A Fast Algorithm for Computing Multivariate Normal Densities using Matérn-like Precision Matrices with Unit Marginal Variances

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Introduction

Let $\mathbf{X} = (X_1, X_2, \dots, X_n)$ be a multivariate random vector with marginal distribution functions F_i for $i = 1, 2, \dots, n$. The joint distribution function of $\mathbf{X}$ can be written as:

$$F_{\mathbf{X}}(\mathbf{x}) = C(F_1(x_1), F_2(x_2), \dots, F_n(x_n)),$$

where C is the Gaussian copula defined by the GMRF precision matrix Q.

The Gaussian copula C is given by:

$$C(u_1, u_2, \dots, u_n) = \Phi_Q(\Phi^{-1}(u_1), \Phi^{-1}(u_2), \dots, \Phi^{-1}(u_n)),$$

where Φ_Q is the joint cumulative distribution function of a multivariate normal distribution with mean vector $\mathbf{0}$ and precision matrix Q, and Φ^{-1} is the inverse of the standard normal cumulative distribution function.

It is imperative that the precision matrix Q governing the GMRF Copula, C, has marginal variance equal to 1 so that is it on the same scale as the transformed data, $\Phi^{-1}(u_i)$. This can be troublesome because GMRFs are defined in terms of their precision matrices, Q, which more often than not have marginal variances that are different from 1.

This paper presents an fast and efficient algorithm for creating a Matérn-like precision matrix, Q, with unit marginal variance, and computing the multivariate Gaussian copula density of $Z = \Phi^{-1}(u)$ where $u \sim \text{Uniform}(0, 1)$.

The matrix, Q, is defined as

$$Q = Q_1 \otimes I + I \otimes Q_1,$$

where Q_1 is the precision matrix of a standardized one-dimensional AR(1) process and $\otimes$ is the kronecker product.

The method leverages the special structure of Q_1 and the use of a kronecker sum in the definitionto avoid explicit formation and inversion of the larger matrix, Q, making it particularly suitable for high-dimensional spatial data.

Methods

Theory

One-Dimensional AR(1) Matrix

The core of our approach is based on the eigendecomposition of an AR(1) precision matrix, which forms the building block of our Matérn-like precision structure. For a one-dimensional AR(1) process with parameter ρ, the precision matrix Q_1 has a tridiagonal structure:

$$Q = \frac{1}{1-\rho^2}\begin{bmatrix} 1 & -\rho & 0 & \cdots & 0 & 0 \\ -\rho & 1+\rho^2 & -\rho & \cdots & 0 & 0 \\ 0 & -\rho & 1+\rho^2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1+\rho^2 & -\rho \\ 0 & 0 & 0 & \cdots & -\rho & 1 \end{bmatrix}$$

Matérn-like Precision Matrix

For two-dimensional spatial fields, we construct a Matérn-like precision matrix Q using Kronecker products:

$$Q = Q_1 \otimes I + I \otimes Q_1$$

where I is the identity matrix and $\otimes$ denotes the Kronecker product The eigenvalues (λ_k) and eigenvectors (v_k) of Q_1 can be calculated numerically and used to evaluate the multivariate Gaussian density, letting us skip out on forming Q entirely. This is due to the following theorem:

Eigendecomposition of Kronecker Sums

Theorem

Let $A \in \mathbb{R}^{n\times n}$ have eigenvalues λ_i, $i \in \{1, \dots, n\}$, and let $B \in \mathbb{R}^{m\times m}$ have eigenvalues μ_j, $j \in \{1, \dots, m\}$. Then the Kronecker sum $A \oplus B = (I_m \otimes A) + (B \otimes I_n)$ has eigenvalues $\lambda_i + \mu_j$, $i \in \{1, \dots, n\}, j \in \{1, \dots, m\}$.

Moreover, if $x_1, \dots, x_p$ are linearly independent right eigenvectors of A corresponding to $\lambda_1, \dots, \lambda_p$ ($p \leq n$), and $z_1, \dots, z_q$ are linearly independent right eigenvectors of B corresponding to $\mu_1, \dots, \mu_q$ ($q \leq m$), then $z_j \otimes x_i \in \mathbb{R}^{mn}$ are linearly independent right eigenvectors of

$A \oplus B$ corresponding to $\lambda_i + \mu_j$, $i \in \{1, \dots, p\}, j \in \{1, \dots, q\}$.

Discussion

This theorem provides a crucial insight that allows us to efficiently construct the eigendecomposition of the full precision matrix Q for two-dimensional spatial fields by leveraging the eigendecomposition of the one-dimensional precision matrix Q_1, avoiding the computationally intensive process of explicitly forming and inverting the large matrix Q.

