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Hierarchical-block conditioning approximations for high-dimensional multivariate normal probabilities

Jian Cao[1] · Marc G. Genton[1] · David E. Keyes[1] · George M. Turkiyyah[1]

Abstract

This paper presents a new method to estimate large-scale multivariate normal probabilities. The approach combines a hierarchical representation with processing of the covariance matrix that decomposes the n-dimensional problem into a sequence of smaller m-dimensional ones. It also includes a d-dimensional conditioning method that further decomposes the m-dimensional problems into smaller d-dimensional problems. The resulting two-level hierarchical-block conditioning method requires Monte Carlo simulations to be performed only in d dimensions, with $d \ll n$, and allows the complexity of the algorithm's major cost to be $O(n \log n)$. The run-time cost of the method depends on two parameters, m and d, where m represents the diagonal block size and controls the sizes of the blocks of the covariance matrix that are replaced by low-rank approximations, and d allows a trade-off of accuracy for expensive computations in the evaluation of the probabilities of m-dimensional blocks. We also introduce an inexpensive block reordering strategy to provide improved accuracy in the overall probability computation. The downside of this method, as with other such conditioning approximations, is the absence of an internal estimate of its error to use in tuning the approximation. Numerical simulations on problems from 2D spatial statistics with dimensions up to 16,384 indicate that the algorithm achieves a 1% error level and improves the run time over a one-level hierarchical Quasi-Monte Carlo method by a factor between 10 and 15.

Keywords Block reordering · d-Dimensional conditioning · Hierarchical representation · Spatial covariance functions · Univariate reordering

1 Introduction

The computation of high-dimensional multivariate normal (MVN) probabilities is required for a variety of applications. For example, in spatial extreme statistics, the max-stable process is extensively used for modeling the maximum of a large

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number of realizations and the commonly used parameterizations involve the multivariate normal distribution (Smith et al. 1990; Schlather 2002; Brown and Resnick 1977). Moreover, the multivariate t-distribution probability can be transformed into a multivariate normal probability (Genz and Bretz 2009) and the multivariate skew-normal distribution (Genton 2004; Azzalini and Capitanio 2014) is defined based on the multivariate normal distribution, both of which have important applications in science and engineering (Gupta and Brown 2001; Kotz and Nadarajah 2004).

The multivariate normal probability is defined as:

$$\Phi_n(\mathbf{a}, \mathbf{b}; \mathbf{0}, \boldsymbol{\Sigma}) = \int_{\mathbf{a}}^{\mathbf{b}} \frac{1}{\sqrt{(2\pi)^n |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}\mathbf{x}^T \boldsymbol{\Sigma}^{-1} \mathbf{x}\right) d\mathbf{x},$$

(1)

where $\mathbf{a}$ and $\mathbf{b}$ are integration limits, the mean vector $\boldsymbol{\mu}$ is assumed to be $\mathbf{0}$, $\boldsymbol{\Sigma}$ is a positive-definite matrix produced by a covariance function, and n is the problem size. Because most covariance functions in spatial statistics are smooth at points

excluding 0, the blocks of the covariance matrix that represent the correlation between two groups of well-separated variables are usually well approximated by low-rank blocks. This approximation provides the potential for using the hierarchical matrix ($\mathcal{H}$ matrix) representation (Hackbusch 2015) for the covariance matrix, $\boldsymbol{\Sigma}$, which substantially reduces the complexity of the matrix-associated operations.

MVN probabilities are generally not analytically tractable and various approximation methods have been studied to generate reliable estimations. Genz (1992) used separation of variables to transform the integration region to the unit hypercube in which a Monte Carlo simulation is performed. Niederreiter (1992), Caflisch (1998) and Owen and Zhou (2000) studied more efficient sampling methods for Monte Carlo simulation. Genz and Bretz (2009) provided a summary of recently developed methods for estimating MVN probabilities. Two state-of-the-art methods, among others, are the bivariate conditioning method (Trinh and Genz 2015) and the hierarchical Quasi-Monte Carlo method (Genton et al. 2018). The bivariate conditioning method provides insights into estimating high-dimensional MVN problems with low-dimensional Monte-Carlo simulations but the univariate reordering has a complexity of $O(n^3)$ which makes working in high dimensions difficult. The hierarchical Quasi-Monte Carlo method utilizes the hierarchical representation of the covariance matrix and reduces the complexity of one Monte Carlo sample to $O(mn + kn \log(n/m))$ from $O(n^2)$, where m and k represent the diagonal block size and the rank of the off-diagonal blocks, respectively.

The purpose of this paper is to generalize the bivariate conditioning method to a d-dimensional conditioning method and combine it with the hierarchical representation of the covariance matrix. Through this combination, we introduce a two-level hierarchical-block conditioning method. In addition, we develop a reordering scheme with a complexity of $O(m^2 n)$ that can maintain the low-rank feature of the off-diagonal blocks, thus making it applicable to high-dimensional MVN problems. The downside of conditioning methods, including this one, is that error estimates of the computed MVN probability approximations are not generated as part of the computations. As a result, apriori assessments are needed to insure that the method is reliable in the contexts where it will be used (Trinh and Genz 2015).

The remainder of the paper is organized as follows. In Sect. 2, we introduce the construction of the hierarchical covariance matrix. In Sect. 3, we propose a generalized d-dimensional conditioning algorithm and present the derivation of the truncated normal expectations and the numerical simulation results for different d. In Sect. 4, we combine the conditioning method with the hierarchical representation of the covariance matrix to develop a two-level hierarchical-block conditioning method that speeds up the MVN integration problem relative to the one-level hierar-

chical Quasi-Monte Carlo method. In Sect. 5, we introduce a block-wise reordering scheme that significantly improves the accuracy level with negligible run-time cost. We discuss the method further in Sect. 6 and conclude in Sect. 7.

2 Building hierarchical representations

2.1 Generating a hierarchical covariance matrix

Hierarchical covariance matrices are shown in Fig. 1a, b. The number of diagonal blocks, denoted by r, expands with a factor of 2 while the off-diagonal part has a total number of $r - 1$ low-rank blocks. In actual construction and storage, the $\mathcal{H}$-matrix assumes a quad-tree structure in which each parent node has two child nodes as well as two low-rank matrices. The green blocks are low-rank representations and the blue blocks signify dense matrices. Hierarchical representation enables faster matrix arithmetic and decreases the storage costs. These improvements are especially significant for high-dimensional problems. Specifically, when two groups are well separated in space, the corresponding off-diagonal block usually has few singular values that are larger than the machine precision. However, the low-rank feature depends on the separation of samples. When the samples are not very distant, the ranks of the off-diagonal blocks grow. Even so, the hierarchical representation still delivers significant computational savings relative to the standard dense representation.

Building a hierarchical covariance matrix requires the input of a covariance model, the spatial geometry of the samples and the indices of the samples. For general covariance models, the low-rank representation of off-diagonal blocks is generated from the dense representation through singular value decomposition (Hackbusch 2015). This is computationally expensive but achieves the goal of examining the efficiencies of different algorithms for solving the MVN problem in high dimensions. We can use the orthonormal polynomial expansions of common covariance functions as an approximation to generate the low-rank representation directly. Both methods approximate the off-diagonal blocks individually and thus require validation for positive-definiteness. In the case where a non-positive-definite approximation is produced, we can decrease the error tolerance level, $\|\mathbf{L} - \mathbf{U}\mathbf{V}^T\|/\|\mathbf{L}\|$, where $\mathbf{L}$ is some matrix block, $\mathbf{U}\mathbf{V}^T$ is the low-rank approximation of $\mathbf{L}$, and $\|\cdot\|$ denotes a valid norm for matrices, or we can increase the number of terms in the orthonormal polynomial expansions.

