Efficiency Assessment of Approximated Spatial Predictions for Large Datasets

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Abstract: Due to the well-known computational showstopper of the exact Maximum Likelihood Estimation (MLE) for large geospatial observations, a variety of approximation methods have been proposed in the literature, which usually require tuning certain inputs. For example, the Tile Low-Rank approximation (TLR) method, a recently developed efficient technique using parallel hardware architectures, involves many tuning inputs including the numerical accuracy, which needs to be selected according to the features of the true process. To properly choose the tuning inputs, it is crucial to adopt a meaningful criterion for the assessment of the prediction efficiency with different inputs. Unfortunately, the most commonly-used mean square prediction error (MSPE) criterion cannot directly assess the loss of efficiency when the spatial covariance model is approximated. In this paper, we present two other criteria, the Mean Loss of Efficiency (MLOE) and Mean Misspecification of the Mean Square Error (MMOM), and show numerically that, in comparison with the common MSPE criterion, the MLOE and MMOM criteria are more informative, and thus more adequate to assess the loss of the prediction efficiency by using the approximated or misspecified covariance models. Thus, our suggested criteria are more useful for the determination of tuning inputs for sophisticated approximation methods of spatial model fitting. To illustrate this, we investigate the trade-off between the execution time, estimation accuracy, and prediction efficiency for the TLR method with extensive simulation studies and suggest proper settings of the TLR tuning inputs. We then apply the TLR method to a large spatial dataset of soil moisture in the area of the Mississippi River basin, showing that with our suggested tuning inputs, the TLR method is more efficient in prediction than the popular Gaussian predictive process method.

Key words: Covariance approximation; Gaussian predictive process; Loss of efficiency; Maximum likelihood estimation; Spatial prediction; Tile Low-Rank approximation.

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1 Introduction

Geostatistical applications include modeling the spatial distribution of a set of observations (e.g., temperature, humidity, soil moisture, wind speed) taken at \( n \) locations regularly or irregularly spaced over a given geographical area. In geostatistics, the spatial datasets are often considered as a realization of a Gaussian process, defined by a mean function and a spatial covariance model. More specifically, we suppose that the data are observed from a stationary, isotropic Gaussian random field \( \{ Z(s) : s \in D \subset \mathbb{R}^d \} \), with mean zero and covariance function \( C(h; \theta) := \text{Cov}_\theta\{Z(s_1), Z(s_2)\} \) for any \( s_1, s_2 \in D \) and \( \|s_1 - s_2\| = h \), where \( \theta \) is the unknown parameter vector. In recent years, the Matérn family has been a popular choice for the covariance function, since it represents a general form of many possible covariance models in the literature, due to its flexibility. The Matérn covariance function is defined as

\[
C(h; \theta) = \sigma^2 \frac{2^{\nu-1}}{\Gamma(\nu)} \nu \frac{h}{\alpha} \mathcal{K}_\nu \left( \frac{h}{\alpha} \right),
\]

(1)

where \( \theta = (\sigma^2, \alpha, \nu)^\top \), \( \sigma^2 > 0, \alpha > 0 \), and \( \nu > 0 \) are the variance, range parameter, and smoothness parameter, respectively, and \( \mathcal{K}_\nu \) is the modified Bessel function of the second kind of order \( \nu \).

The Maximum Likelihood Estimation (MLE) method has been widely used for estimating the parameter vector \( \theta \) of the spatial model. Denoting the spatial dataset by \( Z = \{ Z(s_1), \ldots, Z(s_n) \}^\top \), where \( s_1, \ldots, s_n \) are the observation locations, the MLE of the unknown parameter \( \theta \) can then be obtained by maximizing the following log-likelihood function:

\[
l(\theta) = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log \det\{\Sigma(\theta)\} - \frac{1}{2} Z^\top \Sigma(\theta)^{-1} Z,
\]

(2)

where \( \Sigma(\theta) \) is the covariance matrix, with entries \( [\Sigma(\theta)]_{i,j} = C(\|s_i - s_j\|; \theta) \) for \( i, j = 1, \ldots, n \). Finding the exact MLE requires \( O(n^3) \) computations and \( O(n^2) \) memory, since evaluating the log-likelihood function involves the inverse and the determinant of the covariance ma-
trix. Thus, the exact MLE is not feasible for large spatial datasets in applications, e.g. meteorological data, where $n$ is often of an order of $10^5$ or $10^6$.

