Fast Automatic Bayesian Cubature Using Lattice Sampling

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Abstract Automatic cubatures approximate multidimensional integrals to user-specified error tolerances. For high dimensional problems, it makes sense to fix the sampling density but determine the sample size, \( n \), automatically. Bayesian cubature postulates that the integrand is an instance of a stochastic process. Here we assume a Gaussian process parameterized by a constant mean and a covariance function defined by a scale parameter times a parameterized function specifying how the integrand values at two different points in the domain are related. These parameters are estimated from integrand values or are given non-informative priors. The sample size, \( n \), is chosen to make the half-width of the credible interval for the Bayesian posterior mean no greater than the error tolerance.

The process just outlined typically requires vector-matrix operations with a computational cost of \( O(n^3) \). Our innovation is to pair low discrepancy nodes with matching kernels that lower the computational cost to \( O(n \log n) \). This approach is demonstrated using rank-1 lattice sequences and shift-invariant kernels. Our algorithm is implemented in the Guaranteed Automatic Integration Library (GAIL).

Keywords Bayesian cubature · Fast automatic cubature · GAIL · Probabilistic numeric methods

1 Introduction

Cubature is the problem of inferring a numerical value for an integral, \( \mu := \int g(x) \, dx \), where \( \mu \) has no closed form analytic expression. Typically, \( g \) is accessible as a black-box algorithm. Cubature is a key component of many problems in scientific computing, finance, statistical modeling, and machine learning.

The integral may often be expressed as

\[
\mu := E[f(X)] = \int_{[0,1]^d} f(x) \, dx, \tag{1}
\]

where \( f : [0,1]^d \to \mathbb{R} \) is the integrand, and \( X \sim \mathcal{U}([0,1]^d) \). The process of transforming the original integral into the form of (1) is not addressed here. See [6, Section 2.11] for a discussion of variable transformations. The cubature may be an affine function of integrand values:

\[
\hat{\mu} := w_0 + \sum_{i=1}^{n} f(x_i) w_i, \tag{2}
\]

where the weights, \( w_0 \), and \( \mathbf{w} = (w_i)_{i=1}^{n} \in \mathbb{R}^n \), and the nodes, \( \{x_i\}_{i=1}^{n} \subseteq [0,1]^d \), are chosen to make the error, \( |\mu - \hat{\mu}| \), small. The integration domain \([0,1]^d\) is convenient for the low discrepancy node sets [6,24] that we use. The nodes are assumed to be deterministic.

We construct a reliable stopping criterion that determines the number of integrand values, \( n \), required to ensure that the error is no greater than a user-defined error tolerance denoted by \( \varepsilon \), i.e.,

\[
|\mu - \hat{\mu}| \leq \varepsilon. \tag{3}
\]

Rather than relying on strong assumptions about the integrand, such as an upper bound on its variance or total variation, we construct a stopping criterion that is based on a credible interval arising from a Bayesian approach to the problem. We build upon the work of Briol et al. [1], Diaconis [5], O’Hagan [18], Ritter [22],...
The primary contribution of this article is to demonstrate how the choice of a family of covariance kernels that match the low discrepancy sampling nodes facilitates fast computation of the cubature and the data-driven stopping criterion. Our cubature requires n function values—at a cost of $\mathcal{O}(n \log(n))$ operations to check whether the error tolerance is satisfied. The total cost of our algorithm is then $\mathcal{O}(n \log(n))$ operations to check whether the error tolerance is satisfied. The total cost of our algorithm is then

$$\mathcal{O}(n \log(n)),$$

for all $\alpha \neq 0$, $n \in \mathbb{N}$, $x_1, \ldots, x_n \in [0, 1]^d$. (4)

The function, $C$, and the Gram matrix, $C$ depend implicitly on $\theta$, but the notation may omit this parameter for simplicity’s sake.

For a Gaussian process, all vectors of linear functionals of $f$ have a multivariate Gaussian distribution. Defining $f := \{f(x_j)\}_{j=1}^n$ as the multivariate normal vector of function values, it follows that

$$f \sim \mathcal{N}(m, s^2 C),$$

where $1$ is a vector of all ones, $m \sim \mathcal{N}(m, s^2 c_0)$, (5b)

$$\text{cov}(f, \mu) = \left(\int_{[0,1]^d} C(t, x) \, dt\right)^n =: c.$$

We need the following lemma to derive the distribution of the posterior error of our cubature.

**Lemma 1.**[21] (A.6), (A.11–13)] If $Y = (Y_1, Y_2)^T \sim \mathcal{N}(m, C)$, where $Y_1$ and $Y_2$ are random vectors of arbitrary length, and

$$m = \begin{pmatrix} m_1 \\ m_2 \end{pmatrix} = \begin{pmatrix} E(Y_1) \\ E(Y_2) \end{pmatrix},$$

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = \begin{pmatrix} \text{var}(Y_1) & \text{cov}(Y_1, Y_2) \\ \text{cov}(Y_2, Y_1) & \text{var}(Y_2) \end{pmatrix},$$

then

$$Y_1 | Y_2 \sim \mathcal{N}(m_1 + C_{12} C_{22}^{-1} (Y_2 - m_2), C_{11} - C_{12} C_{22}^{-1} C_{21}).$$

Moreover, the inverse of the matrix $C$ may be partitioned as

$$C^{-1} = \begin{pmatrix} A_{11} & A_{12}^T \\ A_{21} & A_{22} \end{pmatrix},$$

$$A_{11} = (C_{11} - C_{12} C_{22}^{-1} C_{21})^{-1}, \quad A_{21} = -C_{22}^{-1} C_{21} A_{11},$$

$$A_{22} = C_{22}^{-1} + C_{22}^{-1} C_{21} A_{11} C_{22}^{-1}.$$

It follows from Lemma 1 that the conditional distribution of the integral given observed function values,
\( f = y \) is also Gaussian:
\[
\mu(f = y) \sim N(m(1 - c^T \Sigma^{-1}) + c^T \Sigma^{-1} y,
\]
\[
s^2(c_0 - c^T \Sigma^{-1} c)). \tag{6}
\]
The natural choice for the cubature is the posterior mean of the integral, namely,
\[
\hat{\mu}(f = y) = m(1 - T^{-1} c) + T^{-1} y,
\]
which takes the form of \( \hat{\mu} \). Under this definition, the cubature error has zero mean and a variance depending on the choice of nodes:
\[
(m - \hat{\mu})(f = y) \sim N(0, s^2(c_0 - c^T \Sigma^{-1} c)).
\]
A credible interval for the integral is given by
\[
P[f | \mu - \hat{\mu} \leq \epsilon_{CI}] = 99%.
\tag{8a}
\]
\[
\epsilon_{CI} = 2.58s \sqrt{c_0 - c^T \Sigma^{-1} c} \tag{8b}
\]
Naturally, 2.58 and 99% can be replaced by other quantiles and credible levels.

2.2 Parameter estimation

The credible interval in (8) suggests how our automatic Bayesian cubature proceeds. Integrand data is accumulated until the width of the credible interval, \( \epsilon_{CI} \), is no greater than the error tolerance. As \( n \) increases, one expects \( \sqrt{c_0 - c^T \Sigma^{-1} c} \) to decrease for well-chosen nodes, \( \{x_i\}_{i=1} \).