2.2 Hierarchical Cholesky factorization

Both the conditioning method and the Quasi-Monte Carlo method require the Cholesky factor of the covariance matrix.
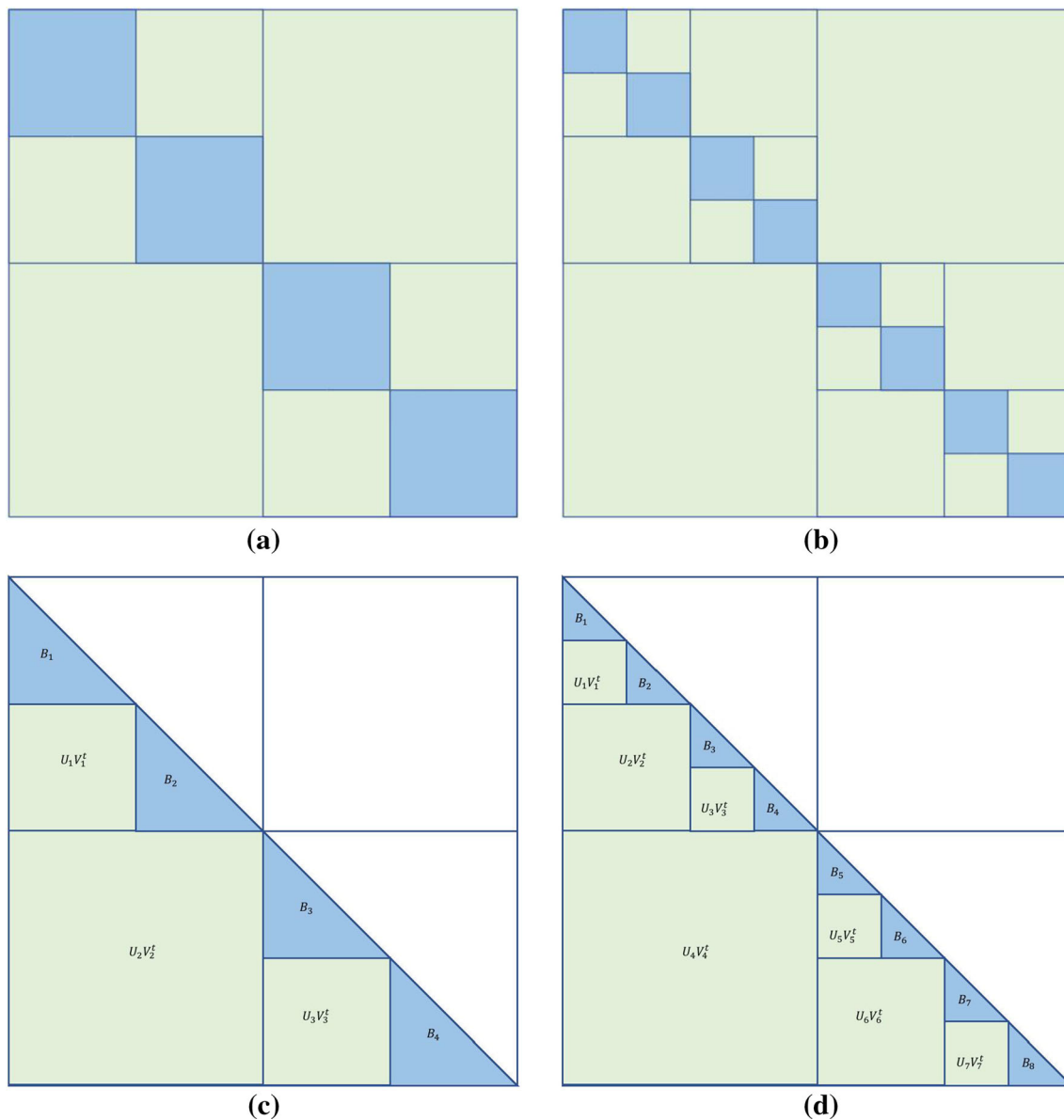
Fig. 1 Hierarchical covariance matrices and Cholesky factors. The green blocks are approximated by low-rank matrices while the blue blocks are stored in the dense form. **a**, **b** are hierarchical matrices with maximum tree depth equal to 2 and 3. **c**, **d** are hierarchical Cholesky factors with maximum tree depth equal to 2 and 3. (Color figure online)

The dense Cholesky factorization has a complexity of $O(n^3)$ and requires $O(n^2)$ amount of memory, which becomes prohibitive on typical workstations when n is much larger than 10^4. Hierarchical Cholesky factorization is much faster in large dimensions (e.g., more than 10,000) even under a strong spatial correlation structure. Table 1 compares two implementations of dense Cholesky factorization and one of hierarchical Cholesky factorization under different matrix dimensions, n. We selected a 2D exponential covariance structure, $\mathrm{corr}(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|/\beta)$, where β is set to 0.3, to compare the time required for these three Cholesky factorization methods. The underlying geometry consists of n points evenly distributed on a grid in the unit square and indexed with Morton's order (Morton 1966). Three implementations, namely the *chol* from R (R Core Team 2016), the *dpotrf* from LAPACK (Anderson et al. 1999), and the *choldecomp_hmatrix* from H2Lib (Hackbusch 2015), are compared as run on an Intel Xeon(R) E5-2680 CPU.

Since we focus on high-dimensional problems, we can reasonably conclude that hierarchical Cholesky factorization is the most efficient among the three although *dpotrf* is highly optimized. The commonly used function, *chol* from R, has

Table 1 Time required for Cholesky factorization (seconds)

n	256	1024	4096	16,384
chol	0.004	0.23	12.66	737.0
dpotrf	0.001	0.02	0.61	41.5
choldecomp_hmatrix	0.003	0.03	0.46	9.3

The covariance matrix is generated from the exponential covariance function with $\beta = 0.3$, based on n points uniformly distributed in the unit square indexed with Morton's order. *chol* refers to the Cholesky factorization implemented in R. *dpotrf* is the Cholesky factorization from the LAPACK library. *choldecomp_hmatrix* is the hierarchical Cholesky factorization from the H2Lib library

a much slower performance than the other two. The cost of hierarchical Cholesky factorization depends on the ranks of the off-diagonal blocks, which usually grow at a much slower rate than $O(n)$ under 2D geometries. The algorithm may involve truncation of the off-diagonal blocks to maintain the low-rank feature. This would introduce little error compared with the overall estimation method discussed in the paper. The resulting hierarchical Cholesky factor has the hierarchical structure shown in Fig. 1c, d.

3 d-Dimensional conditioning approximation

With knowledge of the hierarchical Cholesky factor, $\mathbf{L}$, the n-dimensional MVN problem can be separated into r m-dimensional MVN problems through the change of variable $\mathbf{Y} = \mathbf{L}\mathbf{X}$. For each m-dimensional problem, the Cholesky factor of its covariance matrix is already given from the diagonal blocks of $\mathbf{L}$. In this section, we extend the bivariate conditioning method of Trinh and Genz (2015) to a d-dimensional conditioning method and use it to compute the m-dimensional MVN probabilities and truncated expectations that become the building blocks for solving the n-dimensional MVN problem. To avoid confusion, we will add a tilde to the notations in the n dimension to represent the counterpart in the m dimension. For example, $\tilde{\mathbf{X}}$ represents the normal random variables in the m dimension.

3.1 d-Dimensional LDL decomposition

LDL decomposition is a generalization of the classical Cholesky factorization. In fact, we can produce the Cholesky factors from LDL decomposition and vice versa without tracing back to the original covariance matrix. In calculating MVN probabilities, the variable transformation using the Cholesky factor can make the new integration variables independent from each other. Similarly, transformation with the $\tilde{\mathbf{L}}$ matrix in LDL decomposition can generate integration variables that are block-wise independent. The bivariate

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Algorithm 1 LDL decomposition

1: **procedure** LDL($\tilde{\mathbf{\Sigma}}$)
2: $\quad \tilde{\mathbf{L}} \leftarrow \mathbf{I}_m, \tilde{\mathbf{D}} \leftarrow \mathbf{O}_m$
3: $\quad$ **for** $i = 1 : d : m - d + 1$ **do**
4: $\qquad \tilde{\mathbf{D}}[i : i+d-1, i : i+d-1] \leftarrow \tilde{\mathbf{\Sigma}}[i : i+d-1, i : i+d-1]$
5: $\qquad \tilde{\mathbf{L}}[i+d : m, i : i+d-1] \leftarrow \tilde{\mathbf{\Sigma}}[i+d : m, i : i+d-1]\tilde{\mathbf{D}}^{-1}[i : i+d-1, i : i+d-1]$
6: $\qquad \tilde{\mathbf{\Sigma}}[i+d : m, i+d : m] \leftarrow \tilde{\mathbf{\Sigma}}[i+d : m, i+d : m]$
$\qquad\qquad - \tilde{\mathbf{L}}[i+d : m, i : i+d-1]$
$\qquad \tilde{\mathbf{D}}[i : i+d-1, i : i+d-1]\tilde{\mathbf{L}}^T[i+d : m, i : i+d-1]$
7: $\qquad$ **if** $i + d < m$ **then**
8: $\qquad\qquad \tilde{\mathbf{D}}[i+d : m, i+d : m] \leftarrow \tilde{\mathbf{\Sigma}}[i+d : m, i+d : m]$
9: $\qquad$ **end if**
10: $\quad$ **end for**
11: $\quad$ **return** $\tilde{\mathbf{L}}$ and $\tilde{\mathbf{D}}$
12: **end procedure**