Furthermore, we can compute the log-density of an observation x directly by using just the eigenvalues and eigenvectors og Q_1, thereby enabling efficient computation of the log-density of the multivariate normal distribution even for large spatial fields.

Example: Calculating Eigenvalues and Eigenvectors for Q Using Q_1

To illustrate the application of Theorem 13.16, consider the one-dimensional precision matrix Q_1 with known eigendecomposition. Suppose Q_1 has eigenvalues λ_i and corresponding eigenvectors v_i. For a two-dimensional spatial field, we construct the Matérn-like precision matrix Q using Kronecker products as follows:

$$Q = Q_1 \otimes I + I \otimes Q_1,$$

where I is the identity matrix and $\otimes$ denotes the Kronecker product.

Eigenvalues

The eigenvalues of Q can be determined from the eigenvalues of Q_1. If Q_1 has eigenvalues λ_i for $i = 1, 2, \dots, n$, then the eigenvalues of Q are given by:

$$\lambda_{ij} = \lambda_i + \lambda_j \quad \text{for} \quad i, j = 1, 2, \dots, n.$$

Eigenvectors

Similarly, the eigenvectors of Q can be constructed from the eigenvectors of Q_1. If v_i and v_j are eigenvectors of Q_1 corresponding to eigenvalues λ_i and λ_j respectively, then the eigenvectors of Q are given by:

$$v_{ij} = v_i \otimes v_j \quad \text{for} \quad i, j = 1, 2, ..., n.$$

Here, v_{ij} is the Kronecker product of v_i and v_j.

These relationships allow us to efficiently compute the eigendecomposition of the full precision matrix Q using the eigendecomposition of the smaller matrix Q_1, significantly reducing the computational complexity.

Efficient Density Calculation Using Eigendecomposition

Given the eigendecomposition of Q1, we can efficiently compute the multivariate normal density with respect to the precision matrix Q. Let λ_i and v_i be the eigenvalues and eigenvectors of Q1, respectively. The log-density of a multivariate normal distribution with precision matrix Q is given by:

$$\log p(x) = -\frac{1}{2}(n \log(2\pi) + \log |Q| + x^T Q x)$$

where n is the dimension of x, $|Q|$ is the determinant of Q, and $x^T Q x$ is the quadratic form.

Log-Determinant Calculation

The log-determinant of Q can be computed efficiently using the eigenvalues of Q1:

$$\log |Q| = \sum_{i=1}^{d} \sum_{j=1}^{d} \log(\lambda_i + \lambda_j)$$

where d is the dimension of Q1.

Quadratic Form Calculation

First, we define the product of the eigenvector and the data vector x as:

$$y_{ij} = (v_i \otimes v_j)^T x,$$

where v_i and v_j are the eigenvectors of Q_1 and $\otimes$ denotes the Kronecker product.

Next, we define the eigenvalue sum as:

$$\mu_{ij} = \lambda_i + \lambda_j,$$

where λ_i and λ_j are the eigenvalues of Q_1. Using these definitions, the quadratic form can be expressed as:

$$x^T Q x = \sum_{i=1}^{d} \sum_{j=1}^{d} \mu_{ij} y_{ij}^2.$$

In this way, we calculate the quadratic form without having to form the matrix Q or its full set of eigenvectors or values.

Scaling the Input x

The input vector $x = \Phi^{-1}(u)$ has zero mean and unit marginal variance. Instead of scaling the precision matrix to have $(Q^{-1})_{ii} = 1$, we calculate the marginal standard deviations, σ_k, implied by Q using the eigenstructure of Q_1, then scale the input vector x using those

standard deviations. First we compute the marginal standard deviations:

$$\sigma_k = \sqrt{\sum_{i=1}^{d}\sum_{j=1}^{d} \frac{(v_i \otimes v_j)_k^2}{\lambda_i + \lambda_j}}$$

where $(v_i \otimes v_j)_k$ is the k-th element of the Kronecker product $v_i \otimes v_j$.

Algorithm Implementation

The density calculation is implemented as follows:

- Compute the eigendecomposition of Q_1.
- Calculate the marginal standard deviations σ_k.
- For each observation x:
    a. Standardize x by element-wise multiplication with σ_k.
    b. Compute the log-determinant and quadratic form using the formulas above.
    c. Combine the terms to get the log-density.

This approach avoids explicit formation and inversion of the full precision matrix Q, allowing for efficient computation even for large spatial fields. This method has been implemented in C++ code that can perform a full set of computations for a 200×200 spatial grid (i.e. Q would be 40.000×40.000) in just over one second.