Note that \( \epsilon_{CI} \) has no explicit dependence on the integrand values, even though one would intuitively expect that larger integrand should imply a larger \( \epsilon_{CI} \). This is because parameters, \( m, s, \) and \( \theta \), have not yet been inferred from integrand data. After inferring the parameters, \( \epsilon_{CI} \) does reflect the size of the integrand values. This section describes three approaches to parameter estimation.

2.2.1 Empirical Bayes

One approach is to estimate the parameters via maximum likelihood estimation (MLE). The log-likelihood function of the parameters given the function data \( y \) is:
\[
\ell(s, m, \theta | y) = -\frac{1}{2} s^2(y - m \Sigma^{-1} y) - \frac{1}{2} \log(\det(\Sigma)) - \frac{n}{2} \log(s^2) + \text{constants}.
\]
Maximizing the log-likelihood first with respect to \( m \), then with respect to \( s \), and finally with respect to \( \theta \) yields
\[
m_{\text{MLE}} = \frac{1^T \Sigma^{-1} y}{1^T \Sigma^{-1} 1},
\]
\[
s_{\text{MLE}} = \frac{y - m_{\text{MLE}} 1^T \Sigma^{-1} (y - m_{\text{MLE}})}{n}
\tag{9}
\]
\[
\theta_{\text{MLE}} = \arg \min \left\{ \log \left( y^T \left( \begin{array}{c} C_1 - C_1 1^T \Sigma^{-1} \end{array} \right) y \right) + \frac{1}{n} \log(\det(\Sigma)) \right\}.
\tag{10}
\]
The MLE estimate of \( \theta \) balances minimizing the covariance scale factor, \( s_{\text{MLE}}^2 \), against minimizing \( \det(\Sigma) \).

Under these estimates of \( \theta \) balances the empirical Bayes estimates and the credible interval \( \epsilon_{CI} \) simplify to
\[
\hat{\mu}_{\text{MLE}} = \frac{(1 - 1^T \Sigma^{-1} c) c}{1^T \Sigma^{-1} 1} C_1^{-1} y,
\tag{12}
\]
\[
\epsilon^2_{\text{MLE}} = \frac{2.58^2}{n} y^T \left( \begin{array}{c} C_1 - C_1 1^T \Sigma^{-1} \end{array} \right) y 
\times (c_0 - c^T \Sigma^{-1} c),
\tag{13}
\]
\[
P[f | \mu - \hat{\mu}_{\text{MLE}} \leq \epsilon_{\text{MLE}}] = 99%.
\tag{14}
\]
Here \( c_0, c, \) and \( C \) are assumed implicitly to be based on \( \theta = \theta_{\text{MLE}} \).

2.2.2 Full Bayes

Rather than use maximum likelihood to determine \( m \) and \( s \) one can treat them as hyperparameters with a non-informative, conjugate prior, namely \( p_{m,s}(\xi, \lambda) \propto 1/\lambda \). Then the posterior density for the integral given the data using Bayes theorem is
\[
\rho_{\mu}(z | f = y) = \int \int \rho_{\mu}(z | f = y, m = \xi, s^2 = \lambda) \rho_{f}(\xi, \lambda) p_{m,s}(\xi, \lambda) d\xi d\lambda
\]
\[
\propto \int \frac{1}{\lambda^{(n+3)/2}} \exp \left( \frac{1}{2\lambda} \left( \frac{\|z - (1 - c^T \Sigma^{-1} c) y\|^2}{c_0 - c^T \Sigma^{-1} c} + (y - \xi 1^T \Sigma^{-1} y - \xi 1) \right) \right) d\xi d\lambda
\]
\[
\propto \int \frac{1}{\lambda^{(n+3)/2}} \cdot \cdots \cdot \int \exp \left( - \frac{\alpha^2 - 2\beta \xi + \gamma}{2\lambda(c_0 - c^T \Sigma^{-1} c)} \right) d\xi d\lambda,
\]

\[
\text{where } \alpha, \beta, \gamma \text{ are defined as in (5), (6) and } p_{m,s}(\xi, \lambda) \propto 1/\lambda. \]
where 
\[
\alpha = (1 - c^T C^{-1} 1)^2 + 1^T C^{-1} 1 (c_0 - c^T C^{-1} c), \\
\beta = (1 - c^T C^{-1} 1)(z - c^T C^{-1} y) \\
+ 1^T C^{-1} y (c_0 - c^T C^{-1} c), \\
\gamma = (z - c^T C^{-1} y)^2 + y^T C^{-1} y (c_0 - c^T C^{-1} c).
\]

In the derivation above and below, factors that are independent of \( \xi, \lambda, \) or \( z \) can be discarded since we only need to preserve the proportion. But, factors that depend on \( \xi, \lambda, \) or \( z \) must be kept. Completing the square, \( \alpha \xi^2 - 2 \beta \xi + \gamma = \alpha(\xi - \beta/\alpha)^2 - (\beta^2/\alpha) + \gamma \), allows us to evaluate the integrals with respect to \( \xi, \lambda \):

\[
\rho_{\mu}(z|f = y) = \int_0^\infty \int_0^\infty \frac{1}{\lambda^{(n+3)/2}} \exp\left(-\frac{\gamma - \beta^2/\alpha}{2\lambda(c_0 - c^T C^{-1} c)}\right) \frac{d\xi d\lambda}{2\lambda(c_0 - c^T C^{-1} c)}.
\]

2.2.3 Generalized Cross-Validation

A third parameter optimization technique is leave-one-out cross-validation (CV). Let \( \tilde{y}_i = E[f(x_i)|f_i = y_{\cdot i}] \), where the subscript \(-i\) denotes the vector excluding the \( i \)th component. This is the conditional expectation of \( f(x_i) \) given all data but the function value at \( x_i \). The cross-validation criterion, which is to be minimized, is sum of squares of the difference between these conditional expectations and the observed values:

\[
CV = \sum_{i=1}^n (y_i - \tilde{y}_i)^2.
\]

Let \( A = C^{-1} \), let \( \zeta = A(y - m_1) \), and partition \( C \), \( A \), and \( \zeta \) as

\[
C = \begin{pmatrix} c_{ii} & C_{T_{-i},i}^T \\ C_{T_{-i},i} & C_{-i,-i} \end{pmatrix}, \quad A = \begin{pmatrix} a_{ii} \ A_{T_{-i},i}^T \\ A_{-i,i} \ A_{-i,-i} \end{pmatrix}, \quad \zeta = \begin{pmatrix} \zeta_i \\ \zeta_{-i} \end{pmatrix},
\]

where the subscript \( i \) denotes the \( i \)th row or column, and the subscript \(-i\) denotes all rows or columns except the \( i \)th. Following this notation, Lemma 22 implies that

\[
\tilde{y}_i = m + C_{-i,-i}^{-1} (y_{-i} - m_1) \\
\zeta_i = a_{ii}(y_i - m) + A_{-i,i}^T (y_{-i} - m_1) \\
= a_{ii}(y_i - m) - C_{T_{-i},i} C_{-i,-i}^{-1} (y_{-i} - m_1)
\]

Thus, (17) may be re-written as

\[
CV = \sum_{i=1}^n \left( \frac{\zeta_i}{a_{ii}} \right)^2, \quad \zeta = C^{-1} (y - m_1).
\]

The generalized cross-validation criterion (GCV) replaces the \( i \)th diagonal element of \( A \) by the average diagonal element of \( A \) [10] [25]:

\[
GCV = \frac{\sum_{i=1}^n \zeta_i^2}{(1/n) \sum_{i=1}^n a_{ii}} \\
= \frac{(y - m_1)^T C^{-2} (y - m_1)}{(1/n) \text{trace}(C^{-1})^2}.
\]