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conditioning method from Trinh and Genz (2015) applied the 2-dimensional LDL decomposition and separated the m integration variables into uncorrelated blocks of size 2. We use the LDL decomposition in dimension d to separate the m integration variables into uncorrelated blocks of size d. When m is a multiple of d, the matrices $\tilde{\mathbf{L}}$ and $\tilde{\mathbf{D}}$ can be written as

$$\tilde{\mathbf{L}} = \begin{bmatrix} \mathbf{I}_d & \mathbf{O}_d & \cdots & \mathbf{O}_d \\ \tilde{\mathbf{L}}_{2,1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \mathbf{I}_d & \mathbf{O}_d \\ \tilde{\mathbf{L}}_{s,1} & \cdots & \tilde{\mathbf{L}}_{s,s-1} & \mathbf{I}_d \end{bmatrix}, \tilde{\mathbf{D}} = \begin{bmatrix} \tilde{\mathbf{D}}_1 & \mathbf{O}_d & \cdots & \mathbf{O}_d \\ \mathbf{O}_d & \ddots & \ddots & \vdots \\ \vdots & \ddots & \tilde{\mathbf{D}}_{s-1} & \mathbf{O}_d \\ \mathbf{O}_d & \cdots & \mathbf{O}_d & \tilde{\mathbf{D}}_s \end{bmatrix},$$

where $s = \frac{m}{d}$, $\mathbf{O}_d$ and $\mathbf{I}_d$ are zero and unit matrices of dimension d, $\tilde{\mathbf{D}}_i, i = 1, \ldots, s$, are positive-definite matrices, and $\tilde{\mathbf{L}}_{ij}, i = 2, \ldots, s, j = 1, \ldots, s - 1$, are matrix blocks. If m is not a multiple of d, then the last row of $\tilde{\mathbf{L}}$ and $\tilde{\mathbf{D}}$ has the dimension of the remainder. The algorithm for LDL decomposition is outlined as Algorithm 1. With the change of variable $\tilde{\mathbf{Y}} = \tilde{\mathbf{L}}\tilde{\mathbf{X}}$, we can rewrite an m-dimensional MVN probability as the product of s d-dimensional MVN probabilities

$$\Phi_m(\tilde{\mathbf{a}}, \tilde{\mathbf{b}}; \mathbf{0}, \tilde{\mathbf{\Sigma}}) = \int_{\tilde{\mathbf{a}}_1'}^{\tilde{\mathbf{b}}_1'} \phi_d(\tilde{\mathbf{y}}_1; \tilde{\mathbf{D}}_1) \int_{\tilde{\mathbf{a}}_2'}^{\tilde{\mathbf{b}}_2'} \phi_d(\tilde{\mathbf{y}}_2; \tilde{\mathbf{D}}_2)$$

$$\cdots \int_{\tilde{\mathbf{a}}_s'}^{\tilde{\mathbf{b}}_s'} \phi_d(\tilde{\mathbf{y}}_s; \tilde{\mathbf{D}}_s) \, d\tilde{\mathbf{y}}_s \cdots d\tilde{\mathbf{y}}_2 \, d\tilde{\mathbf{y}}_1, \quad (2)$$

where $\tilde{\mathbf{a}}_i' = \tilde{\mathbf{a}}_i - \sum_{j=1}^{i-1} \tilde{\mathbf{L}}_{ij}\tilde{\mathbf{y}}_j$, $\tilde{\mathbf{b}}_i' = \tilde{\mathbf{b}}_i - \sum_{j=1}^{i-1} \tilde{\mathbf{L}}_{ij}\tilde{\mathbf{y}}_j$, $\tilde{\mathbf{a}}_i$ and $\tilde{\mathbf{b}}_i, i = 1, \ldots, s$, are the corresponding segments of $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{b}}$. When $d = 1$, Eq. (2) leads to the univariate conditioning method (Mendell and Elston 1974; Kamakura 1989), and when $d = 2$, it corresponds to the bivariate conditioning method (Trinh and Genz 2015), for which both accuracy and complexity increase.

3.2 d-dimensional truncated expectations

The integration limits in Eq. (2) depend only on the integration variables to their left. The conditioning method separates the m-dimensional integration into d-dimensional integrations and updates the integration limits with the truncated expectations of the integration variables on the left side. When $d = 2$, Trinh and Genz (2015) employed the method in Muthen (1990) to calculate the bivariate truncated expectations. In this paper, we generalize the truncated normal expectation formula to d-dimensions based on the work of Kan and Robotti (2017). The truncated expectation is expressed as

$$\mathrm{E}(\hat{\mathbf{X}}^{\mathbf{e}_j}) = \frac{1}{\Phi_d(\hat{\mathbf{a}}, \hat{\mathbf{b}}; \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}})} \int_{\hat{\mathbf{a}}}^{\hat{\mathbf{b}}} \hat{x}_j \phi_d(\hat{\mathbf{x}}; \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}) \, \mathrm{d}\hat{\mathbf{x}}, \qquad (3)$$

where $\hat{\mathbf{X}}$ is a d-dimensional MVN random vector, $\phi_d(\cdot)$ denotes the d-dimensional normal probability density, $\mathbf{e}_j$ is a unit vector of length d with 1 in the jth position and 0 elsewhere, and $\hat{\mathbf{X}}^{\mathbf{e}_j}$ denotes the jth random variable in $\hat{\mathbf{X}}$. In this section, we add a hat to the notations to signify the counterparts in d-dimensions. For example, $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ are the corresponding lower and upper integration limits of dimension d while $\hat{\boldsymbol{\mu}}$ and $\hat{\boldsymbol{\Sigma}}$ denote some general mean vector and covariance matrix of the d-dimensional random vector $\hat{\mathbf{X}}$. We define

$$F_j^d(\hat{\mathbf{a}}, \hat{\mathbf{b}}; \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}) = \int_{\hat{\mathbf{a}}}^{\hat{\mathbf{b}}} \hat{x}_j \phi_d(\hat{\mathbf{x}}; \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}) \, \mathrm{d}\hat{\mathbf{x}},$$

which is the numerator of Eq. (3). A recurrence relation for F_j^d can be derived by differentiating the MVN density function, $\phi_d(\hat{\mathbf{x}}; \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}})$, with respect to $\hat{\mathbf{x}}$, then multiplying $\hat{x}_j$ on both sides and integrating the vector, $\hat{\mathbf{x}}$, from $\hat{\mathbf{a}}$ to $\hat{\mathbf{b}}$. The detailed derivation of the recurrence relation can be found in Kan and Robotti (2017). We use parentheses around the subscript to denote the exclusion of the element from the subscript set. Following this relation, we deduce that

$$F_j^d(\hat{\mathbf{a}}, \hat{\mathbf{b}}; \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}) = \hat{\mu}_j \Phi_d(\hat{\mathbf{a}}, \hat{\mathbf{b}}; \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}) + \mathbf{e}_j^T \hat{\boldsymbol{\Sigma}} \mathbf{c}, \qquad (4)$$

where $\mathbf{c}$ is a vector with the lth coefficient defined as

$$c_l = \phi_1(\hat{a}_l, \hat{\mu}_l, \hat{\sigma}_l^2) \Phi_{d-1}(\hat{\mathbf{a}}_{(l)}, \hat{\mathbf{b}}_{(l)}; \check{\boldsymbol{\mu}}_l^1, \check{\boldsymbol{\Sigma}}_l)$$
$$- \phi_1(\hat{b}_l, \hat{\mu}_l, \hat{\sigma}_l^2) \Phi_{d-1}(\hat{\mathbf{a}}_{(l)}, \hat{\mathbf{b}}_{(l)}; \check{\boldsymbol{\mu}}_l^2, \check{\boldsymbol{\Sigma}}_l),$$

$$\check{\boldsymbol{\mu}}_l^1 = \hat{\boldsymbol{\mu}}_{(l)} + \hat{\boldsymbol{\Sigma}}_{(l),l} \frac{\hat{a}_l - \hat{\mu}_l}{\hat{\sigma}_l^2}, \quad \check{\boldsymbol{\mu}}_l^2 = \hat{\boldsymbol{\mu}}_{(l)} + \hat{\boldsymbol{\Sigma}}_{(l),l} \frac{\hat{b}_l - \hat{\mu}_l}{\hat{\sigma}_l^2},$$

$$\check{\boldsymbol{\Sigma}}_l = \hat{\boldsymbol{\Sigma}}_{(l),(l)} - \frac{1}{\hat{\sigma}_l^2} \hat{\boldsymbol{\Sigma}}_{(l),l} \hat{\boldsymbol{\Sigma}}_{l,(l)}.$$

When $d = 2$, $\hat{\boldsymbol{\mu}} = \mathbf{0}$ and $\hat{\sigma}_l = 1, l = 1, \ldots, d$, the above formula turns into the bivariate version used by Trinh and Genz (2015). The computation of the d-dimensional truncated expectation requires the computation of the $(d-1)$-dimensional MVN probability for $2d$ times which becomes the major computational cost for the conditioning algorithm and for the two-level hierarchical-block conditioning algorithm introduced later. Future developments for efficiently estimating the truncated normal expectations would substantially improve the performance of this algorithm.

3.3 The d-dimensional conditioning algorithm

In the m-dimensional MVN probability problem represented by Eq. (2), the d-dimensional conditioning method iterates through s integrations from the left to the right while updating the integration limits after each iteration. The d-dimensional conditioning algorithm is presented as Algorithm 2: A minor change is needed to the algorithm when the remainder of m divided by d is not 0. In the algorithm, $\Phi_d(\tilde{\mathbf{a}}', \tilde{\mathbf{b}}'; \mathbf{0}, \tilde{\mathbf{D}}')$ is approximated with Quasi-Monte Carlo simulation and $\mathrm{E}[\tilde{\mathbf{Y}}']$ is computed from Eqs. (3) and (4). Since $(d-1)$-dimensional MVN probabilities are generated through Quasi-Monte Carlo simulations, the result unavoidably introduces a small error that can be made negligible compared with the error from the conditioning method.

