Advanced Statistical Computing Proejct

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

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1 Introduction

The computation of multivariate normal probability appears various fields. For instance, the inferences based on the central limit theorem, which holds when the sample size is large enough, is widely used in the social sciences and engineering as well as in the natural sciences. Recently, the dimensionality of data and models has been grown significantly, and in this respect, so does a need for the methodology to efficiently calculate high-dimensional multivariate normal probability.

Cao, Genton, Keyes, and Turkiyyah (2019) proposes new approaches to approximate high-dimensional multivariate normal probability

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

using the hierarchical matrix $\mathcal{H}$ (Hackbusch, 2015) for the covariance matrix Σ. The methods are based on two state-of-arts methods, among others, are the bivariate conditioning method (Trinh & Genz, 2015) and the hierarchical Quasi-Monte Carlo method (Genton, Keyes, & Turkiyyah, 2018). Specifically, Cao et al. (2019) generalize the bivariate conditioning method to a d-dimension and combine it with the hierarchical representation of the covariance matrix.

2 Multidimensional Conditioning Approximations

The following methods are generalization of the bivariate conditioning method (Trinh & Genz, 2015).

2.1 d-Dimensional Conditioning Approximation

2.2 CMVN

2.3 RCMVN

3 Hierarchical-Block Approximations

3.1 The Hierarchical-Block Conditioning Method

In this section, we suggest methods to solve the n-dimensional MVN problem with the hierarchical covariance matrix 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.

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 Σ. Then, we can express (1) as

$$\Phi_n(\mathbf{a}, \mathbf{b}; \mathbf{0}, \mathbf{\Sigma}) = \int_{\mathbf{a}'_1}^{\mathbf{b}'_1} \phi_m(\mathbf{x}_1; \mathbf{B}_1\mathbf{B}_1^T) \cdots \int_{\mathbf{a}'_r}^{\mathbf{b}'_r} \phi_r(\mathbf{x}_r; \mathbf{B}_r\mathbf{B}_r^T) d\mathbf{x}_r \cdots d\mathbf{x}_1. \tag{2}$$

Where $\mathbf{a}'$, $\mathbf{b}'$, $i = 1, \cdots, r$, are the corresponding segments of the updated $\mathbf{a}$ and $\mathbf{b}$. Specifficaly, we can compute n-dimensional MVN problem using hierarchical structure as algorithm 1.

Algorithm 1 Hierarchical-block conditioning algorithm

procedure `HMVN`$(a,\ b,\ \Sigma,\ d)$
  $\mathbf{x} \leftarrow \mathbf{0}$ and $P \leftarrow 1$
  $[\mathbf{B}, \mathbf{UV}] \leftarrow$ `choldecomp_hmatrix`(Σ)
  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
    $\mathbf{a}_i \leftarrow \mathbf{a}[j + 1 : j + m]$
    $\mathbf{b}_i \leftarrow \mathbf{b}[j + 1 : j + m]$
    $P = P * \Phi_m(\mathbf{a}_i, \mathbf{b}_i; \mathbf{0}, \mathbf{B}_i\mathbf{B}_i^T)$
    $\mathbf{x}[j + 1 : j + m] \leftarrow \mathbf{B}_i^{-1}\mathbb{E}[\mathbf{X}_i]$
  end for
end procedure

Note the probabilities $\Phi_m(\mathbf{a}_i, \mathbf{b}_i; \mathbf{0}, \mathbf{B}_i\mathbf{B}_i^T)$ can be computed using Quasi-Monte Carlo method (`HMVN`, Method 1 in Cao et al. (2019)), d-dimensional conditioning algorithm (`HCMVN`, Method 2 in Cao et al. (2019)) or with d-dimensional conditioning algorithm with univariate reordering (`HRCMVN`, Method 3 in Cao et al. (2019)). These methods are more effective and easily parallelizable than the classical methods.

3.2 Computational Complexity

For a clearer comparison of the complexities, we decompose the complexity of Algorithm 1 into three parts and list the complexity for each part in Table 1, where $M(\cdot)$ denotes the complexity of the QMC simulation in the given dimension. Table 1 shows that the time efficiency of the d-dimensional conditioning algorithm mainly comes from lowering the dimension in which the QMC simulation is performed.

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. The complexity of the univariate reordering is $O(m^2n)$, the same as the complexity of computing the MVN probabilities in `HCMVN`, resulting in an identical major complexity component for `HCMVN`

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

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

and `HRCMVN`. Since`HCMVN` and `HRCMVN` perform the QMC simulation in d-dimensions, these two methods are not greatly affected by the choice of m.

4 Block Reordering

5 Results

5.1 Data

5.2 Multivariate Normal Probabilities

To implement `*MVN` functions, we need to calculate n-dimensional normal probability (1),

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

numerically. We implement `mvn`, the function that calculate multivariate normal probabilities using Richtmyer Quasi-Monte Carlo(QMC) method proposed by Genz and Bretz (2009).

It is well-known that QMC methods is more effective than classical Monte Carlo(MC) method. All the multivariate normal distribution probabilities required in the next algorithms are calculated using the `mvn` function.

5.3 CMVN

5.4 HMVN

In this section, we implement three methods in the section 3 and compare theirs performance

- `HMVN()`: Calculate multivariate normal probabilities using hierarchical-block approximation
- `HCMVN()`: Calculate multivariate normal probabilities using hierarchical-block conditioning approximation

- `HRCMVN()`: Calculate multivariate normal probabilities using hierarchical-block conditioning approximation with univarite reordering

5.5 Block Reordering

6 Conclusion

References

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