The loss function GCV depends on \( m \) and \( \theta \), but not on \( s \). Minimizing the GCV yields

\[
m_{\text{GCV}} = \frac{1^T C^{-2} y}{1^T C^{-2} 1}.
\]

\[
\theta_{\text{GCV}} = \arg \min_{\theta} \left\{ \log \left( y^T \left[ C^{-2} - \frac{C^{-1} 1 1^T C^{-1}}{1^T C^{-2} 1} \right] y \right) \\
- 2 \log \left( \text{trace}(C^{-1}) \right) \right\}.
\]

Plugging this value of \( m \) into (17) yields

\[
\hat{\mu}_{\text{GCV}} = \left( \frac{(1 - 1^T C^{-1} 1) C^{-1} 1}{1^T C^{-2} 1} + c \right)^T C^{-1} y.
\]
An estimate for \( s \) may be obtained by noting that by Lemma 1
\[
\text{var}(f(x_i)|f_{-i} = y_{-i}) = s^2 a_{ii}^{-1}.
\]
Thus, we may estimate \( s \) using an argument similar to that used in deriving the GCV and then substituting \( s_{GCV}^2 \) for \( m \):
\[
s^2 = \text{var}(f(x_i)|f_{-i} = y_{-i}) a_{ii}
= \frac{1}{n} \sum_{i=1}^{n} (y_i - \tilde{y})^2 a_{ii}
= \frac{1}{n} \sum_{i=1}^{n} \tilde{c}_i^2 a_{ii}
= \frac{1}{n} \sum_{i=1}^{n} \tilde{c}_i^2
= \frac{(y - m)^T C^{-2} (y - m)}{\text{trace}(C^{-1})}
\approx s_{GCV}^2,
\]
where
\[
s_{GCV}^2 := y^T \left[ C^{-2} - \frac{C^{-2} 11^T C^{-2}}{11^T C^{-1}} \right] y \left[ \text{trace}(C^{-1}) \right]^{-1}.
\]
The confidence interval based on GCV corresponds to (8) with the estimated \( C \), is replaced by \( bC \) for some positive constant \( b \), the cubature, \( \tilde{\mu} \), the estimates of \( \theta \), and the cubic interval widths, \( \text{err}_{CI} \), all remain unchanged. The estimates of \( s^2 \) are multiplied by \( b^{-1} \), as would be expected.

2.3 The automatic Bayesian cubature algorithm

The previous section presents three credible intervals, (14), (15), and (21), for the \( \mu \), the desired integral. Each credible interval is based on different assumptions about the hyperparameters \( m \), \( s \), and \( \theta \). We stress that one must estimate these hyperparameters or assume a prior distribution on them because the credible intervals are used as stopping criteria for our cubature rule. Since a credible intervals makes a statement about a typical function—not an outlier—one must try to ensure that the integrand is a typical draw from the assumed Gaussian process.

Our Bayesian cubature algorithm increases the sample size until the width of the credible interval is small enough. This is accomplished through successively doubling the sample size. The steps are detailed in Algorithm 1.

Algorithm 1 Automatic Bayesian Cubature

**Require:** A generator for the sequence \( x_1, x_2, \ldots \); a black-box function, \( f \); an absolute error tolerance, \( \varepsilon > 0 \); the positive initial sample size, \( n_0 \); the maximum sample size \( n_{\max} \)

1: \( n \leftarrow n_0, n' \leftarrow 0, \text{err}_{CI} \leftarrow \infty \)
2: **while** \( \text{err}_{CI} > \varepsilon \) and \( n \leq n_{\max} \) **do**
3: Generate \( \{x_i\}_{i=0}^{n_{\max}+1} \) and sample \( \{f(x_i)\}_{i=0}^{n_{\max}+1} \)
4: Compute \( \theta \) by (11) or (18)
5: Compute \( \text{err}_{CI} \) according to (13), (16), or (20)
6: \( n' \leftarrow n, n \leftarrow 2n' \)
7: **end while**
8: Update sample size to compute \( \hat{\mu} \), \( n \leftarrow n' \)
9: Compute \( \hat{\mu} \), the approximate integral, according to (12) or (19)
10: **return** \( \hat{\mu}, n \) and \( \text{err}_{CI} \)

2.4 Example with the Matérn kernel

To demonstrate automatic Bayesian cubature consider a Matérn covariance kernel:
\[
C_\theta(x, t) = \prod_{k=1}^{d} \exp(-\theta |x_k - t_k|)(1 + \theta |x_k - t_k|),
\]
and Sobol points as the nodes. Also, consider the integration problem of evaluating multivariate normal probabilities:
\[
\mu = \int \frac{\exp(-\frac{1}{2} t^T \Sigma^{-1} t)}{(2\pi)^{d/2} \det(\Sigma)} \, dt,
\]
where \( (a, b) \) is a finite, semi-infinite or infinite box in \( \mathbb{R}^d \). This integral does not have an analytic expression for general \( \Sigma \), so cubatures are required.

Genz [8] introduced a variable transformation to transform (22) into an integral on the unit cube. Let \( \Sigma = LL^T \) be the Cholesky decomposition where \( L = (l_{jk})_{j,k=1}^{d} \) is a lower triangular matrix. Iteratively define
\[
\alpha_1 = \Phi(a_1), \quad \beta_1 = \Phi(b_1)
\]
\[
\alpha_j(x_1, \ldots, x_{j-1}) = \Phi\left( \frac{1}{l_{jj}} \left( a_j - \sum_{k=1}^{j-1} l_{jk} \Phi^{-1}(\alpha_k + x_k(\beta_k - \alpha_k)) \right) \right),
\]
\( j = 2, \ldots, d, \)
\[
\beta_j(x_1, \ldots, x_{j-1}) = \Phi\left( \frac{1}{l_{jj}} \left( b_j - \sum_{k=1}^{j-1} l_{jk} \Phi^{-1}(\alpha_k + x_k(\beta_k - \alpha_k)) \right) \right),
\]
\( j = 2, \ldots, d, \)
\[
f_{\text{Genz}}(x) = \prod_{j=1}^{d} [\beta_j(x) - \alpha_j(x)].
\]
where \( \Phi \) is the cumulative standard normal distribution function. Then, \( \mu = \int_{[0,1]^{d-1}} f_{\text{Genz}}(x) \, dx. \)
We use the following parameter values in the simulation:

\[ d = 3, \quad a = \begin{pmatrix} -6 \\ -2 \\ -2 \end{pmatrix}, \quad b = \begin{pmatrix} 5 \\ 2 \\ 1 \end{pmatrix}, \quad L = \begin{pmatrix} 4 & 1 & 1 \\ 0 & 1 & 0.5 \\ 0 & 0 & 0.25 \end{pmatrix}. \]

The node sets are randomly scrambled Sobol points \( [6, 7] \). The results for \( \varepsilon = 10^{-2}, 10^{-3}, 10^{-4}, \) and \( 10^{-5} \) and 100 scrambles for each \( \varepsilon \) are shown in Figure 2. We observe the algorithm meets the error criterion 95% of the time. As shown in Figure 2, computation time increases rapidly with \( n \). The maximum likelihood estimation of \( \theta \), which requires repeated evaluation of the objective function, is the most time consuming of all. It takes tens of seconds to compute \( \hat{\mu}_n \) once with \( \varepsilon = 10^{-5} \). In contrast, this example in Section 5 take less than a hundredth of a second to compute \( \hat{\mu}_n \) once with \( \varepsilon = 10^{-5} \) using our new algorithm. Not only is the Bayesian cubature with the the Matérn kernel slow, but also \( C \) becomes highly ill-conditioned as \( n \) increases. So, Algorithm 1 in its current form is impractical.