To illustrate the improved accuracy and the effect on computation time when d becomes larger, we simulate 250 MVN problems for different values of m and d. The covariance matrix, $\tilde{\boldsymbol{\Sigma}}$, is simulated through $\tilde{\boldsymbol{\Sigma}} = \tilde{\mathbf{Q}}\tilde{\mathbf{J}}\tilde{\mathbf{Q}}^T$, where $\tilde{\mathbf{Q}}$ is simulated from the Haar distribution over the orthogonal matrix group (Stewart 1980) and $\tilde{\mathbf{J}}$ is a diagonal matrix with the diagonal coefficients independently drawn from $U(0, 1)$. The integration limits are set with $\tilde{\mathbf{a}} = -\infty$ and $\tilde{\mathbf{b}} \overset{i.i.d}{\sim} U(0, m)$ which correspond to the conditions used in Trinh and Genz (2015) for straightforward comparison. Our simulation results are presented in the upper half of Table 2, where the relative errors are benchmarked against the Quasi-Monte

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Algorithm 2 d-dimensional conditioning algorithm

1: **procedure** CMVN($\tilde{\boldsymbol{\Sigma}}, \tilde{\mathbf{a}}, \tilde{\mathbf{b}}, d$)
2:    $\tilde{\mathbf{y}} \leftarrow \mathbf{0}$ and $P \leftarrow 1$
3:    $[\tilde{\mathbf{L}}, \tilde{\mathbf{D}}] = \mathrm{LDL}(\tilde{\boldsymbol{\Sigma}})$ as in Algorithm 1
4:    **for** $i = 1 : s$ **do**
5:        $j \leftarrow (i - 1)d$
6:        $\tilde{\mathbf{g}} \leftarrow \tilde{\mathbf{L}}[j + 1 : j + d, 1 : j]\tilde{\mathbf{y}}[1 : j]$
7:        $\tilde{\mathbf{a}}' \leftarrow \tilde{\mathbf{a}}[j + 1 : j + d] - \tilde{\mathbf{g}}$
8:        $\tilde{\mathbf{b}}' \leftarrow \tilde{\mathbf{b}}[j + 1 : j + d] - \tilde{\mathbf{g}}$
9:        $\tilde{\mathbf{D}}' \leftarrow \tilde{\mathbf{D}}[j + 1 : j + d, j + 1 : j + d]$
10:       $P \leftarrow P \cdot \Phi_d(\tilde{\mathbf{a}}', \tilde{\mathbf{b}}'; \mathbf{0}, \tilde{\mathbf{D}}')$
11:       $\tilde{\mathbf{y}}[j + 1 : j + d] \leftarrow \mathrm{E}[\tilde{\mathbf{Y}}']$
12:    **end for**
13:    **return** P and $\tilde{\mathbf{y}}$
14: **end procedure**

Table 2 Errors and execution times of the d-dimensional conditioning method

(m, d)	1	2	4	8	16
Without univariate reordering					
16	2.1%	1.9%	**1.6%**	1.0%	0.0%
	0.00s	0.00s	**0.00s**	0.04s	0.23s
32	2.5%	2.4%	**2.2%**	1.8%	1.1%
	0.00s	0.01s	**0.01s**	0.06s	0.40s
64	**2.8%**	2.8%	2.7%	2.4%	2.0%
	0.00s	0.01s	0.02s	0.13s	0.79s
128	**2.6%**	2.6%	2.5%	2.4%	2.1%
	0.01s	0.02s	0.04s	0.29s	1.68s
With univariate reordering					
16	0.09%	0.05%	**0.01%**	0.01%	0.01%
	0.001s	0.002s	**0.004s**	0.033s	0.205s
32	0.05%	**0.02%**	0.02%	0.02%	0.02%
	0.002s	**0.004s**	0.008s	0.062s	0.392s
64	**0.03%**	0.03%	0.02%	0.02%	0.02%
	0.005s	0.008s	0.016s	0.126s	0.778s
128	**0.02%**	0.02%	0.02%	0.02%	0.02%
	0.014s	0.020s	0.038s	0.286s	1.625s

The upper half of the table reports results of the non-reordered conditioning method and the lower half reports the results of the reordered conditioning method. The correlation matrix is randomly generated from the correlation matrix space. The absolute error and the time cost are shown for each combination of m and d based on 250 replicates. The bold font represents the smallest error × time under each m

Carlo results with a sample size of 10^4, which can provide an estimation error below 10^{-4}. Since $(d − 1)$-dimensional MVN probabilities need to be evaluated for $2d × s$ times, we use a progressive sample size for the Quasi-Monte Carlo simulations within the d-dimensional conditioning algorithm. Specifically, when $d \leq 4$, $5 × 200$ samples are selected, when $4 < d \leq 8$, $10 × 400$ samples are selected, and when $d > 8$, $10 × 1000$ samples are selected. The estimation error is reduced when d increases with m remaining unchanged because less correlation information is discarded by conditioning when d becomes larger. In the extreme case when $d = m$, we perform the Quasi-Monte Carlo simulation in m-dimensions to approximate the MVN probability directly and no error is caused by the loss of correlation information. The time cost grows close to a linear fashion with m but exponentially with d.

3.4 Reordered d-dimensional conditioning

Trinh and Genz (2015) found that reordering of the integration variables can improve the estimation accuracy of the conditioning method. The reordering precedes the run-

ning of Algorithm 2 and arranges the integration variables with smaller truncated probabilities on the left side. Since the integration limits are affected only by the integration variables to their left as shown in Eq. (2), intuitively the integration variables further to the left have more impact on the estimation accuracy. Univariate reordering is preferred to multivariate reordering because the marginal improvement for the multivariate reordering is insignificant but the increased computational complexity is substantial. The univariate reordering algorithm is presented as Algorithm 2.2 in Trinh and Genz (2015). Here, we extract and rephrase the univariate reordering algorithm for completeness. The d-dimensional conditioning method with univariate reordering is presented as Algorithm 3 here.

The lower half of Table 2 presents the results for the d-dimensional conditioning algorithm with preceding reordering. The simulation conditions are the same as in the upper half of the table. Reordering results in significant improvement in estimation accuracy if we compare the errors with those from the non-reordered conditioning method. We cannot distinguish the conditioning method error from the Monte Carlo error when their estimate difference is below $5 × 10^{-4}$. The time costs, including those from the univariate reordering, decrease on average compared with the case without the univariate reordering, indicating that the univariate reordering can speed up the d-dimensional Monte Carlo simulation performed as part of the conditioning method. The univariate reordering has a complexity of $O(m^3)$ but is still insignificant up to 128-dimensions. Although this complexity increases rapidly as m increases, the size of each diagonal

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Algorithm 3 d-dimensional conditioning algorithm with univariate reordering

1: **procedure** RCMVN($\tilde{\mathbf{\Sigma}}, \tilde{\mathbf{a}}, \tilde{\mathbf{b}}, d$)
2: $\quad \tilde{\mathbf{y}} \leftarrow \mathbf{0}, \tilde{\mathbf{C}} \leftarrow \tilde{\mathbf{\Sigma}}$
3: $\quad$ **for** $i = 1 : m$ **do**
4: $\quad\quad$ **if** $i > 1$ **then**
5: $\quad\quad\quad \tilde{\mathbf{y}}[i − 1] \leftarrow \frac{\phi(\tilde{a}') − \phi(\tilde{b}')}{\Phi(\tilde{b}') − \Phi(\tilde{a}')}$
6: $\quad\quad$ **end if**
7: $\quad\quad j \leftarrow \arg\min_{i \leq j \leq m} \left\{ \Phi\left(\frac{\tilde{\mathbf{b}}[j] − \tilde{\mathbf{C}}[j, 1:i−1] \tilde{\mathbf{y}}[1:i−1]}{\sqrt{\tilde{\mathbf{\Sigma}}[j, j] − \tilde{\mathbf{C}}[j, 1:i−1] \tilde{\mathbf{C}}^T[j, 1:i−1]}} \right) − \Phi\left(\frac{\tilde{\mathbf{a}}[j] − \tilde{\mathbf{C}}[j, 1:i−1] \tilde{\mathbf{y}}[1:i−1]}{\sqrt{\tilde{\mathbf{\Sigma}}[j, j] − \tilde{\mathbf{C}}[j, 1:i−1] \tilde{\mathbf{C}}^T[j, 1:i−1]}} \right) \right\}$
8: $\quad\quad \tilde{\mathbf{\Sigma}}[:, (i, j)] \leftarrow \tilde{\mathbf{\Sigma}}[:, (j, i)], \tilde{\mathbf{\Sigma}}[(i, j), :] \leftarrow \tilde{\mathbf{\Sigma}}[(j, i), :]$
9: $\quad\quad \tilde{\mathbf{C}}[:, (i, j)] \leftarrow \tilde{\mathbf{C}}[:, (j, i)], \tilde{\mathbf{C}}[(i, j), :] \leftarrow \tilde{\mathbf{C}}[(j, i), :]$
10: $\quad\quad \tilde{\mathbf{a}}[(i, j)] \leftarrow \tilde{\mathbf{a}}[(j, i)], \tilde{\mathbf{b}}[(i, j)] \leftarrow \tilde{\mathbf{b}}[(j, i)]$
11: $\quad\quad \tilde{\mathbf{C}}[i, i] \leftarrow \sqrt{\tilde{\mathbf{\Sigma}}[i, i] − \tilde{\mathbf{C}}[i, 1:i−1] \tilde{\mathbf{C}}^T[i, 1:i−1]}$
12: $\quad\quad \tilde{\mathbf{C}}[j, i] \leftarrow (\tilde{\mathbf{\Sigma}}[j, i] − \tilde{\mathbf{C}}[i, 1:i−1] \tilde{\mathbf{C}}^T[j, 1:i−1])/\tilde{\mathbf{C}}[i, i],$ for $j = i + 1, \ldots, m$
13: $\quad\quad \tilde{a}' \leftarrow (\tilde{\mathbf{a}}[i] − \tilde{\mathbf{C}}[i, 1:i−1] \tilde{\mathbf{y}}[1:i−1])/\tilde{\mathbf{C}}[i, i]$
14: $\quad\quad \tilde{b}' \leftarrow (\tilde{\mathbf{b}}[i] − \tilde{\mathbf{C}}[i, 1:i−1] \tilde{\mathbf{y}}[1:i−1])/\tilde{\mathbf{C}}[i, i]$
15: $\quad$ **end for**
16: $\quad$ CMVN($\tilde{\mathbf{\Sigma}}, \tilde{\mathbf{a}}, \tilde{\mathbf{b}}, d$) as in Algorithm 2
17: **end procedure**

