), \ldots, c_3(s)$.

We use the BISQuE strategy to approximate the posterior predictive densities $f(Y_0 | Y)$ and $f(\tilde{Y}_0 | Y)$. In particular, we use the BISQuE strategy to directly approximate $f(\tilde{Y}_0 | Y)$ by letting $h(\theta_1, \theta_2; X)$ in (11) be the conditional cumulative distribution function for $Y_0$. Table 2 connects this example’s notation to that used with BISQuE. When used as the BISQuE conditioning variable $\theta_2$, we map covariance parameters to the real line by log-transforming scale parameters $\sigma^2$ and logit-transforming range parameters $\rho$. All conditional and marginal posterior densities required for BISQuE are computable in closed form up to a proportionality constant; refer to Hewitt et al. (2018) for distributional results.

Posterior inference via BISQuE is effectively identical to posterior inference via Gibbs sampling, but is computed with substantially less effort. Drawing posterior covariance parameter samples takes 8,331 seconds and composition sampling takes an additional 755 seconds, whereas the BISQuE approximations take a total of 118 seconds (Table 2), and posterior inference is nearly identical (e.g., Figure 5). The approximate BISQuE and Gibbs posterior masses $\hat{P}(\tilde{Y}_0(s,t) = v_i | Y)$ agree to at least two decimal places for all 240 locations $s \in D_Y$ and values $v_1, v_2, v_3$; additional computing effort can further reduce approximation errors, but offers limited practical benefit because the discretization is coarse.
5 Discussion

We combine conditioning techniques with sparse grid quadrature rules to develop approximate Bayesian Inference via Sparse grid Quadrature Evaluation (BISQuE). Approximations (11) are developed by reformulating Bayesian posterior quantities, such as densities and expectations, so that they may be approximated as weighted mixtures of conditional quantities \( h(\theta_1, \theta_2; X) \). The integration nodes and weights from sparse grid quadrature rules are used to build mixing weights \( w^{(i, \ell)} \) and conditioning values \( \theta_2^{(i, \ell)} \). In a similar manner as general quadrature techniques and importance sampling methods, the final BISQuE approximation weights \( \tilde{w}^{(i, \ell)} \) use weight ratios \( f(\nu^{(i, \ell)} | X) / w(\nu^{(i, \ell)}, X) \) to align the “theoretical distribution” \( f(\nu | X) \) with the “sampling distribution” \( w(\nu, X) \) (Givens and Hoeting, 2013, pgs. 143, 181). Nested integration strategies enable BISQuE approximations (11) when models do not have closed form expressions for required components (Section 3.4). Posterior approximation via BISQuE is deterministic and computationally efficient, offering faster computation than MCMC methods for a wide range of models (5) and posterior quantities (8). In our applications, we find that BISQuE often reduces overall computing time by at least two orders of magnitude and yields nearly identical inference to standard MCMC approaches (Section 4).

The BISQuE approximation is similar to, and can be combined with Integrated Nested Laplace approximations (INLA) for latent Gaussian models (Rue et al., 2009). Combining BISQuE with INLA can yield an approximation technique that scales better to models with more hyperparameters. Similar to INLA, our framework will be most efficient when used to approximate low-dimensional posterior quantities, like marginal densities or joint densities with computationally tractable closed form expressions (e.g., \( f(X_0 | X) \) in Section 4.2). However, BISQuE does not require that a model have a latent Gaussian structure and is thus applicable to a broad class of models such as the population estimation model of Section 4.1.

We can combine the BISQuE approximation (11) and INLA because both methods
use conditioning and integration grids to yield fast deterministic posterior approximation.

In terms of the general hierarchical model (5), INLA specifies a hierarchical parameter model \( f(\theta_1, \theta_2) = f(\theta_1 | \theta_2)f(\theta_2) \) in which \( f(\theta_1 | \theta_2) \) is Gaussian and \( f(\theta_2) \) is a prior distribution for relatively low-dimensional hyperparameters \( \theta_2 \). Rue et al. (2009) define \( \theta_1 = (\theta_{11}, \ldots, \theta_{1i}, \ldots, \theta_{1n}) \), develop an integration grid, and use Laplace approximations for \( f(\theta_1 | \theta_2, X) \) and \( f(\theta_2 | X) \) to approximate the marginal posterior density \( f(\theta_{1i} | X) \). The nested Laplace approximations can be embedded in the BISQuE approximation (11), yielding posterior approximation that uses an alternate integration grid to INLA. The embedding can be beneficial because sparse grid quadrature rules allow for more computationally efficient approximation in models with higher dimensional hyperparameters \( \theta_2 \). Specifically, Rue et al. (2009) suggest creating integration grids for models with high-dimensional \( \theta_2 \) by using central composite design (CCD) methods—an experimental design and response surface technique for approximating second order surfaces with relatively few function evaluations (Box and Wilson, 1951). When integration is the main concern, sparse grid quadrature methods can require substantially fewer integration nodes in high dimensions (Novak and Ritter, 1999, Table 2, \( \ell = 3 \)) than CCD-based grids (Sanchez and Sanchez, 2005, Table 3).