3 Fast Automatic Bayesian Cubature

The generic automatic Bayesian cubature algorithm described in the last section requires \( O(n^3) \) operations to estimate \( \theta \), compute the credible interval width, and compute the cubature. Now we explain how to speed up the calculations. A key is to choose kernels that match the nodes, \( \{x_i\}_{i=1}^n \), so that the vector-matrix operations required by Bayesian cubature can be accomplished using fast transforms at a cost of \( O(n \log(n)) \).

3.1 Fast Transform Kernel

We make some assumptions about the relationship between the covariance kernel and the nodes, which will be shown to hold in Section 4 for rank-1 lattices and shift-invariant kernels. First we introduce the notation

\[ C = \left( C_{\theta}(x_i, x_j) \right)_{i,j=1}^n = \left( C_1, \ldots, C_n \right) \]

\[ = \frac{1}{n} \mathbf{V} \Lambda \mathbf{V}^H, \quad \mathbf{V}^H = n \mathbf{V}^{-1}, \quad \mathbf{V} = (v_1, \ldots, v_n)^T = (V_1, \ldots, V_n), \]

\[ C^p = \frac{1}{n} \mathbf{V} \Lambda^p \mathbf{V}^H, \quad \forall p \in \mathbb{Z}, \]

where \( \mathbf{V}^H \) is the Hermitian of \( \mathbf{V} \). The columns of matrix \( \mathbf{V} \) are eigenvectors of \( \mathbf{C} \), and \( \Lambda \) is a diagonal matrix of eigenvalues of \( \mathbf{C} \). For any \( n \times n \) vector \( b \), define the notation \( \tilde{b} := \mathbf{V}^H b \).

We make three assumptions that allow the fast computation:

\[ \mathbf{V} \] may be identified analytically, \quad (25a)

\[ v_1 = V_1 = 1, \quad (25b) \]

\[ \mathbf{V}^H b \] requires only \( O(n \log(n)) \) operations \( \forall b \). \quad (25c)

We call the transformation \( b \mapsto \mathbf{V}^H b \) a fast transform and \( C \) a fast transform kernel.
Under assumptions (25) the eigenvalues may be identified as the fast transform of the first column of $\mathbf{C}$:
\[
\mathbf{\lambda} = \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_n \end{pmatrix} = \Lambda \mathbf{1} = \Lambda \mathbf{v}_1^T = \left( \frac{1}{n} \mathbf{V}^H \mathbf{V} \right) \Lambda \mathbf{v}_1^T = \mathbf{V}^H \left( \frac{1}{n} \mathbf{V} \Lambda \mathbf{v}_1 \right) = \mathbf{V}^H \mathbf{C}_1 = \tilde{\mathbf{C}}_1, \tag{26}
\]
Where $\mathbf{1}$ is the identity matrix. Also note that the fast transform of $\mathbf{1}$ has a simple form
\[
\tilde{\mathbf{1}} = \mathbf{V}^H \mathbf{1} = \mathbf{V}^H \mathbf{V} \mathbf{1} = \begin{pmatrix} n \\ 0 \\ \vdots \\ 0 \end{pmatrix}.
\]

Many of the terms that arise in the calculations in Algorithm 1 take the form $a^T \mathbf{C}^p b$ for real $a$ and $b$ and integer $p$. These can be calculated via the transforms $\tilde{a} = \mathbf{V}^H a$ and $\tilde{b} = \mathbf{V}^H b$ as
\[
a^T \mathbf{C}^p b = \frac{1}{n} a^T \mathbf{V} \Lambda^p \mathbf{V}^H b = \frac{1}{n} \tilde{a}^T \Lambda^p \tilde{b} = \frac{1}{n} \sum_i \lambda_i^p \tilde{a}_i \tilde{b}_i.
\]
In particular,
\[
\tilde{\mathbf{1}} = \mathbf{V}^H \mathbf{1} = \mathbf{V}^H \mathbf{V} \mathbf{1} = \begin{pmatrix} n \\ 0 \\ \vdots \\ 0 \end{pmatrix}.
\]

3.2 Empirical Bayes

Under assumptions (25), the empirical Bayes parameters in (9), (10), (11), (12), and (13) can be expressed in terms of the fast transforms of the function data, the first column of the Gram matrix, and $\mathbf{c}$ as follows:
\[
m_{\text{MLE}} = \frac{\hat{y}_1}{n} = \frac{1}{n} \sum_{i=1}^n y_i,
\]
\[
s_{\text{MLE}}^2 = \frac{1}{n^2} \sum_{i=2}^n \frac{|\tilde{y}_i|^2}{\lambda_i},
\]
\[
\theta_{\text{MLE}} = \arg\min_{\theta} \left[ \log \left( \sum_{i=2}^n \frac{|\tilde{y}_i|^2}{\lambda_i} \right) \right. + \left. \frac{1}{n} \sum_{i=1}^n \log(\lambda_i) \right]. \tag{28}
\]
\[
\hat{\mu}_{\text{MLE}} = \frac{\hat{y}_1}{n} + \frac{1}{n} \sum_{i=2}^n \frac{\tilde{c}_i \tilde{y}_i}{\lambda_i}.
\]
\[
\text{err}_{\text{MLE}} = \frac{2.58}{n} \sqrt{\sum_{i=2}^n \frac{|\tilde{y}_i|^2}{\lambda_i} \left( c_0 - \frac{1}{n} \sum_{i=1}^n \frac{|\tilde{c}_i|^2}{\lambda_i} \right)}.
\]

Since all the quantities on the right hand sides can be obtained in $O(n \log(n))$ operations by fast transforms, the left hand sides are all computable using the asymptotic computational cost.

Under the further assumption (27), it follows that
\[
\hat{\mu}_{\text{MLE}} = \frac{\hat{y}_1}{n} = \frac{1}{n} \sum_{i=1}^n y_i,
\]
\[
\text{err}_{\text{MLE}} = \frac{2.58}{n} \sqrt{\sum_{i=2}^n \frac{|\tilde{y}_i|^2}{\lambda_i} \left( 1 - \frac{n}{\lambda_1} \right)} \tag{29}.
\]
Thus, in this case $\hat{\mu}$ is simply the sample mean.

