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

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Introduction

Introduction

- The computation of the multivariate normal (MVN) probability

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

  where $\mathbf{a}$ and $\mathbf{b}$ are integration limits, the mean vector μ is assumed to be 0, $\mathbf{\Sigma}$ is a positive-definite covariance matrix, is required for a variety of applications.
- Various methods to compute MVN probability are suggested such as Richtmyer Quasi-Monte Carlo(QMC) (Genz and Bretz, 2009)
- However, In high-dimensional settings (large n), it is hard to compute (1) directly.
- We review new approaches proposed by Cao et al. (2019) to approximate high-dimensional multivariate normal probability (1) using the hierarchical matrix $\mathcal{H}$ (Hackbusch, 2015) for the covariance matrix $\mathbf{\Sigma}$.

Key Ideas

The methods are based on the concepts of

1. The bivariate conditioning method (Trinh and Genz, 2015)
   - LDL decomposition and truncated expectations
   - Generalized to d-dimensioned-case
2. The hierarchical QMC method (Genton et al., 2018)
   - Hierarchical cholseky decomposition: efficient and fast computation
   - QMC: beneficial on computation complexity and memory management
3. Reordering (Trinh and Genz, 2015)
   - Univariate reordering (Trinh and Genz, 2015)
   - Generalized the upper case to blockwise reordering

Multidimensional Conditioning Approximations

Quasi Monte Carlo Method

- Monte Carlo Error bound : $O(N^{-1/2})$ for monte carlo(MC) method
- Genz and Bretz (2009) claimed independent sample points is the reason of slow convergence.
- Via employing low discrepancy sets for sequence, QMC is asymptotically efficient than MC.
- With $\mathbf{\Delta} \sim U[0,1]^n$,

$$L_N = \{\mathbf{z} + \mathbf{\Delta} \bmod 1 : \mathbf{z} \in K_N\}$$

$$K_N = \{i\mathbf{q} \bmod 1, i = 1, \cdots, N\}$$

  where $\mathbf{q} = \sqrt{\mathbf{p}}$ and $\mathbf{p}$ is set of prime numbers.
- Since square root of prime numbers is irrational and linear independent over the rational numbers,

Quasi Monte Carlo Method

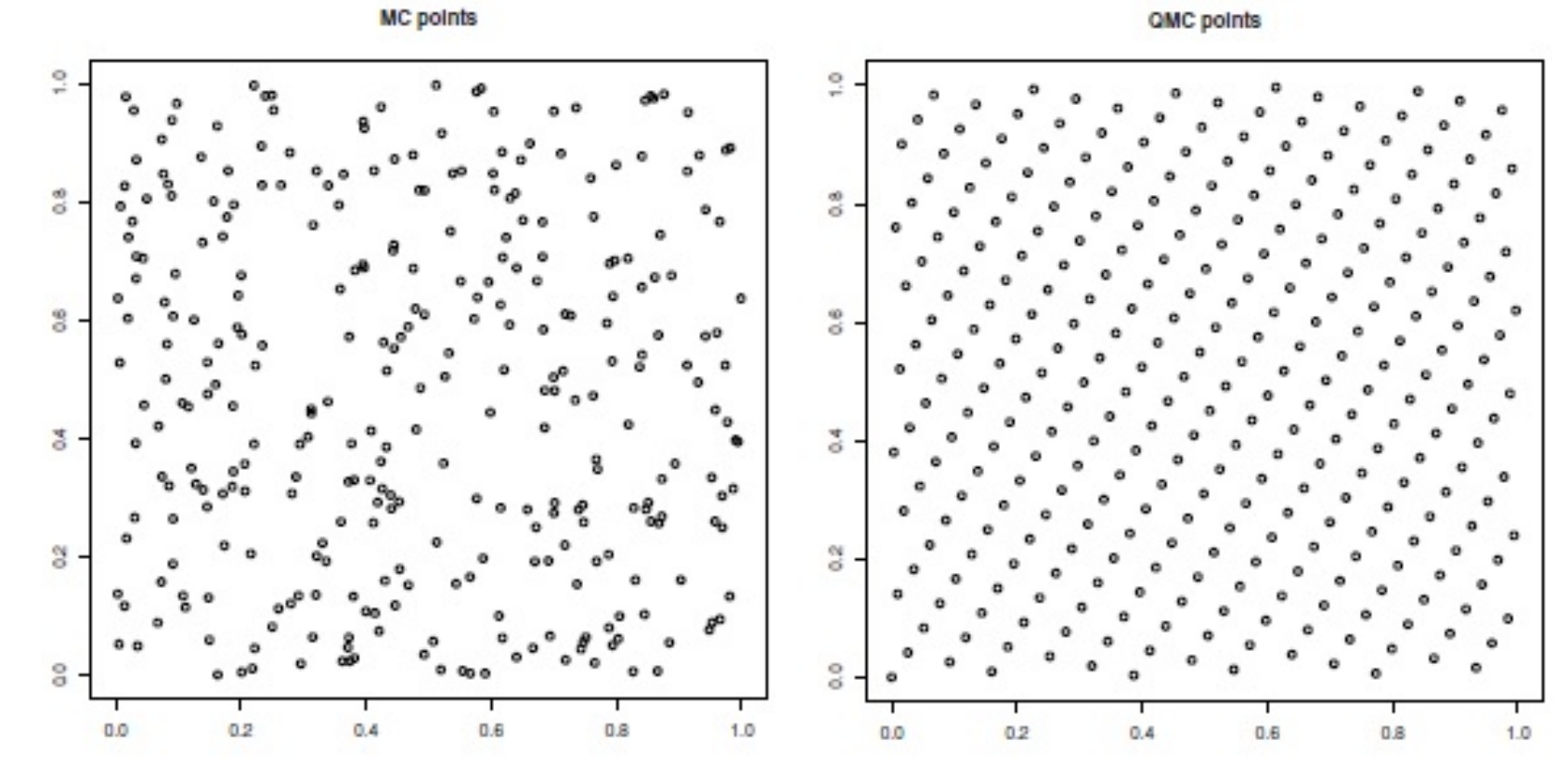


Figure 1: Comparison of MC and QMC sample points(Genz and Bretz, 2009)