Our BISQuE approximation advances Bayesian computing for hierarchical models, but open questions remain for wider application of the method. Notably, our approximation requires the ability to evaluate \( h(\theta_1, \theta_2; X) \) quickly, so may often be limited to marginal posterior inference for \( \theta_1 \) with relatively small dimension. Our approximation also relies on the availability of nested quadrature rules for \( \theta_2 \). It is difficult to develop quadrature rules for discrete variables, thus practical use of our approximation may be limited to models with parameters \( \theta_2 \) defined on continuous spaces \( \Omega_2 \). Fast convergence of our approximation also relies on the availability of accurate approximations to \( f(\theta_2 | X) \). If the BISQuE approximation (11) has not converged, intuition about numerical integration suggests the resulting approximation will likely underestimate posterior variability (Rue et al., 2009). However, Rue et al. (2009, Section 6.5) also point out that \( f(\theta_2 | X) \) often becomes increasingly Gauss-
sian as the dimension of $\theta_2$ grows since the Bayesian structure will increase variability and regularity will the dimension, which will help accelerate convergence.

The BISQuE methodology suggests continued development in several areas. Additional diagnostics should be developed for wider practical application of the BISQuE approximation (11). The approximation’s convergence can be monitored by checking the approximation’s stability as the level $q$ of the underlying sparse grid quadrature rule (4) is increased (Laurie, 1985). However, this does not necessarily provide a diagnostic that can assess how well conditioned a model (5) or posterior quantity (8) is for use with BISQuE. Drawing from importance sampling, studying the weight ratio $f(\nu^{(i,\ell)}|X)/w(\nu^{(i,\ell)}, X)$ in (11) at quadrature nodes $\nu^{(i,\ell)}$ may help diagnose practical issues. Theoretical smoothness properties of $h(\theta_1, \theta_2; X)$ or concentration of the posterior density $f(\theta_2|X)$ may also provide insight into the conditioning for specific models.

Software is available for implementing BISQuE approximations. We have developed the bisque package for R that computes BISQuE approximations for user-specified models. Custom implementations of BISQuE can also be developed for specific, high performance applications with the use of software libraries, including the mvQuad package for R and the SGMGA libraries for C and C++ (Burkardt, 2007; Weiser, 2016). These libraries contain tables and routines that compute sparse grid quadrature nodes and weights if $w(\nu, X)$ is a member of a standard family of weight functions (Givens and Hoeting, 2013, Table 5.6).

**Supplementary materials**

Additional information and supporting material for this article is available online at the journal’s website.
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Figure 1: Fur seals example: A) BISQuE (x) and Gibbs (□) approximations to the posterior density for total number of fur seal pups $f(N|c,r)$ are nearly identical. B) BISQuE (—) and Gibbs (⋯) approximations to the joint posterior density $f(U_1|c,r)$ are nearly identical.
Figure 2: Fur seals example: BISQuE (—) and Gibbs (---) approximations to the posterior densities $f(\alpha_i | c, r)$ are nearly identical.
Figure 3: Spatial model example: Relative differences between BISQuE and Gibbs approximations $\Delta(Y) = (Y_{BISQuE} - Y_{Gibbs})/Y_{Gibbs} \times 100\%$ for the posterior predictive means (A) and standard errors (B) for the field $\{X(s)\}_{s \in D}$ at unobserved locations $S_0$. Nearly all (95%) relative differences in the posterior mean (A) are less than 5.5% (median=0.4%); relative differences in the mean are artificially large in regions where the posterior mean is near 0. All relative differences in the posterior standard errors (B) are below 3.3% (median=1.4%).
Figure 4: Spatial model example: A, B, C) Sparse grid quadrature (—) and Gibbs (--) approximations to the posterior densities for the spatial covariance parameters \( \sigma^2, \rho, \nu \) are nearly identical. The true values of the parameters are marked by grey vertical lines. D) BISQuE (—) and Gibbs (--) approximations to the posterior density for new observation \( X(s_0) \) is nearly identical at \( s_0 = (.5, .2) \), for example.
Figure 5: BISQuE and Gibbs approximations to the mode of the discretized posterior predictive distributions $f(\tilde{Y}_0|Y)$ are nearly identical.
Table 1: Summary of steps to develop a BISQuE approximation.