3.3 Full Bayes

For the full Bayes approach the cubature is the same as for empirical Bayes. We also defer to empirical Bayes to estimate the parameter $\theta$. The width of the confidence interval is $\text{err}_{\text{full}} := t_{n-1,0.995} \hat{\sigma}_{\text{full}}$, where $\hat{\sigma}^2_{\text{full}}$ can also be computed swiftly under assumptions (25):
\[
\hat{\sigma}^2_{\text{full}} = \frac{1}{n(n-1)} \sum_{i=2}^n \frac{|\tilde{y}_i|^2}{\lambda_i}
\]
\[
\times \left[ \frac{\lambda_1}{n} \left( 1 - \frac{\tilde{c}_1}{\lambda_1} \right)^2 + c_0 - \frac{1}{n} \sum_{i=1}^n \frac{|\tilde{c}_i|^2}{\lambda_i} \right],
\]
Under assumption (27) further simplification can be made:
\[
\hat{\sigma}^2_{\text{full}} = \frac{1}{n(n-1)} \sum_{i=2}^n \frac{|\tilde{y}_i|^2}{\lambda_i} \left( \frac{\lambda_1}{n} - 1 \right),
\]
It follows that
\[
\text{err}_{\text{full}} = t_{n-1,0.995} \sqrt{\frac{1}{n(n-1)} \sum_{i=2}^n \frac{|\tilde{y}_i|^2}{\lambda_i} \left( \frac{\lambda_1}{n} - 1 \right)} \tag{30}.
\]
3.4 Generalized Cross-Validation

GCV yields a different cubature, which nevertheless can also be computed quickly using the fast transform. Under assumptions [25],

$$m_{\text{GCV}} = m_{\text{MLE}} = \frac{\hat{y}_1}{n} = \frac{1}{n} \sum_{i=1}^{n} y_i,$$

$$s_{\text{GCV}}^2 = \frac{1}{n} \sum_{i=2}^{n} \frac{\|\tilde{y}_i\|^2}{\lambda_i^2} \left[ \frac{1}{n} \sum_{i=1}^{n} \lambda_i \right]^{-1},$$

$$\theta_{\text{GCV}} = \arg\min_\theta \left[ \log \left( \frac{\sum_{i=1}^{n} \|\tilde{y}_i\|^2}{\lambda_i^2} \right) - 2 \log \left( \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\lambda_i} \right) \right], \quad (31)$$

$$\hat{\mu}_{\text{GCV}} = \hat{\mu}_{\text{MLE}} = \frac{\hat{y}_1}{n} + \frac{1}{n} \sum_{i=2}^{n} \frac{\tilde{c}_i \tilde{y}_i}{\lambda_i},$$

$$\text{err}_{\text{GCV}} = \frac{2.58}{n} \left\{ \frac{1}{2} \left[ \frac{1}{n} \sum_{i=1}^{n} \lambda_i \right] \right\}^{1/2} \times \left( c_0 - \frac{1}{n} \sum_{i=1}^{n} \frac{\tilde{c}_i \tilde{y}_i}{\lambda_i} \right)^{1/2}. \quad (32)$$

Moreover, under further assumption [27], it follows that

$$\hat{\mu}_{\text{GCV}} = \hat{\mu}_{\text{MLE}} = \hat{\mu}_{\text{ml}} = \frac{\hat{y}_1}{n} = \frac{1}{n} \sum_{i=1}^{n} y_i, \quad (33)$$

In this case too, \( \hat{\mu} \) is simply the sample mean.

4 Integration Lattices and Shift Invariant Kernels

The preceding sections lay out an automatic Bayesian cubature algorithm whose computational cost is only \( O(n \log(n)) \) if \( n \) function values are used. However, this algorithm relies on covariance kernel functions, \( C \) and node sets, \( \{x_i\}_{i=1}^{n} \) that satisfy assumptions [25]. We also want to satisfy assumption [27]. To facilitate the fast transform, \( n \) must be power of 2.

4.1 Extensible Integration Lattice Node Sets

The set of nodes used is defined by a shifted extensible integration lattice node sequence, which takes the form

$$x_i = h\phi(i - 1) + \Delta \mod 1, \quad i \in \mathbb{N}.$$

Here, \( h \) is a \( d \)-dimensional generating vector of positive integers, \( \Delta \) is some point in \([0, 1)^d\), often chosen at random, and \( \{\phi(i)\}_{i=0}^{n} \) is the van der Corput sequence, defined by reflecting the binary digits of the integer about the decimal point, i.e.,

$$i = 0 \ 1 \ 2 \ 3 \ 4 \ 5 \ 6 \ 7 \ \cdots \quad i = 0.0 \ 1.0 \ 2.0 \ 3.0 \ 4.0 \ 5.0 \ 6.0 \ 7.0 \ \cdots \quad \phi(i) = 0.025 \ 0.05 \ 0.075 \ 0.125 \ 0.15 \ 0.2 \ 0.3 \ 0.4 \ 0.5 \ \cdots \quad (34)$$

An example of 64 nodes is given in Figure 3. The even coverage of the unit cube is ensured by a well chosen generating vector. The choice of generating vector is typically done offline by computer search. See [9][13] for more on extensible integration lattices.

![Fig. 3: Example of a shifted integration lattice node set in \( d = 2 \). This figure can be reproduced using PlotPoints.m in GAIL](image)

4.2 Shift Invariant Kernels

The covariance functions \( C \) that match integration lattice node sets have the form

$$C(t, x) = K(t - x \mod 1). \quad (35)$$

This is called a shift invariant kernel because shifting both arguments of the covariance function by the same amount leaves the value unchanged. By a proper scaling of the kernel \( K \) it follows that assumption [27] is satisfied. Of course, \( K \) must also be of the form that ensures that \( C \) is symmetric and positive definite, as assumed in [4].

A family of shift invariant kernels is constructed via even degree Bernoulli polynomials:

$$C_{\theta}(t, x) = \prod_{i=1}^{d} \left[ 1 - (-1)^r \gamma B_{2r}(|x_1 - t_1|) \right], \quad \forall t, x \in [0, 1)^d, \ \theta = (r, \gamma), \ r \in \mathbb{N}, \ \gamma > 0. \quad (36)$$
Symmetric, periodic, positive definite kernels of this form appear in [6]. Bernoulli polynomials are described in [19, Chapter 24].

Larger $r$ implies a greater degree of smoothness of the kernel. Larger $\gamma$ implies greater fluctuations of the output with respect to the input. Plots of $C'(0, 0.3)$ are given in Figure 4 for various $r$ and $\gamma$ values.

4.3 Eigenvectors

For general shift-invariance covariance functions, the Gram matrix takes the form

$$C = (C(x_i, x_j))_{i,j=1}^n = \left(K(h(\phi(i - 1) - \phi(j - 1)) \mod 1)\right)_{i,j=1}^n.$$ 

We now demonstrate that the eigenvector matrix for $C$ is

$$V = \left(e^{2\pi n \sqrt{-1} \phi(i-1)\phi(j-1)}\right)_{i=1}^n. \quad (37)$$

Assumption (25a) follows automatically. Now, note that the $k, j$ element of $V^H V$ is

$$\sum_{i=1}^n e^{2\pi \sqrt{-1} \phi(i-1)(\phi(j-1) - \phi(k-1))}.$$ 

Noting that the sequence $\{\phi(i-1)\}_{i=1}^n$ is a re-ordering of $0, \ldots, 1 - 1/n$ for $n$ a power of 2, this sum may be re-written by replacing $\phi(i - 1)$ by $(i - 1)/n$:

$$\sum_{i=1}^n e^{2\pi \sqrt{-1}(i-1)(\phi(j-1) - \phi(k-1))}.$$ 

Since $\phi(j-1) - \phi(k-1)$ is some integer multiple of $1/n$, it follows that this sum is $n\delta_{j,k}$, where $\delta$ is the Kronecker delta function. This establishes that $V^H = nV^{-1}$ as in (24).