block in the hierarchical covariance matrix, $\mathcal{H}$, is usually taken from a range much smaller than the problem size, n, which makes univariate reordering a feasible option for solving the small MVN problem presented by each diagonal block.

4 The hierarchical-block conditioning method

The simulations for the d-dimensional conditioning method in Sect. 3 indicate that the algorithm coupled with univariate reordering could be an efficient alternative to Monte-Carlo-based methods. Genton et al. (2018) found that building the Quasi-Monte Carlo method on top of a hierarchical representation reduces the computational complexity per sample from $O(n^2)$ to $O(mn + kn \log(n/m))$, which is especially significant when the problem size, n, is large. As an additional benefit, the memory required for storage is also minimized when a hierarchical representation is used. In this section, we solve the n-dimensional MVN problem with the hierarchical covariance matrix and compare the efficiency of using the d-dimensional conditioning method with that of the Monte-Carlo-based method for solving the m-dimensional MVN problems presented by the diagonal blocks.

4.1 The hierarchical-block conditioning algorithm

The hierarchical-block conditioning method uses the conditioning technique with the hierarchical representation of the covariance matrix, which decomposes the n-dimensional integration into:

$$
\Phi_n(\mathbf{a}, \mathbf{b}; \mathbf{0}, \boldsymbol{\Sigma}) = \int_{\mathbf{a}_1'}^{\mathbf{b}_1'} \phi_m(\mathbf{x}_1; \mathbf{B}_1 \mathbf{B}_1^T) \int_{\mathbf{a}_2'}^{\mathbf{b}_2'} \phi_m(\mathbf{x}_2; \mathbf{B}_2 \mathbf{B}_2^T)
$$
$$
\cdots \int_{\mathbf{a}_r'}^{\mathbf{b}_r'} \phi_m(\mathbf{x}_r; \mathbf{B}_r \mathbf{B}_r^T) \, d\mathbf{x}_r \cdots d\mathbf{x}_2 \, d\mathbf{x}_1,
$$
$$(5)$$

where $\mathbf{a}_i'$ and $\mathbf{b}_i'$, $i = 1, \ldots, r$, are the corresponding segments of the updated $\mathbf{a}$ and $\mathbf{b}$. Truncated expectations are computed for each diagonal block, $\mathbf{B}_i \mathbf{B}_i^T$, and used for updating the integration limits to the right as shown in Eq. (5). The hierarchical-block conditioning algorithm is presented as Algorithm 4. It transforms the n-dimensional MVN problem into r m-dimensional problems. For clarity of presentation, we assume that n and m are both powers of 2. The dimension function, dim, therefore returns an integer and the offset refers to the number of rows or columns leading the matrix block, $\mathbf{U}_{i-1} \mathbf{V}_{i-1}^T$. The function *choldecomp_hmatrix* implements the hierarchical Cholesky factorization and returns $\mathbf{B}$

and $\mathbf{UV}^T$ as a vector of matrices. A slight modification is needed when n and m assume arbitrary values from the set of positive integers.

To compute the MVN probability and truncated expectations in m-dimensions, we can either perform the Monte-Carlo-based method directly or use the d-dimensional conditioning algorithm introduced in Sect. 3 as a second level of conditioning. In fact, the former method is a special case of the latter when $d = m$ and has much higher complexity because the simulations are performed in m-dimensions. The latter method further transforms each m-dimensional MVN problem into s d-dimensional MVN problems as shown in Eq. (2) although additional error can be introduced by the conditioning technique on the second level. In Sects. 4.2 and 4.3, we compare the two methods for solving the m-dimensional problem under simple covariance structures.

4.2 Simulation with a constant covariance matrix

We first use the constant covariance structure to compare the performance of applying the d-dimensional conditioning method with that of the Monte-Carlo-based method to each m-dimensional MVN problem. The covariance matrix is ideal for hierarchical representation because any off-diagonal block can be written exactly as the product of two rank-1 matrices. However, the correlation does not decay with the distance between indices and a stronger correlation usually leads to a larger error for the conditioning method (Trinh and Genz 2015). In this section, we progressively define three methods to highlight the efficiencies gained from the conditioning method and the accuracy gained from the univariate reordering. Method 1 applies Eqs. (3) and (4) to compute the m-dimensional MVN probability and truncated expectations

---

Algorithm 4 Hierarchical-block conditioning algorithm

1: **procedure** HCMVN($\mathbf{a}$, $\mathbf{b}$, $\boldsymbol{\Sigma}$, d)
2:      $\mathbf{x} \leftarrow \mathbf{0}$ and $P \leftarrow 1$
3:      $[\mathbf{B}, \mathbf{UV}] \leftarrow choldecomp\_hmatrix(\boldsymbol{\Sigma})$
4:      **for** $i = 1 : r$ **do**
5:          $j \leftarrow (i-1)m$
6:          **if** $i > 1$ **then**
7:              $o_r \leftarrow$ row offset of $\mathbf{U}_{i-1} \mathbf{V}_{i-1}^T$, $o_c \leftarrow$ column offset of $\mathbf{U}_{i-1} \mathbf{V}_{i-1}^T$
8:              $l \leftarrow \dim(\mathbf{U}_{i-1} \mathbf{V}_{i-1}^T)$
9:              $\mathbf{g} \leftarrow \mathbf{U}_{i-1} \mathbf{V}_{i-1}^T \mathbf{x}[o_c + 1 : o_c + l]$
10:             $\mathbf{a}[o_r + 1 : o_r + l] \leftarrow \mathbf{a}[o_r + 1 : o_r + l] - \mathbf{g}$
11:             $\mathbf{b}[o_r + 1 : o_r + l] \leftarrow \mathbf{b}[o_r + 1 : o_r + l] - \mathbf{g}$
12:          **end if**
13:          $\mathbf{a}_i \leftarrow \mathbf{a}[j+1 : j+m]$, $\mathbf{b}_i \leftarrow \mathbf{b}[j+1 : j+m]$
14:          $P \leftarrow P \cdot \Phi_m(\mathbf{a}_i, \mathbf{b}_i; \mathbf{0}, \mathbf{B}_i \mathbf{B}_i^T)$
15:          $\mathbf{x}[j+1 : j+m] \leftarrow \mathbf{B}_i^{-1} \mathrm{E}[\mathbf{X}_i]$
16:      **end for**
17:      **return** P
18: **end procedure**

Table 3 Errors and execution times under the constant covariance structure and 1D exponential covariance structure

m	16			32			64		
n	512	1024	2048	512	1024	2048	512	1024	2048
Constant covariance structure									
M1	11.9%	13.6%	10.9%	11.8%	13.6%	10.9%	11.9%	13.6%	10.9%
	7.6s	14.7s	30.7s	16.7s	33.0s	59.9s	41.2s	78.1s	133.3s
M2	11.9%	13.6%	10.9%	11.8%	13.7%	10.9%	11.9%	13.7%	11.0%
	0.1s	0.3s	0.7s	0.1s	0.3s	0.6s	0.1s	0.3s	0.6s
M3	11.9%	13.6%	10.9%	11.8%	13.7%	10.9%	11.9%	13.6%	11.0%
	0.1s	0.3s	0.7s	0.1s	0.3s	0.6s	0.2s	0.3s	0.6s
1D exponential covariance structure									
M1	10.6%	8.4%	8.0%	3.4%	3.9%	4.1%	1.2%	1.1%	2.2%
	18.8s	38.1s	77.1s	36.5s	75.0s	152.1s	66.3s	141.5s	295.5s
M2	22.2%	29.1%	29.2%	23.1%	16.1%	31.9%	15.8%	21.2%	20.9%
	0.4s	0.8s	1.8s	0.4s	0.8s	1.7s	0.4s	0.9s	1.8s
M3	**10.3%**	**8.4%**	**7.8%**	**2.9%**	**3.6%**	**4.0%**	**1.1%**	**1.0%**	**2.2%**
	0.4s	**0.8s**	**1.8s**	**0.4s**	**0.8s**	**1.7s**	**0.4s**	**0.8s**	**1.7s**

Method 1 depends on the Monte-Carlo-based method for the MVN probability and truncated expectations. Method 2 applies the d-dimensional conditioning method. Method 3 employs the d-dimensional conditioning method with univariate reordering. The constant correlation is set at 0.7. The time and absolute error are based on 20 replicates. The bold font represents the smallest error × time under each combination of m and n

directly. Method 2 employs the d-dimensional conditioning method as described in Algorithm 2 to compute the m-dimensional MVN probability and truncated expectations. Method 3 begins with univariate reordering as described in Algorithm 3 and then uses the d-dimensional conditioning method. We select $d = 4$ for Method 2 and Method 3 because it provides a more balanced trade-off between the error and the computation time given the results in Table 2.