Quasi Monte Carlo Method

$$\begin{aligned}
\mathbf{\Phi}_n(\mathbf{a} \le \mathbf{x} \le \mathbf{b}; \mathbf{\Sigma}) &= \mathbf{\Phi}_n(a \le \mathbf{L}\mathbf{y} \le \mathbf{b}; I_n) \\
&= \int_{a_1 \le l_{11} y_1 \le b_1} \phi(y_1) \cdots \int_{a_n \le \mathbf{l}_n^t \mathbf{y} \le b_n} \phi(y_n) d\mathbf{y} \\
&= \int_{\tilde{a}_1}^{\tilde{b}_1} \phi(y_1) \int_{\tilde{a}_2(y_1)}^{\tilde{b}_2(y_1)} \phi(y_2) \cdots \int_{\tilde{a}_n(y_1, \cdots, y_{n-1})}^{\tilde{b}_n(y_1, \cdots, y_{n-1})} \phi(y_n) d\mathbf{y}
\end{aligned}$$

$$\text{with } \tilde{a}_i(y_1, \cdots, y_{i-1}) = \frac{a_i - \sum_{j=1}^{i-1} l_{ij} y_j}{l_{ii}}$$

$$\text{and } (\tilde{b}_i(y_1, \cdots, y_{i-1})) = \frac{b_i - \sum_{j=1}^{i-1} l_{ij} y_j}{l_{ii}}$$

$$\begin{aligned}
&= \int_{\Phi(\tilde{a}_1)}^{\Phi(\tilde{b}_1)} \int_{\Phi(\tilde{a}_2(\Phi^{-1}(z_1)))}^{\Phi(\tilde{b}_2(\Phi^{-1}(z_1)))} \cdots \int_{\Phi(\tilde{a}_n(\Phi^{-1}(z_1), \cdots, \Phi^{-1}(z_{n-1})))}^{\Phi(\tilde{b}_n(\Phi^{-1}(z_1), \cdots, \Phi^{-1}(z_{n-1})))} d\mathbf{z} (y_i = \Phi^{-1}(z_i)) \\
&= (e_1 - d_1) \int_0^1 (e_2(w_1) - d_2(w_1)) \cdots \\
&\int_0^1 (e_n(w_1, \cdots, w_{n-1}) - d_n(w_1, \cdots, w_{n-1}))) \int_0^1 d\mathbf{w}
\end{aligned}$$

$$\text{with } z_i = d_i + (e_i - d_i) w_i \qquad (2)$$

Quasi Monte Carlo Method

1: **procedure** MVN($\boldsymbol{\mu}$, $\boldsymbol{\Sigma}$, $\mathbf{a}$, $\mathbf{b}$, ns, N)
2: $\mathbf{L} = \text{cholesky}(\boldsymbol{\Sigma})$
3: $\mathbf{a} = \mathbf{a} - \boldsymbol{\mu}$; $\mathbf{b} = \mathbf{b} - \boldsymbol{\mu}$
4: $T = 0$, $N = 0$, $V = 0$
5: $\mathbf{p} = \text{vector of primes less than } \frac{5n \log n + 1}{4}$; $\mathbf{q} = \sqrt{\mathbf{p}}$
6: $\mathbf{P} = \mathbf{1}_{ns}$
7: $ans = 0$
8: **for** $i = 1, \cdots, ns$ **do**
9: $I_i = 0$, $\boldsymbol{\Delta} \sim U(0,1)^n$
10: **for** $j = 1, \cdots, N$ **do**
11: $\mathbf{X}[1:n, j] = (j+1)\mathbf{q} + \boldsymbol{\Delta}$
12: $\mathbf{X}[1:n, j] = 2|\mathbf{X}[1:n, j] - \text{floor}(\mathbf{X}[1:n, j])| - 1$
13: **end for**
14: **sample** $= \mathbf{O}_{n,N}$
15: $\mathbf{s}$, $\mathbf{c}$, $\mathbf{d}$, $\mathbf{dc}$, $\mathbf{P} = \mathbf{0}_N$
16: **for** $j = 1, \cdots, n$ **do**
17: **if** $j > 1$ **then**
18: $c = \min(1, c + X[j-1, :] \odot dc)$
19: **sample**$[i-1, 1:N] = \Phi^{-1}(c)$
20: $s =$ **sample**$[1:i-1, 1:N]^T L[1:i-1, i]$
21: **end if**
22: $\mathbf{P}* = \Phi(\frac{b-s}{L[i,i]}) - \Phi(\frac{a-s}{L[i,i]})$
23: **end for**
24: ans+ $= \text{mean}(\mathbf{P})$
25: **end for**
26: **return** ans$/ns$
27: **end procedure**

Algorithm 1: Multivariate Normal Probability with Quasi Monte Carlo Method

Conditioning Approximation

- Mendell and Elston (1974), Kamakura (1989), and Trinh and Genz (2015) exploit Cholesky factors from LDL decomposition rather than dealing with original covariance matrix.
- Biviarate example is follow:

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma}_{1,1} & \mathbf{R}^T \\ \mathbf{R} & \hat{\mathbf{\Sigma}} \end{pmatrix}, \text{ with } \mathbf{L} = \begin{pmatrix} \mathbf{I}_2 & \mathbf{O} \\ 1:\mathbf{M} & \mathbf{L} \end{pmatrix} \text{ and } \mathbf{D} = \begin{pmatrix} \mathbf{D}_1 & \mathbf{O} \\ \mathbf{O} & \widehat{\mathbf{D}}, \end{pmatrix}$$

  where $\mathbf{\Sigma}_{1,1}, \mathbf{D}_1$ is a 2×2 matrix.
- From $\mathbf{D}_1 = \mathbf{\Sigma_{1,1}}$, $\mathbf{M} = \mathbf{R}\mathbf{D}_1^{-1}$, $\widehat{\mathbf{D}} = \hat{\mathbf{\Sigma}} - \mathbf{M}\mathbf{D}_1\mathbf{M}^T$

$$\mathbf{\Phi}_n(\mathbf{a}, \mathbf{b}; \mathbf{0}, \mathbf{\Sigma}) = \frac{1}{\sqrt{|\mathbf{D}|(2\pi)^n}} \int_{\alpha_1}^{\beta_1} \int_{\alpha_2}^{\beta_2} e^{-\frac{1}{2}\mathbf{x_2}^T \mathbf{D}_1^{-1} \mathbf{x}_2} \cdots \int_{\alpha_{2k-1}}^{\beta_{2k-1}} \int_{\alpha_{2k}}^{\beta_{2k}} e^{-\frac{1}{2}\mathbf{x_{2k}}^T \mathbf{D}_1^{-1} \mathbf{x}_{2k}} \tag{3}$$