Next, let $\omega_{k,\ell}$ denote the $k, \ell$ element of $V^H CV$, which is given by the double sum

$$\omega_{k,\ell} = \sum_{i,j=1}^n K(h(\phi(i - 1) - \phi(j - 1)) \mod 1)$$

$$\times e^{-2\pi n \sqrt{-1} \phi(k-1)(\phi(i-1) - \phi(j-1))} e^{2\pi \sqrt{-1} \phi(\ell-1)}.$$ 

Noting that the sequence $\{\phi(i - 1)\}_{i=1}^n$ is a re-ordering of $0, \ldots, 1 - 1/n$ for $n$ a power of 2, this sum may be re-written by replacing $\phi(i - 1)$ by $(i - 1)/n$ and $\phi(j - 1)$ by $(j - 1)/n$:

$$\omega_{k,\ell} = \sum_{i,j=1}^n K\left(h\left(\frac{i - j}{n}\right) \mod 1\right)$$

$$\times e^{-2\pi \sqrt{-1} \phi(k-1)(\frac{i - j}{n})} e^{2\pi \sqrt{-1} \phi(\ell-1)}.$$ 

This sum also remains unchanged if $i$ is replaced by $i + m$ and $j$ is replaced by $j + m$ for any integer $m$:

$$\omega_{k,\ell} = \sum_{i,j=1}^n K\left(h\left(\frac{i - j}{n}\right) \mod 1\right)$$

$$\times e^{-2\pi \sqrt{-1} \phi(k-1)(\frac{i - j}{n})} e^{2\pi \sqrt{-1} \phi(\ell-1)} = \omega_{k,\ell} e^{2\pi \sqrt{-1} \phi(k-1) - \phi(\ell-1)}.$$ 

For this last equality to hold for all integers $m$, we must have $k = \ell$ or $\omega_{k,\ell} = 0$. Thus,

$$\omega_{k,\ell} = n\delta_{k,\ell} \sum_{i=1}^n K\left(h\left(\frac{i - j}{n}\right) \mod 1\right)$$

$$\times e^{-2\pi \sqrt{-1}(i - j)\phi(k-1)}.$$ 

This establishes $V^H CV$ as a diagonal matrix whose diagonal elements are $n$ times the eigenvalues, i.e., $\lambda_k = \omega_{k,k}/n$. Furthermore, $V$ is the matrix of eigenvectors, which satisfies assumption (25a).

4.4 Iterative Computation of the Fast Transform

Assumption (25a) is that computing $V^H b$ requires only $O(n \log(n))$ operations. Recall that we assume that $n$ is a power of 2. This can be accomplished by an iterative algorithm. Let $V^{(n)}$ denote the $n \times n$ matrix $V$ defined in (37). We show how to compute $V^{(2n)} V b$ quickly for all $b \in \mathbb{R}^{2^n}$ assuming that $V^{(n)} V b$ can be computed quickly for all $b \in \mathbb{R}^n$.

From the definition of the van der Corput sequence in (34), it follows that

$$\phi(2^i) = \phi(i)/2, \phi(2^i + 1) = [\phi(i) + 1]/2, \quad i \in \mathbb{N}_0 \quad (38)$$

$$\phi(i + n) = \phi(i) + 1/(2n), \quad i = 0, \ldots, n - 1, \quad (39)$$

$$n\phi(i) \in \mathbb{N}_0, \quad i = 0, \ldots, n - 1. \quad (40)$$
still assuming that \( n \) is an integer power of two. Let 
\[
\tilde{b} = \mathcal{V}(2n)^H b
\]
for some arbitrary \( b \in \mathbb{R}^{2n} \), and define 
\[
\tilde{b} = \begin{pmatrix} b_1 \\ \vdots \\ b_{2n} \end{pmatrix}, \quad \tilde{b}^{(1)} = \begin{pmatrix} b_1 \\ \vdots \\ b_{n+1} \end{pmatrix}, \quad \tilde{b}^{(2)} = \begin{pmatrix} b_2 \\ \vdots \\ b_{2n} \end{pmatrix}.
\]

It follows from these definitions and the definition of \( \mathcal{V} \) in (37) that 
\[
\tilde{b}^{(1)} = \left( \sum_{j=1}^{2n} e^{-4\pi n \sqrt{-1} \phi(2i-2) \phi(j-1)} b_j \right)_{i=1}^n
\]
by (38) 
\[
= \left( \sum_{j=1}^{2n} e^{-2\pi n \sqrt{-1} \phi(i-1) \phi(j-1)} b_j \right)_{i=1}^n
\]
\[
= \left( \sum_{j=1}^{n} e^{-2\pi n \sqrt{-1} \phi(i-1) \phi(j-1)} b_j \right)_{i=1}^n
\]
\[
+ \left( \sum_{j=1}^{n} e^{-2\pi n \sqrt{-1} \phi(i-1) \phi(n+j-1) \phi(n-j+1)} b_{n+j} \right)_{i=1}^n
\]
\[
= \mathcal{V}(n)^H b^{(1)} + \left( e^{-\pi \sqrt{-1} \phi(i-1)} \right)_{i=1}^n \times \left( e^{-2\pi n \sqrt{-1} \phi(i-1) \phi(j-1) \phi(n-j+1)} b_{n+j} \right)_{i=1}^n
\]
\[
= \mathcal{V}(n)^H b^{(1)} + e^{-\pi \sqrt{-1} \phi(i-1)} \otimes (\mathcal{V}(n)^H b^{(2)}),
\]
where \( \otimes \) denotes the Hadamard (term-by-term) product. By a similar argument,
\[
\tilde{b}^{(2)} = \left( \sum_{j=1}^{2n} e^{-4\pi n \sqrt{-1} \phi(2i-1) \phi(j-1)} b_j \right)_{i=1}^n
\]
by (38) 
\[
= \left( \sum_{j=1}^{2n} e^{-2\pi n \sqrt{-1} \phi(i-1) \phi(j-1)} b_j \right)_{i=1}^n
\]
\[
= \left( \sum_{j=1}^{n} e^{-2\pi n \sqrt{-1} \phi(i-1) \phi(j-1)} b_j \right)_{i=1}^n
\]
\[
+ \left( \sum_{j=1}^{n} e^{-2\pi n \sqrt{-1} \phi(i-1) \phi(n+j-1) \phi(n-j+1)} b_{n+j} \right)_{i=1}^n
\]
\[
= \mathcal{V}(n)^H b^{(1)} + \left( e^{-\pi \sqrt{-1} \phi(i-1)} \right)_{i=1}^n \times \left( e^{-2\pi n \sqrt{-1} \phi(i-1) \phi(j-1) \phi(n-j+1)} b_{n+j} \right)_{i=1}^n
\]
\[
= \mathcal{V}(n)^H b^{(1)} + \left( e^{-\pi \sqrt{-1} \phi(i-1)} \right)_{i=1}^n \otimes (\mathcal{V}(n)^H b^{(2)}).
\]

The computational cost to compute \( \mathcal{V}(2n)^H b \) is then twice the cost of computing \( \mathcal{V}(n)^H b^{(1)} \) plus 2n multiplications plus 2n additions. An inductive argument shows that \( \mathcal{V}(n)^H b \) requires only \( \mathcal{O}(n \log(n)) \) operations.

### 4.5 Overcoming Cancellation Error

For the kernels used in our computation, it may happen that \( n/\lambda_1 \) is close to 1. Thus, the term \( 1 - n/\lambda_1 \), which appears in the credible interval widths, \( \text{err}_{\text{MLE}}, \text{err}_{\text{full}}, \) and \( \text{err}_{\text{CCV}} \), may suffer from cancellation error. We can avoid this cancellation error by modifying how we compute the Gram matrix and its eigenvalues.