In this experiment, the correlation of the constant covariance matrix is set at 0.7 for a medium correlation strength. The lower integration bound, **a**, is set at $-\infty$ and the upper bound is independently generated from U(0, n), which makes the expectation of the simulated probability roughly 0.7. The upper half of Table 3 summarizes the time and relative error of the three methods under the constant covariance structure based on 20 replicates. We use 20 as the sample size instead of 250 as in Table 2 because the covariance structure is fixed, leading to a much smaller standard deviation for the estimators. Unlike for other covariance structures, the benchmark for the constant correlation case can be accurately calculated with a 1-dimensional integration

$$\Phi_n(-\infty, \mathbf{b}; \mathbf{0}, \mathbf{\Sigma}_{const})$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2} \prod_{i=1}^{n} \Phi_1\left(\frac{b_i + \sqrt{\theta}x}{1 - \theta}\right) dx, \quad (6)$$

where θ is the constant correlation coefficient. The estimation errors from the three methods are very close under the same set of constant-covariance MVN problems, indicating that

the dominant error comes from the first level of conditioning and the d-dimensional conditioning methods can estimate the MVN probability of size m almost as accurately as the Quasi-Monte Carlo method. Thus the estimation accuracy of the three methods cannot be clearly distinguished. By comparing the time costs, we can conclude that the d-dimensional conditioning method leads to significant efficiencies. In addition, the complexities of all methods appear to be in a linear relationship with n while the complexities of Method 2 and Method 3 are not sensitive to m.

For a clearer comparison of the complexities, we decompose the complexity of Algorithm 4 into three parts and list the complexity for each part in Table 4, where $M(\cdot)$ denotes the complexity of the Quasi-Monte Carlo simulation in the given dimension. Table 4 shows that the time efficiency of the d-dimensional conditioning algorithm mainly comes from lowering the dimension in which the Quasi-Monte Carlo simulation is performed. The complexity of the univariate reordering is $O(m^2n)$, the same as the complexity of computing the MVN probabilities in Method 2, resulting in an identical major complexity component for Method 2 and Method 3. Since Methods 2 and 3 perform the Quasi-Monte Carlo simulation in d-dimensions, these two methods are not greatly affected by the choice of m.

4.3 Simulation with 1D exponential covariance matrix

The second covariance structure used for comparing the accuracy and efficiency of the three methods is the 1D

Table 4 Complexity decomposition of the three methods

	MVN prob	Trunc exp	Upd limits
M1	$\frac{n}{m}M(m)$	$2nM(m) + O(nm^2)$	$O(mn + kn\log(n/m))$
M2	$\frac{n}{d}M(d) + O(m^2n)$	$2nM(d) + O(nd^2)$	$O(mn + kn\log(n/m))$
M3	$\frac{n}{d}M(d) + O(m^2n)$	$2nM(d) + O(nd^2)$	$O(mn + kn\log(n/m))$

Method 1 depends on the Monte-Carlo-based method for the MVN probability and truncated expectations. Method 2 applies the d-dimensional conditioning method. Method 3 employs the d-dimensional conditioning method with univariate reordering. The three parts of the complexity are the calculation of the MVN probability (MVN prob), the calculation of the truncated expectations (Trunc exp), and the update of the integration limits with truncated expectations (Upd limits). The latter two share the same asymptotic order in all three complexity terms. The updating cost is independent of the method

exponential covariance structure. Under this structure, the correlation is $\rho(X_i, X_j) = \exp(-d_{ij}/\beta)$, where d_{ij} is the distance between X_i and X_j, and β is the coefficient controling the correlation decay rate. After the random variables are indexed with a geometrically increasing order, the off-diagonal blocks can be written accurately as the product of two rank-1 matrices as in the case of the constant covariance. However, unlike the constant covariance example, the 1D exponential correlation decays quickly along with the distance between indices. In this experiment, n points are selected on the real line with neighboring distance 1, β is set to 10. Here, **a**, **b** and d are selected in the same fashion as in Sect. 4.2. Results from the Quasi-Monte Carlo simulation with a sample size of 100×10^4 are used as the benchmark, whose error level is below 10^{-4} in general. The lower half of Table 3 describes the average time and error of the three methods based on 20 replicates.

We find that the errors of the three methods under the 1D exponential structure fall into two bins. The error from Method 1 is close to that from Method 3, and both are much smaller than that from Method 2, indicating that univariate reordering effectively reduces the estimation error and even makes up for the loss of information resulting from the second level of conditioning. In contrast, under the constant covariance structure, a relatively large error is already generated from the first level of conditioning, which makes the improvement from univariate conditioning insignificant. Since there are two levels of conditioning in Method 2 and Method 3, we refer to both methods as two-level hierarchical-block conditioning methods hereafter. A similar conclusion about algorithmic efficiencies can be drawn from the results of the 1D exponential covariance structure that Methods 2 and 3 are more efficient. However, it is worth noting that the computation time for the same combination of (n, m) and the computational method is smaller under the 1D exponential covariance structure, probably because the Quasi-Monte Carlo simulation is faster under the weaker covariance structure. By comparing the results of the two covariance structures in Table 3, we may also conclude that increasing the diagonal block size, m, reduces the estimation error under a decaying correlation

structure because, intuitively, a larger m captures more correlation information. This is less obvious for Method 2 and Method 3, however, because the second level of conditioning unavoidably causes some of the correlation information within each diagonal block to be discarded.

Based on the results from the constant covariance structure and the 1D exponential covariance structure, we argue that Method 3 has the best combination of efficiency and accuracy. Hence from this point on, we consider only Method 3, the two-level hierarchical-block conditioning method proceded by univariate reordering for each diagonal block. We compare results from Method 3 with those from the hierarchical Quasi-Monte Carlo method (Genton et al. 2018), which could be considered the state-of-the-art technique for high-dimensional MVN problems at the time of this writing. To test the efficiencies of both methods on general MVN problems, we use a covariance structure in two dimensions.

4.4 Simulation with a 2D exponential covariance matrix

The covariance matrix from 1-dimensional geometry has a bounded rank for off-diagonal blocks under most covariance models because the sample points are distinctly separable. However, in two and higher dimensions, a proper indexing scheme needs to be implemented to maintain the locality of the samples despite the fact that the rank of the off-diagonal blocks usually grows in a log fashion. Morton's order is extensively used for reducing the dimensionality of data to one while leaving the sample points in the geometric vicinity still closer in indices. In this section, we assume a 2D exponential covariance structure and use Morton's order for indexing the sample points on the plane. As a result, the ranks of the off-diagonal blocks grow with their block sizes but at a much slower rate than $O(n)$. This is visible in the second column of Table 5. The diagonal block size m and the second conditioning dimension, d, collectively determine the amount of correlation information that is captured. Here, m reduces the estimation error at the cost of increased univariate reordering time for each diagonal block while d improves the result by performing Quasi-Monte Carlo simulation in higher

dimensions. In Sects. 4.2 and 4.3, we found that the two-level hierarchical-block conditioning methods are insensitive to the choice of m. We therefore fix $m = 64$ for the 2D covariance structure in this section and examine the effectiveness of our algorithm when the second conditioning dimension, d, is set to 1, 2, and 4. To test the sensitivity with respect to the correlation strength, we perform the estimation under $\beta = 0.3, 0.1$, and 0.03, representing strong, medium, and weak correlation strengths.