Conditioning Approximation

Cao et al. (2019) generalizes bivariate method of Trinh and Genz (2015) to d-dimensional. The details are Algorithms 2

procedure LDL($\mathbf{\Sigma}$)
  $\mathbf{L} \leftarrow \mathbf{I}_m, \mathbf{D} \leftarrow \mathbf{O}_m$
  for $i = 1 : d : m - d + 1$ **do**
    $\mathbf{D}[i : i + d - 1, i : i + d - 1] \leftarrow \mathbf{\Sigma}[i : i + d - 1, i : i + d - 1]$
    $\mathbf{L}[i + d : m, i : i + d - 1] \leftarrow \mathbf{\Sigma}[i + d : m, i : i + d - 1]\mathbf{D}^{-1}[i : i + d - 1, i : i + d - 1]$
    $\mathbf{\Sigma}[i + d : m, i + d : m] \leftarrow \mathbf{\Sigma}[i + d : m, i + d : m] - \mathbf{L}[i + d : m, i : i + d - 1]\mathbf{D}^{-1}[i : i + d - 1, i : i + d - 1]\mathbf{L}[i : i + d - 1, i + d : m]$
    if $i + d < m$ **then**
      $\mathbf{D}[i + d : m, i + d : m] \leftarrow \mathbf{\Sigma}[i + d : m, i + d : m]$
    end if
  end for
  return L and **D**
end procedure

Algorithm 2: LDL decomposition

Conditioning Approximation

When $s = \frac{m}{d}$ is integer, results of Algorithm 2, $\mathbf{L}, \mathbf{D}$ can be written as

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

with d-dimensional identitiy matrix $\mathbf{I}_d$ and d-dimensional zero matrix $\mathbf{O}_d$ and d-dimensional positive-definite matrix $\mathbf{D}_1, \cdots, \mathbf{D}_s$.

As in (3), tranformation, $Y = LX$ provides m-dimensional multivariate normal prabability as the product of s d-dimensional multivariate normal probabilities as

$$\mathbf{\Phi}_{\boldsymbol{m}}(\mathbf{a}, \mathbf{b}; \mathbf{0}, \mathbf{\Sigma}) = \int_{\alpha_1}^{\beta_1} \phi_d(\mathbf{y}_1; \mathbf{D}_1) \int_{\alpha_2}^{\beta_2} \phi_d(\mathbf{y}_2; \mathbf{D}_2) \tag{4}$$

$$\cdots \int_{\alpha_s}^{\beta_s} \phi_d(\mathbf{y}_s; \mathbf{D}_s) d\mathbf{y}_s \cdots d\mathbf{y}_2 d\mathbf{y}_1, \tag{5}$$

where $\boldsymbol{\alpha}_i = \mathbf{a}_i - \sum_{j=1}^{i-1} \mathbf{L}_{ij}\mathbf{y}_j, \boldsymbol{\beta}_i = \mathbf{b}_i - \sum_{j=1}^{i-1} \mathbf{L}_{ij}\mathbf{y}_j$

Conditioning Approximation

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

Algorithm 3: d-dimensional conditioning algorithm

Multidimensional Truncated Expectations

- The truncated expectation is expressed as

$$E(X^{e_j}) = \frac{1}{\mathbf{\Phi}(\mathbf{a}, \mathbf{b}; \boldsymbol{\mu}, \boldsymbol{\Sigma})} \int_{\mathbf{a}}^{\mathbf{b}} x_j \phi_d(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{x}$$
$$= \frac{1}{\mathbf{\Phi}(\mathbf{a}, \mathbf{b}; \boldsymbol{\mu}, \boldsymbol{\Sigma})} F_j^d(\mathbf{a}, \mathbf{b}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Theore 1 has same form with bivariate version of Trinh and Genz (2015) with $d = 2$
- It allows us to calculate $E[Y']$ in Algorithm 3 with $\mathbf{\Phi}$ which can be obtained with quasi monte calro method proposed by Genz (1992)

Multidimensional Truncated Expectations

Theorem
Kan and Robotti (2017)

$$F_j^d(\mathbf{a}, \mathbf{b}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mu_j \boldsymbol{\Phi}_d(\mathbf{a}, \mathbf{b}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) + \mathbf{e}_j^T \boldsymbol{\Sigma} \mathbf{c},$$

where c is a vector with lth component defined as

$$\begin{aligned} c_l = {} & \phi_1(a_l; \mu_l, \sigma_l^2) \Phi_{d-1}(\mathbf{a}_{-l}, \mathbf{b}_{-l}; \hat{\boldsymbol{\mu}}^1, \hat{\boldsymbol{\Sigma}}_l) \\ & - \phi_1(b_l; \mu_l, \sigma_l^2) \Phi_{d-1}(\mathbf{a}_{-l}, \mathbf{b}_{-l}; \hat{\boldsymbol{\mu}}^2, \hat{\boldsymbol{\Sigma}}_l) \end{aligned}$$

$$\hat{\boldsymbol{\mu}}_l^1 = \mu_{-l} + \boldsymbol{\Sigma}_{-l,l} \frac{a_l - \mu_l}{\sigma_l^2}, \hat{\boldsymbol{\mu}}_l^2 = \mu_{-l} + \boldsymbol{\Sigma}_{-l,l} \frac{b_l - \mu_l}{\sigma_l^2},$$

$$\hat{\boldsymbol{\Sigma}}_l = \boldsymbol{\Sigma}_{-l,-l} - \frac{1}{\sigma_l^2} \boldsymbol{\Sigma}_{-l,l} \boldsymbol{\Sigma}_{l,-l}$$