1. Write posterior quantity of interest in BISQuE form (8).
   
   Computable approximations or exact expressions must exist for the components \( h(\theta_1, \theta_2; X) \) and \( f(\theta_2 | X) \). Section 3.4 proposes nested integration strategies (15) and (16) if approximation is necessary; nested Laplace approximations can also be used for components in latent Gaussian models (cf. Rue et al., 2009).

2. Select transformation \( \nu = T(\theta_2) \) to map \( \theta_2 \in \Omega_2 \) to \( \nu \in \mathbb{R}^p \).
   
   Favor transformations \( T \) that yield an approximately Gaussian posterior density \( f(\nu | X) \).

3. Apply the BISQuE approximation that uses unstandardized (11) or standardized (13) weights.
   
   The level \( q \in \mathbb{N} \) of the underlying sparse grid quadrature rule (4) determines the integration nodes \( \nu^{(i, \ell)} \) and weights \( w^{(i, \ell)} \).

4. Increase the level \( q \) of underlying quadrature rule (4) until the approximation (11) or (13) converges.
   
   Nested quadrature rules allow the level \( q \) approximation to reduce computational cost by reusing quadrature nodes and weight ratios from the level \( q - 1 \) approximation.
Table 2: Definitions of the parameters and posterior quantities for the BISQuE approximations in Section 4. $X = (c, r)$ for the fur seals example (Section 4.1), and $X = Y$ for the Remote effects spatial process model example (RESP, Section 4.3). The marginal posterior densities for the covariance parameters $(\sigma^2, \rho, \nu)$ in the spatial example (Section 4.2) are computed using sparse-grid quadrature methods (4) to directly marginalize the joint posterior distribution $f(\sigma^2, \rho, \nu | X)$ at each evaluation point. Computation times are also presented. For the RESP example, let $\theta^* = (\sigma_w^2, \sigma^2, \rho_w, \rho, \rho_\alpha)$ and $I(s) = (c_{i-1}(s), c_i(s))$.

| Example     | $h(\theta_1; X)$ | $h(\theta_1, \theta_2; X)$ | $\theta_1$ | $\theta_2$ | BISQuE | Gibbs |
|-------------|------------------|------------------------------|------------|------------|--------|-------|
| Fur seals   | $f(N|c, r)$      | $f(N|\theta_2, c, r)$       | $N (\alpha, U_1)$ | $0.3$ | $298$  |
|             | $f(\alpha_i|c, r)$ | $f(\alpha_i|\theta_2, c, r)$ | $\alpha_i (N, U_1)$ | $0.1$ | $298$  |
|             | $f(U_1|c, r)$    | $f(U_1|\theta_2, c, r)$    | $U_1 \alpha$ | $5.0$ | $298$  |
| Spatial     | $E[X_0|X]$       | $E[X_0|\theta_2, X]$       | $X_0 (\sigma^2, \rho, \nu)$ | $6$  | $2,651$|
|             | $\text{Var}(X_0|X)$ | (10)                       | $X_0 (\sigma^2, \rho, \nu)$ | $6$  | $2,651$|
|             | $f(X_0|X)$       | $f(X_0|\theta_2, X)$       | $X_0 (\sigma^2, \rho, \nu)$ | $6$  | $2,651$|
|             | $f(\sigma^2|X)$ | $\text{N/A}$               | $\sigma^2 (\rho, \nu)$ | $74$ | $2,043$|
|             | $f(\rho|X)$     | $\text{N/A}$               | $\rho (\sigma^2, \nu)$ | $74$ | $2,043$|
|             | $f(\nu|X)$      | $\text{N/A}$               | $\nu (\sigma^2, \rho)$ | $74$ | $2,043$|
| RESP        | $f(Y_0|Y)$       | $f(Y_0|\theta_2, Y)$       | $Y_0 \theta^*$ | $118$ | $9,086$|
|             | $f(\tilde{Y}_0|Y)$ | $P(Y_0(s,t) \in I(s)|\theta_2, Y)$ | $Y_0 \theta^*$ | $118$ | $9,086$|