Table 5 presents the results for the two-level hierarchical-block conditioning method. The algorithm is implemented in C++ and compared with that in Genton et al. (2018). Table 5 shows the relative error and time, averaged from the same set of 20 problem replicates for each dimension n. For each replicate, the upper bound, **b**, is generated from U$(0, n)$ and the lower bound **a** is assumed to be $-\infty$ as in Trinh and Genz (2015). We construct the hierarchical covariance matrix, $\mathcal{H}$, prior to Cholesky factorization, and we use an adaptively decreasing tolerance level, starting at 5×10^{-4}, for building $\mathcal{H}$ to guarantee the positive-definiteness of $\mathcal{H}$. The second column describes the ranks of the off-diagonal blocks of $\mathcal{H}$ that grow approximately in a $\log n$ fashion. The last five columns correspond to the error and time for the three techniques evaluated in this section, namely the Quasi-Monte Carlo method (with a sample size of 10,000), the hierarchical Quasi-Monte Carlo method (with a sample size of 10,000), and the two-level hierarchical-block conditioning method with $d = 1, 2$, and 4. The benchmarks are more accurate hierarchical Quasi-Monte Carlo simulations with increased sample size. Specifically, the sample size is 10^6 for $n = 1024$ or 4096 and 5×10^6 for $n = 16,384$, which produces estimation error below 5×10^{-4} under all correlation strengths and below 1×10^{-4} under the weak correlation. The normal Quasi-Monte Carlo simulation is not used as a benchmark because of the huge computational cost in 16,384 dimensions (around 35,000 s). The two-level hierarchical-block conditioning method provides a poor estimation, indicating that the conditioning method by itself is not very suitable for high-dimensional MVN probability estimation when the correlation strength exceeds the level corresponding to $\beta = 0.03$ and $n = 256$. It is worth mentioning that the correlation strength is essentially increased when n increases while β remains unchanged because the samples are from the unit hypercube. Also the increase of d will reduce the estimation error but is still unable to reach a satisfactory level. The method, when used without a reordering strategy, does not produce sufficiently accurate results. This motivated the development of the reordering strategy described in the next section. We note that the time difference between this paper and Genton et al. (2018) for the Quasi-Monte Carlo method and the hierarchical Quasi-Monte Carlo method is due to different hardware and machine-level implementations.

Algorithm 5 Block-wise reordering

1: **procedure** BLOCKREORDER(**G**, ρ, **a**, **b**, m, **ind**)
2:      **for** $i = 1 : m : n - m + 1$ **do**
3:          subind $\leftarrow$ **ind**$[i : i + m - 1]$
4:          **A** $\leftarrow \rho($**G**, **subind**$)$
5:          **a**$' \leftarrow$ **a**[**subind**]
6:          **b**$' \leftarrow$ **b**[**subind**]
7:          **P** = [**P**,RCMVN(**A**, **a**$'$, **b**$'$, 1)$.P$] as in Algorithm 3
8:      **end for**
9:      sort(**ind**, **P**, m)
10:     **return ind**
11: **end procedure**

---

5 Block reordering

In the context of conditioning algorithms, the integration variables on the farther left, which also have higher priority in terms of calculation, tend to have more impact on the accuracy of the estimation. Univariate reordering can effectively reduce the estimation error for low-dimensional MVN problems (Trinh and Genz 2015) but applying it to n integration variables has a complexity of $O(n^3)$ and is likely to spoil the low-rank feature of the off-diagonal blocks, which is not desirable for an efficiency-oriented algorithm. The construction of the hierarchical covariance matrix essentially assumes that the correlation within each m-sized block of variables is strong while the correlation between these blocks is weak. Building on this idea, we rearrange the diagonal blocks of size m with their probabilities increasing from left to right, which is consistent with the idea of univariate reordering. The reordering of the blocks is implemented only once instead of recursively due to the high complexity of calculating the truncated expectations in m-dimensions. The probability for each block is estimated with the conditioning method introduced in Algorithm 2 and d is set to 1. Hence, the univariate reordering is performed at the same time. The algorithm for the block-wise reordering is summarized as Algorithm 5. For clarity, we use $\rho($**G**, **ind**$)$ for constructing a correlation matrix based on the correlation function, ρ, geometry, **G**, and indices, **ind**. Here, sort(**ind**, **P**, m) stands for rearranging the size-m segments of **ind** based on the vector, **P**, in an increasing order.

To examine the increased accuracy from the preceding block reordering, we implemented the 2D exponential experiments the same way as in Sect. 4.4 with an extra reordering layer before the two-level hierarchical-block conditioning algorithm. The benchmarks are computed the same way as in Table 5. Table 6 compares the reordered conditioning algorithm with the Monte-Carlo-based algorithms and the additional time cost from block reordering is measured separately and shown in the last column. The original Morton's order is disturbed by the block reordering. As a result, the ranks and the memory cost of the off-diagonal blocks increase as indicated in the second and third columns. The resulting

Table 5 Performance of the two-level hierarchical-block conditioning method without reordering

n	$k_{min}, k_{avg}, k_{max}$	$\mathcal{H}$ (Megabytes)	mvn	hmvn	hccmvn$_1$	hccmvn$_2$	hccmvn$_4$
$\beta = 0.3$							
256	15, 20, 30	0.22	**0.4%**	0.4%	19.7%	18.5%	16.1%
			0.2s	0.6s	0.0s	0.1s	0.2s
1024	14, 24, 60	1.58	**0.5%**	0.5%	27.6%	26.0%	24.7%
			2.0s	2.7s	0.1s	0.5s	1.1s
4096	14, 26, 116	11.67	0.9%	**0.9%**	47.8%	46.8%	43.6%
			30.7s	**20.0s**	1.2s	2.9s	5.4s
16,384	13, 26, 222	87.09	0.7%	**0.7%**	52.8%	50.9%	48.7%
			1161.1s	**91.5s**	6.9s	14.4s	26.2s
$\beta = 0.1$							
256	13, 18, 28	0.21	**0.2%**	0.2%	14.5%	12.1%	9.3%
			0.2s	0.6s	0.0s	0.1s	0.2s
1024	14, 23, 58	1.55	**0.5%**	0.5%	31.9%	29.5%	24.8%
			1.8s	2.5s	0.1s	0.4s	1.1s
4096	14, 26, 117	11.81	0.6%	**0.6%**	26.6%	24.5%	22.9%
			26.6s	**11.2s**	0.4s	2.1s	4.7s
16,384	13, 27, 229	89.63	0.8%	**0.8%**	54.9%	53.5%	51.7%
			1161.8s	**53.9s**	4.1s	10.4s	20.9s
$\beta = 0.03$							
256	8, 12, 18	0.18	**0.0%**	0.0%	1.2%	0.8%	0.6%
			0.2s	2.6s	0.0s	0.0s	0.1s
1024	12, 20, 50	1.39	**0.1%**	0.1%	6.2%	5.7%	3.5%
			2.0s	2.6s	0.1s	0.4s	1.0s
4096	13, 25, 112	11.22	0.5%	**0.5%**	26.8%	24.0%	19.8%
			26.8s	**11.2s**	0.5s	2.1s	4.5s
16,384	14, 27, 227	88.90	0.5%	**0.5%**	28.3%	26.5%	24.0%
			1166.8s	**43.2s**	3.4s	9.3s	19.6s

The covariance matrix is generated from the exponential covariance function based on n points randomly distributed in the unit square indexed with Morton's order. The Quasi-Monte Carlo method (mvn), the hierarchical Quasi-Monte Carlo method (hmvn) and the two-level hierarchical-block conditioning method (hccmvn$_d$) with $d = 1, 2$ and 4 are compared. The bold font represents the smallest error $\times$ time under each n

estimation error for the two-level hierarchical-block conditioning method is significantly reduced by the preceding block reordering but still affected by the correlation strength. For isotropic exponential covariance models, we use their effective ranges as a proxy for the correlation strength. When β is equal to 0.3, 0.1, and 0.03 respectively, the effective ranges are 0.90, 0.30, and 0.09, which can provide a reference for the level of estimation error when the integration region is scaled to the unit hypercube. The error is below 3% overall with strong correlation, while below 1% with medium and weak correlations. Errors of such magnitude can make the conditioning method a good substitute for Monte-Carlo-based methods. The run time costs for the two-level hierarchical-block conditioning method are not sensitive to the ranks of the off-diagonal blocks. Columns 6 to 8 of Table 6 indicate similar time performance compared with Table 5

because each matrix-vector multiplication is performed only once in the conditioning algorithm as described in Algorithm 4. The choice of d has little impact on the estimation accuracy when the preceding block reordering exists due to the fact that the accuracy level is already very high when $d = 1$. Thus, we use $d = 1$ as the benchmark for comparing the time efficiencies of the hierarchical-block conditioning method and the hierarchical Quasi-Monte Carlo method. On average, the two-level hierarchical-block conditioning method, $hccvn_1$, has the best combination of error $\times$ time and is eleven times faster than the hierarchical Quasi-Monte Carlo method, $hmvn$, but slightly more sensitive to the correlation strength. The extra time used for block reordering is negligible compared with the overall time costs of the conditioning methods.