Multidimensional Conditioning Approximation with Univariate Reordering

Appropriate integration order on conditioning algorithm possibly improves estiation accuracy

- Schervish (1984) : integral with shortest integration interval widths be the outermost integration variables
- Gibson et al. (1994) : variables which have smallest expected values be the outermost integration variables.
  Since innermost integrals which have smaller variation have the most influence with this order, overall variance reduces.
- Trinh and Genz (2015) also employs this ordering, and Cao et al. (2019) generalized it to d-dimensional problem.

Multidimensional Conditioning Approximation with Univariate Reordering

procedure RCMVN($\mathbf{\Sigma}$, $\mathbf{a}$, $\mathbf{b}$, d)

  $\mathbf{y} \leftarrow \mathbf{0}$, $\mathbf{C} \leftarrow \mathbf{\Sigma}$

  for $i = 1 : m$ **do**

    if $i > 1$ **then**

      $\mathbf{y}[i-1] \leftarrow \frac{\phi(a') - \phi(b')}{\Phi(b') - \Phi(a')}$

    end if

    $j \leftarrow \text{argmin}_{i \le j \le m} \{ \Phi(\frac{\mathbf{b}[j] - \mathbf{C}[j, 1:i-1]\mathbf{y}[1:i-1]}{\sqrt{\mathbf{\Sigma}[j,j] - \mathbf{C}[j, 1:i-1]\mathbf{C}^T[j, 1:i-1]}}) - \Phi(\frac{\mathbf{a}[j] - \mathbf{C}[j, 1:i-1]\mathbf{y}[1:i-1]}{\sqrt{\mathbf{\Sigma}[j,j] - \mathbf{C}[j, 1:i-1]\mathbf{C}^T[j, 1:i-1]}}) \}$

    $\mathbf{\Sigma}[:, (i, j)] \leftarrow \mathbf{\Sigma}[:, (j, i)]$; $\mathbf{\Sigma}[(i, j), :] \leftarrow \mathbf{\Sigma}[(j, i), :]$

    $\mathbf{C}[:, (i, j)] \leftarrow \mathbf{C}[:, (j, i)]$; $\mathbf{C}[(i, j), :] \leftarrow \mathbf{C}[(j, i), :]$

    $\mathbf{a}[(i, j)] = \mathbf{a}[(j, i)]$

    $\mathbf{b}[(i, j)] = \mathbf{b}[(j, i)]$

    $\mathbf{C}[i, i] \leftarrow \sqrt{\mathbf{\Sigma}[i, i] - \mathbf{C}[i, 1 : i-1]\mathbf{C}^T[i, 1 : i-1]}$

    $\mathbf{C}[j, i] \leftarrow \frac{\mathbf{\Sigma}[j, i] - \mathbf{C}[i, 1:i-1]\mathbf{C}^T[j, 1:i-1]}{\mathbf{C}[i, i]}$, for $j = i+1, \cdots, m$

    $a' = \frac{\mathbf{a}[i] - \mathbf{C}[i, 1:i-1]y[1:i-1]}{\mathbf{C}[\mathbf{i}, \mathbf{i}]}$

    $b' = \frac{\mathbf{b}[i] - \mathbf{C}[i, 1:i-1]y[1:i-1]}{\mathbf{C}[\mathbf{i}, \mathbf{i}]}$

  end for

  return CMVN($\mathbf{\Sigma}$, $\mathbf{a}$, $\mathbf{b}$, d) as in Algorithm 3

end procedure

Algorithm 4: d-dimensional conditioning algorithm with univariate reordering

Hierarchical-Block Approximation

Hierarchical Cholesky Decomposition

- Hackbusch (2015) proposed hiarchical matrix and its cholesky decomposition method.
- $A = LU$ have the structure

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} L_{11} & O \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} L_{11}^T & L_{12}^T \\ O & L_{22}^T \end{pmatrix}$$

  with lower triangular matrix L_{11}, L_{22}.
- It leads to four tasks:
  (a) compute L_{11} via Cholesky decomposition of A_{11}
  (b) compute L_{12} from $L_{21}L_{11}^T = A_{21}$
  (c) low rank approximation of $L_{12} = UV^T$
  (d) compute L_{22} via Cholesky decomposition of $A_{22} - L_{21}L_{21}^T$
- We have applied low rank approximation with svd to (c) each block of its decomposition to make implementation efficiently and save storage while accuracy is preserved, i.e.
  $A = UDV^T = \sum_{i=1}^{n} d_i u_i v_i^T \approx \sum_{i=1}^{k} d_i u_i v_i^T$.

Hierarchical Cholesky Decomposition

Hierachical cholesky decomposition of $n \times n$ matrix into $m \times m$ blocks is implemented like below.