Define a new function \( \hat{C} := C - 1 \), and its associated Gram matrix \( \hat{C} = C - 11^T \). Note that \( \hat{C} \) inherits the shift-invariant properties of \( C \). Since \( 1 \) is the first eigenvector of \( C \), it follows that the eigenvalues of \( \hat{C} \) are \( \hat{\lambda}_1 = \lambda_1 - n, \lambda_2, \ldots, \lambda_n \). Moreover, 
\[
1 - \frac{n}{\lambda_1} = \frac{\lambda_1 - n}{\lambda_1} = \frac{\lambda_1}{\lambda_1 + n},
\]
where now the right hand side is free of cancellation error.

We show how to compute \( \hat{C} \) without introducing round-off error. The covariance functions that we use are of product form, namely,
\[
C(t, x) = \prod_{\ell=1}^{d} \left[ 1 + \hat{C}_\ell(t, x) \right], \quad \hat{C}_\ell : [0, 1]^2 \rightarrow \mathbb{R}.
\]
Direct computation of \( \hat{C}(t, x) = C(t, x) - 1 \) introduces cancellation error if the \( \hat{C} \) are small. So, we employ the iteration
\[
\hat{C}(t, x) = \hat{C}_1(t_1, x_1),
\]
\[
\hat{C}(t, x) = \hat{C}^{(\ell)}(t, x) + \hat{C}_\ell(t, x),
\]
where \( \hat{C}_\ell(t, x) = \hat{C}^{(\ell-1)}(t, x) \) and \( \ell = 2, \ldots, d \).

In this way, the Gram matrix \( \hat{C} \), whose \( i, j \)-element is \( \hat{C}(x_i, x_j) \) can be constructed with minimal round-off error.

Computing the eigenvalues of \( \hat{C} \) via the procedure given in [29] yields \( \lambda_1 = \lambda_1 - \lambda_1 \). The estimates of \( \theta \) are computed in terms of the eigenvalues of \( \hat{C} \), so (42a) and (42b) become
\[
\theta_{\text{MLE}} = \arg \min \left[ \log \left( \sum_{i=2}^{n} \frac{y_i^2}{\lambda_i} \right) + \frac{n}{n} \sum_{i=1}^{n} \log(\lambda_i) \right],
\]
\[
\theta_{\text{GCV}} = \arg \min \left[ \log \left( \sum_{i=2}^{n} \frac{y_i^2}{\lambda_i} \right) - 2 \log \left( \frac{n}{n} \sum_{i=1}^{n} \frac{1}{\lambda_i} \right) \right],
\]
where \( \lambda_1 = \lambda_1 + \lambda_1 \). The widths of the credible intervals in (29), (30), and (33) become
\[
\text{err}_{\text{MLE}} = 2.58 \frac{\lambda_1}{n} \sum_{i=2}^{n} \frac{|y_i|^2}{\lambda_i},
\]
\[
\text{err}_{\text{FULL}} = \frac{t_{n-1,0.995}}{n} \sqrt{\frac{\lambda_1}{n-1} \sum_{i=2}^{n} \frac{|y_i|^2}{\lambda_i}},
\]
\[
\text{err}_{\text{GCV}} = 2.58 \frac{\lambda_1}{n} \sum_{i=2}^{n} \frac{|y_i|^2}{\lambda_i} \left[ \frac{1}{n-1} \sum_{i=1}^{n} \frac{1}{\lambda_i} \right].
\]

Since \( \hat{\lambda}_1 = \lambda_1 - \lambda_1 \) and \( \lambda_1 \) is small for large \( n \), the credible intervals via empirical Bayes and full Bayes are similar, since \( t_{n-1,0.995} \) is approximately 2.58. The computational steps for the improved, faster, automatic Bayesian cubature are detailed in Algorithm 2.

We summarize the results of this section and the previous one as follows:

**Proposition 1** Any periodic, symmetric, positive definite, shift-invariant covariance kernel of the form \( [27] \), when matched with rank-1 lattice data-sites, must satisfy assumptions \( [25] \). The fast Fourier transform (FFT) can be used to expedite the estimates of \( \theta \) in (41) and the credible interval widths \( [42] \) in \( O(n \log(n)) \) operations. The cubature, \( \hat{\mu} \), is just the sample mean.

We have implemented the fast adaptive Bayesian cubature algorithm in MATLAB as part of the Guaranteed Adaptive Integration Library (GAIL) [2] as \( \text{cubBayesLattice.m} \). This algorithm uses the kernel defined in \( [34] \), \( r = 1, 2 \) and the periodizing variable transforms in Section 5.1. The rank-1 lattice node generator is taken from \( [17] \) (exod2_base2.m20).

## 5 Numerical Experiments

### 5.1 Periodizing Variable Transformations

The shift-invariant covariance kernels underlying our Bayesian cubature assume that the integrand has a degree of periodicity, with the smoothness assumed depending on the smoothness of the kernel. While integrands arising in practice may be smooth, they might not be periodic. Variable transformations can be used to ensure periodicity.

Suppose that the original integral has been expressed as
\[
\mu := \int_{[0,1]^d} g(t) \, dt
\]
where \( g \) has sufficient smoothness, but lacks periodicity. The Baker’s transform,
\[
\Psi : x \mapsto (\Psi(x_1), \ldots, \Psi(x_d)),
\]
\[
\Psi(x) = 1 - 2|x - 1/2|, \quad (43)
\]
allows us to write \( \mu \) in the form of (1), where \( f(x) = g(\Psi(x)) \).

A family of variable transforms take the form
\[
\Psi : x \mapsto (\Psi(x_1), \ldots, \Psi(x_d)), \quad \Psi : [0, 1] \mapsto [0, 1],
\]
which allows us to write \( \mu \) in the form of (1) with
\[
f(x) = g(\Psi(x)) \prod_{i=1}^{d} \Psi'(x_i).
\]

If \( \Psi \) is sufficiently smooth, \( \lim_{x \to 0} x^{-r} \Psi'(x) = \lim_{x \to 1} (x-1)^{-r} \Psi'(x) = 0 \) for \( r \in \mathbb{N}_0 \), and \( g \in C^{(r-1)}[0, 1]^d \), then \( f \) has continuous, periodic derivatives up to order \( r \) in
each direction. Examples of this kind of transform include [23]:

Sidi's $C_1$: \[ \Psi(x) = x - \frac{\sin(2\pi x)}{2\pi}, \]
\[ \Psi'(x) = 1 - \cos(2\pi x), \]

Sidi's $C_2$: \[ \Psi(x) = \frac{8 - 9\cos(\pi x) + \cos(3\pi x)}{16}, \]
\[ \Psi'(x) = \frac{3\pi[3\sin(\pi x) - \sin(3\pi x)]}{16}. \]

Periodizing variable transforms are used for the numerical examples below. In some cases, they can speed the convergence of the Bayesian cubature.

5.2 Test Results and Observations

Three integrals were evaluated using the GAIL algorithm $\text{cubBayesLattice}$: a multivariate normal probability, the Keister’s example, and an option pricing example. Four different error tolerances, $\varepsilon$, were set for each example, with the tolerances chosen depending on the difficulty of the problem. The sequences $\{x_i\}_{i=1}^\infty$ were the randomly shifted lattice node sequences supplied by GAIL. The accuracy of the algorithm differs depends on the shift. For each integral, each tolerance, and each of our stopping criteria—empirical Bayes, full Bayes, and generalized cross-validation—our algorithm was run for 100 different random shifts. For each test, the execution times were plotted against $|\mu - \hat{\mu}|/\varepsilon$. We expect $|\mu - \hat{\mu}|/\varepsilon$ to be no greater than one, but hope that it is not too much smaller than one, which would indicate a stopping criterion that is too conservative.