Table 6 Performance of the two-level hierarchical-block conditioning method with reordering

n	$k_{min}, k_{avg}, k_{max}$	$\mathcal{H}$ (MB)	mvn	hmvn	hccmvn$_1$	hccmvn$_2$	hccmvn$_4$	Reorder (s)
$\beta = 0.3$								
256	11, 20, 37	0.22	0.4%	0.4%	**1.3%**	1.1%	1.1%	0.00
			0.2s	0.6s	**0.0s**	0.1s	0.2s	
1024	1, 21, 82	1.73	0.5%	0.5%	**1.0%**	1.0%	1.0%	0.01
			2.0s	2.7s	**0.1s**	0.5s	1.1s	
4096	1, 22, 151	13.94	0.9%	0.9%	**3.1%**	3.1%	3.1%	0.03
			30.7s	20.0s	**1.2s**	2.9s	5.4s	
16,384	1, 24, 287	114.14	0.7%	0.7%	**3.0%**	3.0%	3.0%	0.14
			1161.1s	91.5s	**7.0s**	14.0s	25.5s	
$\beta = 0.1$								
256	10, 18, 34	0.21	0.2%	0.2%	**0.7%**	0.6%	0.6%	0.00
			0.2s	0.6s	**0.0s**	0.1s	0.1s	
1024	1, 19, 82	1.70	0.5%	0.5%	**0.9%**	0.9%	0.9%	0.01
			1.8s	2.5s	**0.1s**	0.5s	1.0s	
4096	1, 22, 151	13.9	0.6%	0.6%	**0.5%**	0.5%	0.5%	0.03
			26.6s	11.2s	**0.5s**	2.1s	4.4s	
16,384	1, 25, 287	115.75	0.9%	0.9%	**0.4%**	0.3%	0.3%	0.14
			1161.8s	53.9s	**4.4s**	10.5s	20.5s	
$\beta = 0.03$								
256	6, 12, 23	0.18	0.0%	0.0%	**0.0%**	0.0%	0.0%	0.00
			0.2s	0.6s	**0.0s**	0.0s	0.1s	
1024	1, 17, 81	1.60	0.1%	0.1%	**0.1%**	0.1%	0.1%	0.01
			1.8s	2.6s	**0.1s**	0.4s	1.0s	
4096	1, 20, 149	13.57	0.5%	0.5%	**0.0%**	0.0%	0.0%	0.04
			26.8s	11.2s	**0.6s**	2.0s	4.4s	
16,384	1, 25, 287	115.71	0.5%	0.5%	**0.0%**	0.0%	0.0%	0.12
			1166.8s	43.2s	**3.4s**	9.3s	19.0s	

The covariance matrix is generated from the exponential covariance function based on n points randomly distributed in the unit square indexed first with Morton's order and then with block reordering as in Algorithm 5. The Quasi-Monte Carlo method (mvn), the hierarchical Quasi-Monte Carlo method (hmvn) and the two-level hierarchical-block conditioning method (hccmvn$_d$) with $d = 1, 2$ and 4 are compared. MB in the third column is short for megabytes. The bold font represents the smallest error $\times$ time under each n

6 Discussion

Despite the broad success of conditioning approximation methods (Kamakura 1989) for computing MVN probabilities, one problem with them is that additional guidance is needed as to when the approximations can be used reliably and when one needs to fall back on more expensive Monte Carlo simulation methods that can produce approximations to a specified accuracy. This concern has been recognized in the literature, and the general practice (Connors et al. 2014; Trinh and Genz 2015) is for potential users to perform careful comparisons with MC methods to assess empirically whether the conditioning approximations are appropriate for their problems, as we have done, for example, in Sect. 5.

However it is possible in principle to perform additional computations to obtain indicators for the errors that are introduced by the basic substitutions adopted in these approximations. One potential strategy combines the conditioning approximation substitution with sampling at the block level, to provide a means for producing error estimates. Consider for example the "conditioned" form of an m-dimensional MVN problem:

$$\Phi_m(\mathbf{a}, \mathbf{b}; \mathbf{0}, \boldsymbol{\Sigma}) = \int_{a'_1}^{b'_1} \phi(x_1; D_1) \int_{a'_2(x_1)}^{b'_2(x_1)} \phi(x_2; D_2)$$
$$\cdots \int_{a'_m(x_1,\ldots,x_{m-1})}^{b'_m(x_1,\ldots,x_{m-1})} \phi(x_m; D_m) \, dx_m \cdots dx_2 \, dx_1.$$

The key substitution in the univariate ($d = 1$) conditioning approximation replaces the x_i values in the limits of the integrals by their expected values μ_i, instead of generating them as random samples from a truncated normal and using these

values to update all integration limits for every sample, as one would do in a Monte Carlo simulation. The justification for these substitutions is that these μ_i values are the average values that the x_i would have if sampled from the truncated normal in $[a_i', b_i']$.

This suggests a possible way to assess the quality of this substitution: instead of using the expected value μ_i, one may use N samples for every integration and use the mean $\bar{\mu}_i$ of the samples to update the integration limits to produce an approximation Φ_m^j of the MVN integration. Repeating this process for $j \in 1 : M$ produces estimates whose variance is an error indicator for Φ_m. A large value of the error indicator implies that the conditioning approximation is not adequate for the problem at hand. One would either need to increase the conditioning dimension d to increase the coupling that was implicitly ignored, or fall back on Monte Carlo simulations.

For the proposed hierarchical block-conditioning method, the MVN integration was written in Eq. (5) as:

$$\Phi_n(\mathbf{a}, \mathbf{b}; \mathbf{0}, \mathbf{\Sigma}) = \int_{\mathbf{a}_1'}^{\mathbf{b}_1'} \phi_m(\mathbf{x}_1; \mathbf{B}_1 \mathbf{B}_1^T) \int_{\mathbf{a}_2'(\mathbf{x}_1)}^{\mathbf{b}_2'(\mathbf{x}_1)} \phi_m(\mathbf{x}_2; \mathbf{B}_2 \mathbf{B}_2^T)$$
$$\cdots \int_{\mathbf{a}_r'(\mathbf{x}_1,\ldots,\mathbf{x}_{r-1})}^{\mathbf{b}_r'(\mathbf{x}_1,\ldots,\mathbf{x}_{r-1})} \phi_m(\mathbf{x}_r; \mathbf{B}_r \mathbf{B}_r^T) \, d\mathbf{x}_r \cdots d\mathbf{x}_2 \, d\mathbf{x}_1.$$

The key substitution here replaced $\mathbf{x}_i$ in the integration limits by their expected values $\boldsymbol{\mu}_i \in \mathbb{R}^m$. In order to assess the effect of these substitutions, one can similarly compute approximations by using N samples for every m-dimensional integration $i \in 1 : r$, and update the integration limits on the right of i using the sample expectation. Repeating this process M times provides a variance that is indicative of the error. Large error indicators would require using larger block sizes (for example $2m$) or falling back on a Monte Carlo simulation. We note here that this computation is far less costly than a full Monte Carlo solution, because the integration limits affected by $\mathbf{x}_i$ are not updated for every sample but only once for the N samples used in the ith integration.

It remains for future work to develop general error indicators and estimates to be used with these conditioning approximations, in order to make them more general-purpose black boxes. In the current state of the practice, the hierarchical-block conditioning method proposed here and the class of approximations to which it belongs are intended to be used when fast computations are desired, but on problems where the user has established that the approximations introduced are of acceptable accuracy for the intended application purpose.

The suitability of the hierarchical conditioning method depends on the covariance structure, the correlation strength, and the accuracy requirement. When the covariance structure is random, for example in Table 2, the non-hierarchical method works better because the cost of building the hier-

archical covariance matrix may not outweigh the savings from matrix manipulations. However, in most circumstances, the covariance function is smooth and adopting the hierarchical representation will greatly improve the efficiency. In cases where the estimation error or a high accuracy level is required, the Monte Carlo method is more suitable than the conditioning method since the latter method in its basic version does not generate an internal estimate of its error. When the MVN probabilities need to be estimated a large number of times, the conditioning method can be based on the correlation strength and the practitioner's error tolerance level. The estimation error is generally below 1% when the correlation strength is lower than or comparable to the medium correlation strength for the exponential covariance, as discussed in Sect. 5. Unlike the Monte Carlo method, the estimate of the conditioning method is not stochastic given a MVN specific problem, $\Phi_n(\mathbf{a}, \mathbf{b}; \mathbf{0}, \mathbf{\Sigma})$, assuming the errors from the d-dimensional Monte Carlo simulations are ignored while the Monte Carlo method can produce an estimate arbitrarily close to the true value through increasing the sample size.

7 Summary and conclusions

We presented a d-dimensional conditioning algorithm as an extension of the bivariate conditioning algorithm from Trinh and Genz (2015) and, based on it, we described a hierarchical-block conditioning method for estimating MVN probabilities that is suitable for high-dimensional problems. The d-dimensional conditioning algorithm delivers more accurate estimation under randomly generated covariance structures as d increases. The hierarchical technique takes advantage of the low-rank features of the common covariance models used in spatial statistics, which significantly reduce the computation time and the storage cost. We also introduced a block reordering scheme that preserves the low-rank feature and significantly improves the estimation accuracy with little additional cost. Combining the three, we introduced a two-level hierarchical-block conditioning algorithm that can further shorten the computation time of MVN probabilities based on the hierarchical Quasi-Monte Carlo method. There are two parameters for the algorithm, namely the diagonal block size, m, and the conditioning dimension, d, which collectively control the accuracy and the complexity of the algorithm. The dimension, m, should be large enough to yield savings from low-rank structures in the off-diagonal blocks yet not too large to make computation of the diagonal blocks too costly. The dimension, d, increases the estimation accuracy for the probability and truncated expectations within each diagonal block but also increases the complexity quickly because of the calculations of truncated expectations. The algorithm provides a practical method for calculating the MVN probabilities in tens of thousands of dimensions.

The estimation for the truncated expectations makes up the largest computational complexity in the current algorithm and is calculated based on Eqs. (3) and (4). Future progress in estimating the truncated expectations of MVN random variables is expected to reduce the run time of this algorithm significantly.

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