1: **procedure** HCHOL(A, n,m,rank)
2: **for** $i = 1 : log_2(\frac{n}{m})$ **do**
3: $nb = n/2^i$
4: x = 0, y = nb
5: **for** $j = 1 : 2^{i-1}$ **do**
6: $\mathbf{U}, \mathbf{D}, \mathbf{V} = lowrankSVD(A[xbegin + 1 : xbegin + nb, ybegin + 1 : ybegin + nb], rank)$
7: $\mathbf{A}[x + 1 : x + nb, y + 1 : y + rank] = \mathbf{UD}$
8: $\mathbf{A}[x + 1 : x + nb, y + rank + 1 : y + nb] = \mathbf{O}$
9: $\mathbf{A}[y + 1 : y + nb, x + 1 : x + rank] = \mathbf{VD}$
10: $\mathbf{A}[y + 1 : y + nb, x + rank + 1 : x + nb] = \mathbf{O}$
11: $x+ = 2nb, y+ = 2nb$
12: **end for**
13: **end for**
14: **end procedure**

Algorithm 5: Hierachical cholesky decomposition

The Hierarchical-Block Conditioning Method

- Let $\phi_m(\mathbf{x}; \mathbf{\Sigma})$ be a pdf of the m-dimensional normal distribution $N(\mathbf{0}, \mathbf{\Sigma})$ and $(\mathbf{B}, \mathbf{U}\mathbf{V}^T)$ be the hierarchical Cholesky decompostion of the covariance matrix $\mathbf{\Sigma}$.
- Then,

$$\Phi_n(\mathbf{a}, \mathbf{b}; \mathbf{0}, \mathbf{\Sigma}) = \int_{\mathbf{a}_1'}^{\mathbf{b}_1'} \phi_m(\mathbf{x}_1; \mathbf{B}_1\mathbf{B}_1^T) \cdots \int_{\mathbf{a}_r'}^{\mathbf{b}_r'} \phi_r(\mathbf{x}_r; \mathbf{B}_r\mathbf{B}_r^T) d\mathbf{x}_r \cdots d\mathbf{x}_1, \tag{6}$$

  where $\mathbf{a}'$, $\mathbf{b}'$, $i = 1, \cdots, r$, are the corresponding segments of the updated $\mathbf{a}$ and $\mathbf{b}$.
- Note the probabilities $\Phi_m(\mathbf{a}_i, \mathbf{b}_i; \mathbf{0}, \mathbf{B}_i\mathbf{B}_i^T)$ can be computed using
  1. Quasi-Monte Carlo method (`HMVN`)
  2. d-dimensional conditioning algorithm (`HCMVN`)
  3. d-dimensional conditioning algorithm with univariate reordering (`HRCMVN`)

The Hierarchical-Block Conditioning Method

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

Algorithm 6: Hierarchical-block conditioning algorithm

Computational Complexity

- Let $M(\cdot)$ be the complexity of the QMC simulation in the given dimension.
- Cao et al. (2019) summarize the time efficiency of the d-dimensional conditioning algorithm as Table 1.

	MVN prob	Trunc exp	Upd limits
`HMVN`	$\frac{n}{m}M(m)$	$2nM(m) + O(nm^2)$	$O(mn + knlog(n/m))$
`HCMVN`	$\frac{n}{d}M(d) + O(m^2 n)$	$2nM(d) + O(nd^2)$	$O(mn + knlog(n/m))$
`HRCMVN`	$\frac{n}{d}M(d) + O(m^2 n)$	$2nM(d) + O(nd^2)$	$O(mn + knlog(n/m))$

Table 1: Complexity decomposition of the `HMVN`, `HCMVN`, and `HRCMVN`

Block Reordering

Block Reordering

- The value of probability based on n-dimensioned multivariate normal random variable comprises of m multiplications of d-dimensional integrals.
- Recall the `RCMVN` algorithm(3) : as computing each d-dimensional integral values, integration variables were arranged in order of increasing order of `CMVN` probability values, from outer to inner
- Permutes the block of LDL-decomposed covariance matrix, in order of `RCMVN` probability values of each blocks
- Result accuracy and time cost is compared among `HMVN`, `HCMVN`, `HRCMVN` with/without block reordering.

Block Reordering

procedure BLOCKREORDER(G, ρ, a, b, m, ind)
  G, ρ, a, b, m, ind given, $\mathbf{P} \leftarrow 0$
  for $i = 1 : m : n - m + 1$ **do**
    $\mathbf{s} \leftarrow ind[i : i + m - 1]$
    $\mathbf{A} \leftarrow \rho(G, \mathbf{s})$
    $a' \leftarrow a[\mathbf{s}]$
    $b' \leftarrow b[\mathbf{s}]$
    $\mathbf{P} \leftarrow [\mathbf{P}, \mathtt{RCMVN}(\mathbf{A}, a', b', 1).P]$
  end for
  sort(ind, **P**, m)
  return ind
end procedure

Algorithm 7: Blockwise reordering

Block Reordering

procedure HCMVN_BRO(a, b, Σ, d)
  $\mathbf{x} \leftarrow \mathbf{0}$, $P \leftarrow 1$, ind $\leftarrow [1, \ldots, n]$
  $[\mathbf{B}, \mathbf{UV}] \leftarrow$ choldecomp_hmatrix(Σ)
  $\mathbf{B} \leftarrow$ Blockreorder(G, ρ, a, b, m, ind)
  for $i = 1 : r$ **do**
    $j \leftarrow (i-1)m$
    if $i > 1$ **then**
      $o_r \leftarrow$ row offset of $\mathbf{U}_{i-1}\mathbf{V}_{i-1}^T$
      $o_c \leftarrow$ column offset of $\mathbf{U}_{i-1}\mathbf{V}_{i-1}^T$
      $l \leftarrow \dim(\mathbf{U}_{i-1}\mathbf{V}_{i-1}^T)$
      $\mathbf{g} \leftarrow \mathbf{U}_{i-1}\mathbf{V}_{i-1}^T\mathbf{x}[o_c + 1 : o_c + l]$
      $\mathbf{a}[o_r + 1 : o_r + l] = \mathbf{a}[o_r + 1 : o_r + l] - \mathbf{g}$
      $\mathbf{b}[o_r + 1 : o_r + l] = \mathbf{a}[o_r + 1 : o_r + l] - \mathbf{g}$
    end if
    $\mathbf{a}_i \leftarrow \mathbf{a}[j + 1 : j + m]$
    $\mathbf{b}_i \leftarrow \mathbf{b}[j + 1 : j + m]$
    $P = P * \Phi_m(\mathbf{a}_i, \mathbf{b}_i; \mathbf{0}, \mathbf{B}_i\mathbf{B}_i^T)$
    $\mathbf{x}[j + 1 : j + m] \leftarrow \mathbf{B}_i^{-1}E[\mathbf{X}_i]$
  end for
end procedure

Algorithm 8: Hierarchical-block conditioning algorithm with Block Reordering

Numerical Examples

Data

Exponential covariance matrix, $\mathbf{\Sigma}_{ij} = exp(-\|\mathbf{s}_i - \mathbf{s}_j\|/\beta)$ is set with $\beta = 0.3$. n points, $\mathbf{s}_1, \cdots, \mathbf{s}_n$ is evenly distributed over unique square with Morton's order which defined recursively as described in figure 2.