Figures 5 to 13 can be reproduced using the script $\text{cubBayesLattice\_guaranteed\_plots.m}$ in GAIL.

**Multivariate Normal Probability.** This example was already introduced in Section 2.4, where we used the Matérn covariance kernel. Here we apply Sidi’s $C_2$ periodization to $f_{\text{Genz}}$ [23], choose $d = 3$ and $r = 2$. The simulation results for this example function are summarized in Figures 5, 6, and 7. In all cases, the Bayesian cubature returns an approximation within the prescribed error tolerance. We used the same setting as before with generic slow Bayesian cubature in Section 2.4 for comparison. For error threshold $\varepsilon = 10^{-5}$ with the empirical Bayes stopping criterion, our fast algorithm takes just under 0.01 second as shown in Figure 5 whereas the basic algorithm takes over 20 seconds as shown in Figure 2.

Fig. 5: Multivariate normal probability example using the empirical Bayes stopping criterion.

Fig. 6: Multivariate normal probability example using the full Bayes stopping criterion.

Fig. 7: Multivariate normal probability example using the GCV stopping criterion.

Amongst the three stopping criteria, GCV achieves the desired tolerance faster than the others. One can also observe from the figures, the credible intervals are in general much wider than the true error. This could be due to the periodized integrand being smoother than the $r = 2$ kernel assumes. Perhaps one should consider smoother covariance kernels.

**Keister’s Example.** This multidimensional integral function comes from [19] and is inspired by a physics application:

\[
\mu = \int_{\mathbb{R}^d} \cos(||t||) \exp(-||t||^2) \, dt = \int_{[0,1]^d} f_{\text{Keister}}(x) \, dx,
\]

where $f_{\text{Keister}}(x)$ is a function that models a physical phenomenon. The integral represents the distribution of a certain property in a physical system. The function $f_{\text{Keister}}(x)$ can be used to simulate the behavior of particles in a given environment.
where
\[ f_{\text{Keister}}(x) = \pi^{d/2} \cos \left( \| \Phi^{-1}(x) \| /2 \right), \]
and again \( \Phi \) is the standard normal distribution. The true value of \( \mu \) can be calculated iteratively in terms of a quadrature as follows:
\[ \mu = \frac{2\pi^{d/2} I_c(d)}{T (d/2)}, \quad d = 1, 2, \ldots \]
where \( T \) denotes the gamma function, and
\[ I_c(1) = \int_{x=0}^{\infty} \exp(-x^T x) \sin(x) \, dx = 0.4244363835020225, \]
\[ I_c(2) = \frac{1 - I_c(1)}{2}, \quad I_c(2) = \frac{I_c(1)}{2} \]
\[ I_c(j) = \frac{(j - 2)I_c(j - 2) - I_c(j - 1)}{2}, \quad j = 3, 4, \ldots \]
\[ I_c(j) = \frac{(j - 2)I_c(j - 2) - I_c(j - 1)}{2}, \quad j = 3, 4, \ldots \]

Figures 8, 9 and 10 summarize the numerical tests for this integral. We used the Sidi’s \( C^1 \) periodization, dimension \( d = 4 \), and \( r = 2 \). As we can see, the GCV stopping criterion achieves faster results than the other stopping criteria, similarly to the multivariate normal case.

**Option Pricing.** The price of financial derivatives can often be modeled by high dimensional integrals. If the underlying asset is described in terms of a discretized geometric Brownian motion, then the fair price of the option is:
\[ \mu = \int_{x \in \mathbb{R}^d} \text{payoff}(x) \frac{\exp(x^T \Sigma^{-1} z)}{(2\pi)^d \sqrt{\det(\Sigma)}} \, dz = \int_{[0,1]^d} f(x) \, dx, \]
where \( \text{payoff}(\cdot) \) defines the discounted payoff of the option,
\[ \Sigma = (T/d) (\min(j, k))^d_{j,k=1} = \text{LL}^T, \]
\[ f(x) = \text{payoff} \left( \text{L} \left( \Phi^{-1}(x_1), \ldots, \Phi^{-1}(x_d) \right) \right). \]
The Asian arithmetic mean call option has a payoff of the form
\[ \text{payoff}(z) = \max \left( \frac{1}{d} \sum_{j=1}^{d} S_j(z) - K, 0 \right) e^{-rT}, \]
where \( S_j(z) = S_0 \exp((r - \sigma^2/2)T/d + \sigma \sqrt{T/d} z_j) \).
Here, \( T \) denotes the time to maturity of the option, \( d \) the number of time steps, \( S_0 \) the initial price of the stock, \( r \) the interest rate, \( \sigma \) the volatility, and \( K \) the strike price.

Figures 11, 12 and 13 summarize the numerical results for this example using \( T = 1/4, \quad d = 13, \quad S_0 = 100, \quad r = 0.05, \quad \sigma = 0.5, \quad K = 100 \). Moreover, \( L \) is chosen to be the matrix of eigenvectors of \( \Sigma \) times the square root of the diagonal matrix of eigenvalues of \( \Sigma \). Because the integrand has a kink caused by the max function, it does not help to use a periodizing transform that is very smooth. We choose the Baker’s transform \([43]\) and \( r = 1 \).

In summary, the Bayesian cubature algorithm computes the integral within the user-specified threshold in nearly all of the test cases. The rare exceptions occurred in the option pricing example for \( \varepsilon = 10^{-4} \).
algorithm used the maximum allowed sample size and still did not reach the stopping criterion $\epsilon_{\text{CI}} \leq \varepsilon$, due to the complexity and high dimension of the integrand.

A noticeable aspect from the plots is how much the error bounds differ from the true error. For option pricing example, the error bound is not as conservative as it is for the multivariate normal and Keister examples. A possible reason is that the latter integrands are significantly smoother than the covariance kernel assumed. This is a matter for further investigation.

6 Discussion and Further Work

We have developed a fast, automatic Bayesian cubature that estimates a multidimensional definite integral within a user defined error tolerance. The stopping criteria arise from assuming the integrand to be a Gaussian process. There are three approaches: empirical Bayes, full Bayes, and generalized cross-validation. The computational cost of the automatic Bayesian cubature can be dramatically reduced if the covariance kernel matches the nodes. One such match in practice is rank-1 lattice nodes and shift-invariant kernels. The matrix-vector multiplications can be accomplished using the fast Fourier Transform. The performance of our automatic Bayesian cubature are illustrated using three integration problems.

Digital sequences and digital shift and/or scramble invariant kernels have the potential of being another match that satisfies the conditions in Section 3. The fast transform would correspond to a fast Walsh transform.

One should be able to adapt our Bayesian cubature to control variates, i.e., assuming

\[ f = GP \left( \beta_0 + \beta_1 g_1 + \cdots + \beta_p g_p, \sigma^2 C \right), \]

for some choice of $g_1, \ldots, g_p$ whose integrals are known, and some parameters $\beta_0, \ldots, \beta_p$ in addition to $s$ and $C$. The efficacy of this approach has not yet been explored.

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