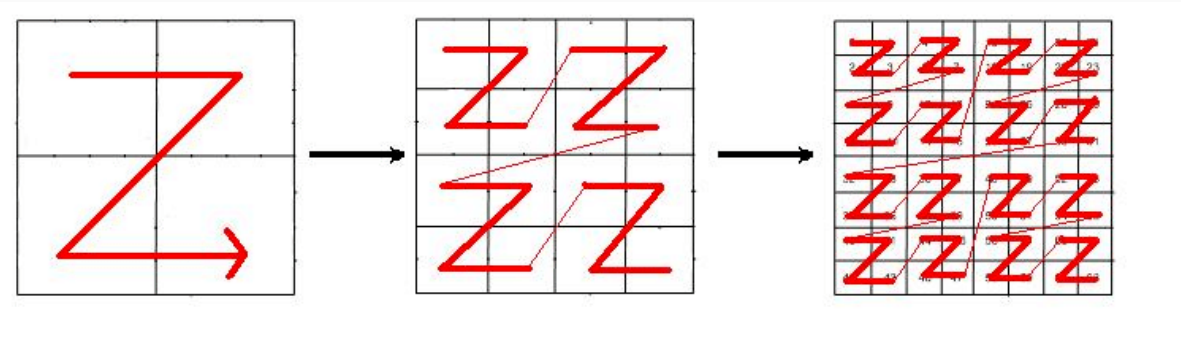


Figure 2: Morton's order (Salem and Arab, 2016)

Cholesky Factorization

Methods

1. The *chol* function from **LinearAlgebra** package
2. The *dpotrf* from **LAPACK** package
3. Hierarchical cholesky decomposition which suggested by Hackbusch (2015) are implemented.

- With various n, three Cholesky methods are applied and results are below table 2.
- In low rank approximation at algorithm 5, rank is about $n^{1/4}$.
- Hierarchical cholesky decomposition provides $\mathbf{\Sigma} \approx L_H L_H^T$.
- Its relative error is defined as $\dfrac{\|\mathbf{\Sigma} - L_H L_H^T\|_2}{\|\mathbf{\Sigma}\|_2}$

Cholesky Factorization

n	256	1024	4096	16384
chol	0.001s	0.0097s	0.414s	156.3s
dpotrf	0.0007s	0.0132s	0.431s	154.1s
hierarchical cholesky	0.153s	0.076s	0.916s	37.3s
Error of hierarchical cholesky	1.06e-7	9.97e-7	1.11e-3	1.87e-3

Table 2: Excution times for Cholesky factorization

Results

- Hierarchical cholesky decomposition is more efficient than other classical cholesky method with large dimension.
- Table 2 ensures accuracy of hierarchical cholesky decomposition proposed by Hackbusch (2015).

Multivariate Normal Probabilities

Methods

1. Classical Monte Carlo(MC) is estimate probabilities from acceptance ratio,
2. Richtmyer Quasi-Monte Carlo(QMC) introduced in the section 2.

Settings

- Varying sample size N and dimension d, two Monte Carlo methods are compared and results are below table 3 and 4.
- Set $\Sigma = I_d$, $\mathbf{a}_i = -\infty$ and $\mathbf{b}_i = 0$, i.e. true probabilities are $1/2^d$s
- Repeat 20 times.

Multivariate Normal Probabilities

(n, d)	4	8	12	16	20
500	12.2%	56.8%	161.9%	100.0%	100.0%
	0.294ms	0.016ms	0.018ms	0.019ms	0.019ms
1000	9.5%	50.6%	193.8%	100.0%	100.0%
	0.046ms	0.041ms	0.028ms	0.028ms	0.034ms
1500	8.9%	38.7%	150.2%	100.0%	100.0%
	0.055ms	0.046ms	0.042ms	0.048ms	0.045ms
2000	5.4%	26.5%	102.4%	100.0%	100.0%
	0.070ms	0.065ms	0.072ms	0.058ms	0.055ms
2500	5.1%	32.0%	100.1%	100.0%	100.0%
	0.073ms	0.092ms	0.081ms	0.083ms	0.076ms

Table 3: Results for the classical Monte Carlo

Multivariate Normal Probabilities

(n, d)	4	8	12	16	20
500	0.0% 0.058ms	0.0% 0.003ms	0.0% 0.006ms	0.0% 0.006ms	0.0% 0.011ms
1000	0.0% 0.003ms	0.0% 0.009ms	0.0% 0.013ms	0.0% 0.017ms	0.0% 0.020ms
1500	0.0% 0.006ms	0.0% 0.011ms	0.0% 0.016ms	0.0% 0.019ms	0.0% 0.030ms
2000	0.0% 0.011ms	0.0% 0.012ms	0.0% 0.013ms	0.0% 0.025ms	0.0% 0.036ms
2500	0.0% 0.009ms	0.0% 0.022ms	0.0% 0.033ms	0.0% 0.038ms	0.0% 0.056ms

Table 4: Results for the Richtmyer Quasi-Monte Carlo

Multidimensional Conditioning Approximations

Results

- MC fails even d is not large enough.
- QMC is numerically stable and faster than MC
- All the multivariate normal distribution probabilities required in the next experiments are calculated using QMC.

d-dimensional Conditioning Algorithm without/with Reordering

Settings

- 250 MVN problems with various values of m and d
- $\mathbf{\Sigma} = \mathbf{QJQ}^T$ is simulated with $\mathbf{Q} \sim$ *Haar distribution* and $J = diag(j_i)$ where $j_1, \cdots, j_m \sim U(0,1)$
- Integration limits $a_i = -\infty$ and $b_i \sim (U, m)$ for $i = 1 \cdots, m$

Theorem

Stewart (1980) Let the independent vectors $x_1, \cdots, x_n$ *be distributed* $N(0, \sigma^2\mathbf{I})$. *For* $j = 1, 2, \cdots, n-1$, *let* $\mathbf{H}_{x_j}$ *be the Householder transformation that reduces* x_j *to* $r_{jj}e_1$, *where* r_{ij} *is obtained in QR decomposition of* $[x_1, \cdots, x_n]$ *Let* $\mathbf{H}_j = diag(\mathbf{I}_{j-1}, \bar{\mathbf{H}}_j)$. *Let* $\mathbf{D} = diag(sign(r_{11}), \cdots, sign(r_{nn}))$. *Then the product* $\mathbf{Q} = \mathbf{DH_1} \cdots \mathbf{H_{n-1}}$ *follows Haar Distribution.*

d-dimensional Conditioning Algorithm without/with Reordering

(m, d)	1	2	4	8	16
Without univariate reordering					
16	3.7% 0.029ms	3.5% 0.201ms	3.6% 0.431ms	3.8% 0.676ms	2.9% 1.372ms
32	2.4% 0.001ms	2.9% 0.390ms	2.9% 0.833ms	3.3% 1.283ms	2.7% 2.545ms
64	1.9% 0.004ms	2.1% 0.762ms	2.1% 1.686ms	1.8% 2.545ms	1.9% 5.004ms
128	1.3% 0.024ms	1.5% 1.505ms	1.3% 3.333ms	1.2% 5.146ms	1.4% 10.548ms
With univariate reordering					
16	3.3% 0.007ms	3.1% 0.203ms	3.3% 0.439ms	3.6% 0.680ms	2.7% 1.363ms
32	2.3% 0.004ms	2.6% 0.393ms	2.6% 0.841ms	3.2% 1.289ms	2.6% 2.544ms
64	2.0% 0.014ms	2.1% 0.773ms	2.1% 1.695ms	1.9% 2.552ms	1.9% 5.022ms
128	1.2% 0.097ms	1.5% 1.593ms	1.4% 3.462ms	1.2% 5.268ms	1.4% 10.7861ms

Table 5: Errors and execution times of the d-dimensional conditioning method

Multidimensional Conditioning Approximations

Results

- Estimated value is compared with approximated value obtained via quasi monte carlo method with a sample size of 10^4, which ensures error below 10^{-4}
- Estimation error tended to decrease as d increases with each m since lager d implers less discarded correlation information.
- Spent time grows to a linear fashion with m while it grows exponentially with d.

Hierarchical-Block Approximations

Methods

- M1, `HMVN()`: Calculate multivariate normal probabilities using hierarchical-block approximation
- M2, `HCMVN()`: Calculate multivariate normal probabilities using hierarchical-block conditioning approximation
- M3, `HRCMVN()`: Calculate multivariate normal probabilities using hierarchical-block conditioning approximation with univarite reordering

Data

1. Constant covariance matrix: $k(x_i, x_j) = \theta + (1 - \theta)\delta_{ij}$ for some $|\theta| < 1$.
2. 1D exponential covariance matrix: $k(x_i, x_j) = \exp(-d_{ij}/\beta)$ for some $\beta > 0$, where d_{ij} is the distance between x_i and x_j.

Hierarchical-Block Approximations

Settings

- Simulation size $= 20$
- Integration limits $a_i = -\infty$ and $b_i \sim (U, n)$ for $i = 1 \cdots, n$
- $\theta = 0.7$, $d_{ij} = 1$, and $\beta = 10$ as in Cao et al. (2019)
- Fix $d = 4$ for `HCMVN` and `HRCMVN`.

Table 6, Figure 3 and 4 are errors and execution times under the constant covariance structure and 1D exponential covariance structure respectively.

Hierarchical-Block Approximations

m	16			32			64		
n	256	512	1024	256	512	1024	256	512	1024
Constant covariance structure									
M1	8.22%	7.11%	8.66%	8.94%	7.88%	6.68%	10.58%	8.05%	9.78%
M2	8.37%	7.08%	8.60%	8.91%	7.77%	6.61%	10.58%	8.26%	9.91%
M3	8.51%	7.10%	8.70%	9.51%	7.92%	7.00%	10.68%	7.94%	9.63%
1D exponential covariance matrix									
M1	2.87%	0.00%	0.01%	0.07%	1.31%	0.00%	2.65%	0.27%	0.57%
M2	3.28%	0.01%	0.90%	0.07%	1.31%	0.01%	2.65%	0.28%	0.57%
M3	4.73%	0.09%	2.11%	2.17%	1.90%	0.16%	3.72%	1.25%	0.66%

Table 6: Relative errors under the constant covariance structure and 1D exponential covariance structure

Hierarchical-Block Approximations- Execution Time i

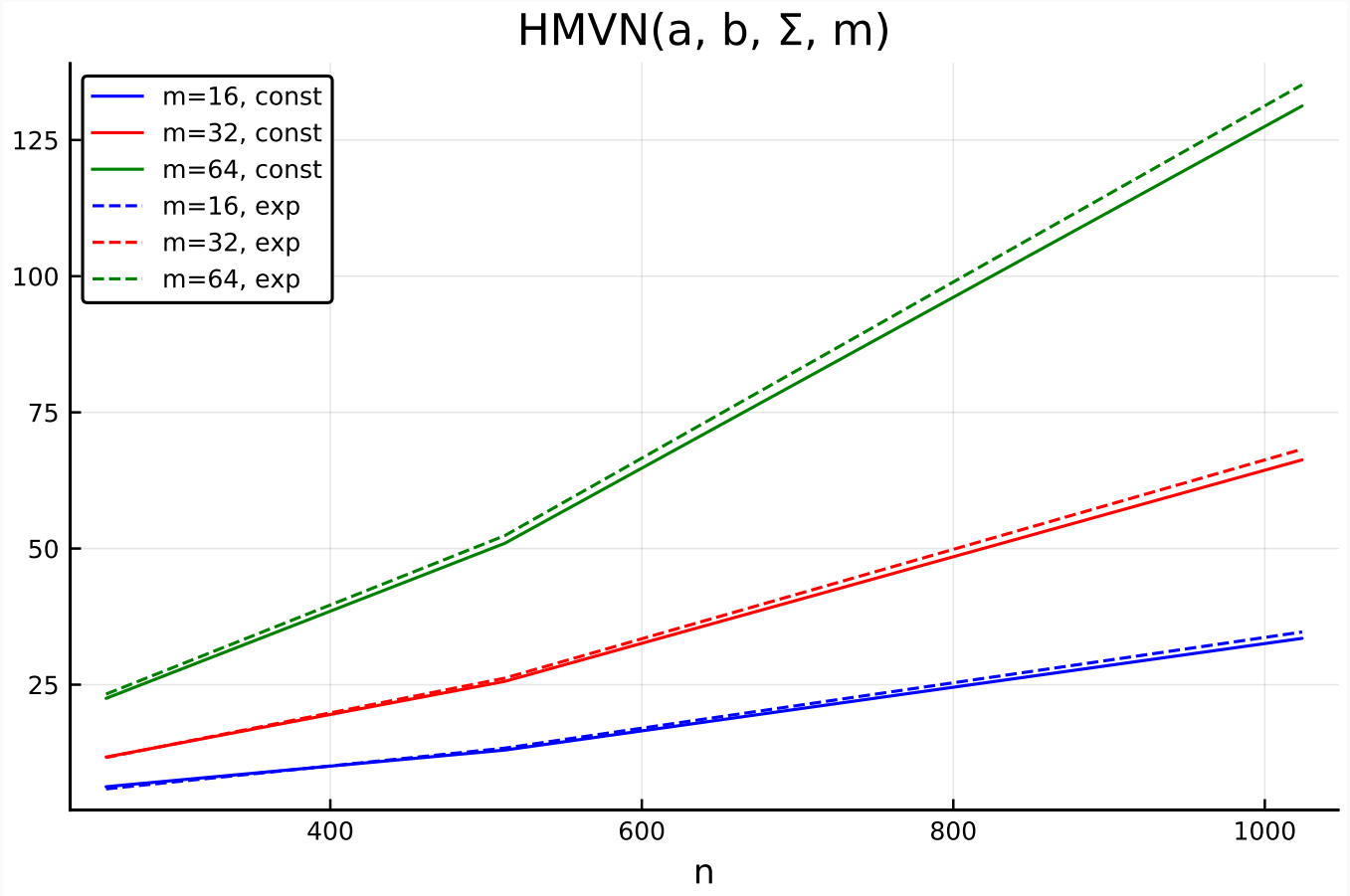
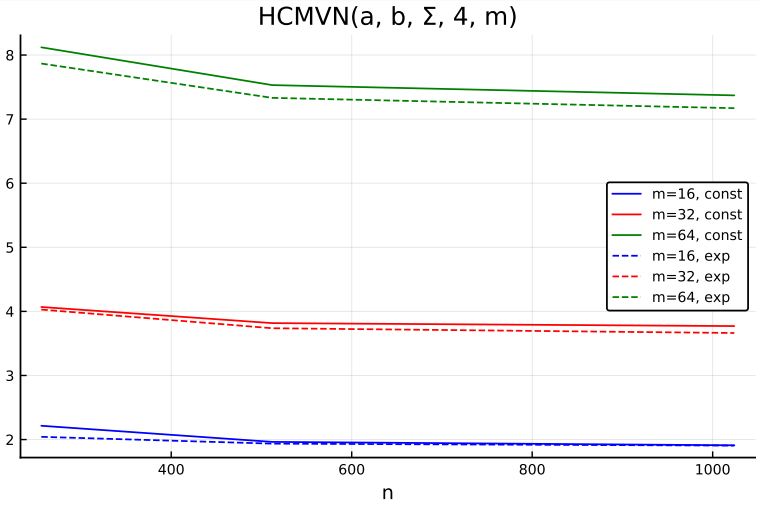
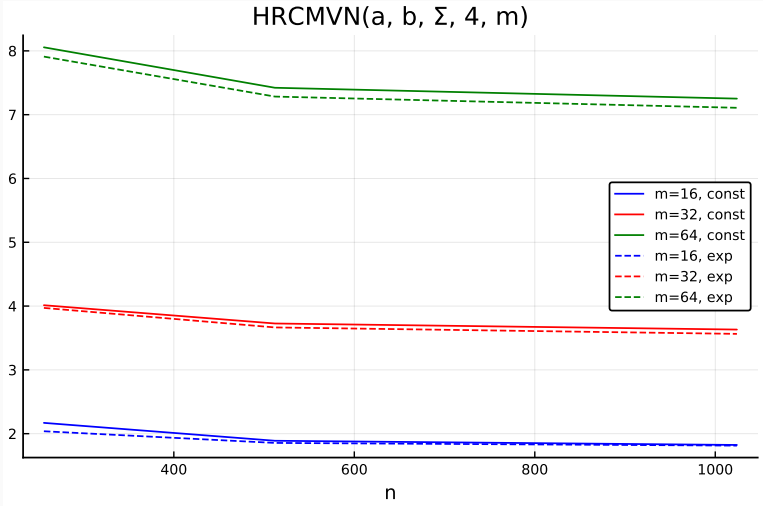


Figure 3: Execution time (seconds) for the hierarchical-block approximation

Hierarchical-Block Approximations- Execution Time ii



(a) `HCMVN`



(b) `HRCMVN`

Figure 4: Execution time (seconds) for the hierarchical-block conditioning approximation

Conclusion

Conclusion

- d-dimensional conditioning and block reordering scheme improved accuracy under the exponential covariance structure, with negligible amount of computing time and cost.
- The hierarchical decomposition method is effective approach for the case of smooth covariance function, such as exponential covariance structure.
- Numerical results were not perfectly homogenous with these of Cao et al. (2019) mainly due to distinct computing environment.

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