To overcome this computational problem, finding approximation methods to compute the MLE has drawn considerable attention. For instance, Kaufman et al. (2008) proposed the covariance tapering method, where the covariance matrix is multiplied element-wise by a sparse covariance matrix. Vecchia (1988) and Curriero and Lele (1999) introduced the composite likelihood approach, approximating the log-likelihood function by ignoring the correlation of the observations at distant locations. Banerjee et al. (2008) proposed the Gaussian predictive process, where the spatial model is approximated by a low-rank model plus a nugget effect. Many of these approximation methods have been reviewed in Sun et al. (2012). The recently proposed Tile Low-Rank (TLR) approximation method (Abdulah et al., 2018b) is a more general method that divides the covariance matrix into several tiles and performs low-rank approximations on the off-diagonal tiles. It improves the performance of the computation of the likelihood function on parallel architectures such as shared-memory, GPU, and distributed-memory systems.

All the above approximation methods require certain types of tuning, to some extent. We call them ‘tuning inputs’ to distinguish them from model parameters that need to be estimated from the data. For instance, for the covariance tapering method (Kaufman et al. 2008), the taper range is a tuning input. The composite likelihood method (Vecchia 1988) approximates the conditional density $p(s_i|s_1, \ldots, s_{i-1})$ conditioning on a subset of $s_1, \ldots, s_{i-1}$, such as $m$ nearest neighbors of $s_i$, for which $m$ is a tuning input. In the Gaussian predictive process model (Banerjee et al. 2008), the predetermined knots are tuning inputs. The TLR approximation (Abdulah et al. 2018b) involves several tuning inputs introduced in Table 1. The tuning inputs should balance the computational burden and the estimation or prediction accuracy, so it is crucial to understand the impact of the tuning inputs on the statistical properties of the approximation methods. The estimation perfor-
mance is often evaluated via summary statistics and the plot of the estimations, such as the estimation variance (Kaufman et al., 2008) or the box-plots (Abdulah et al., 2018b), but the prediction performance is not so straightforward to assess.

In the literature, the prediction performance is often evaluated by cross-validation. This method randomly leaves out $p$ locations $s_1, \ldots, s_p$ from observation locations, and predicts the $Z(s_1), \ldots, Z(s_p)$ using the rest of the data at all other locations. Denote these predictions by $\hat{Z}(s_1), \ldots, \hat{Z}(s_p)$. The prediction performance is assessed by the deviation between the true and the predicted values, such as the Mean Square Prediction Error or Mean Square Kriging Error (Abdulah et al., 2018b)

$$\text{MSPE} = \frac{1}{p} \sum_{i=1}^{p} \{ \hat{Z}(s_i) - Z(s_i) \}^2,$$

or the Mean Square Relative Prediction Error (Yan and Genton, 2018)

$$\text{MSRPE} = \frac{1}{p} \sum_{i=1}^{p} \left( \frac{\hat{Z}(s_i) - Z(s_i)}{Z(s_i)} \right)^2,$$

or the empirical coverage of 95% prediction intervals on the left-out locations (Banerjee et al., 2008). For more cross-validation based criteria, see Dai et al. (2007) and Hengl et al. (2004). These criteria provide a straightforward measure of the performance of the prediction. However, they do not directly assess the loss of statistical efficiency when the approximated model is adopted instead of the true model.

In the context of covariance model misspecification, Stein (1999) proposed the Loss of Efficiency (LOE) and the Misspecification of the MSE (MOM) criteria, based on the comparison of the Mean Square Errors (MSEs) between the true and the misspecified models. Using these criteria, Stein (1999) deduced that the simple kriging prediction is asymptotically optimal when the misspecified covariance model is equivalent to the true model. Stein (1999) also performed some simulations to assess the prediction performance of the kriging prediction under different settings of observation locations. However, all the results presented in Stein (1999) are for the case of a single prediction location.

In this article, we aim to give more appropriate criteria for the assessment of the loss
of prediction efficiency when the true covariance model is approximated. For instance, our suggested criteria can be used to assess the prediction efficiency of the TLR approximation method with different tuning inputs. We suggest to use the Mean Loss of Efficiency (MLOE) and the Mean Misspecification of the Mean Square Error (MMOM) criteria for multiple prediction locations as a generalization of the criteria proposed by [Stein (1999)](http://example.com). Since the approximated covariance model can be viewed as a type of model misspecification, to show the MLOE and MMOM criteria are appropriate to assess the loss of prediction efficiency, we perform a similar simulation study from [Stein (1999)](http://example.com), where the exponential covariance model is misspecified as a Whittle covariance model plus a nugget effect, implying that the approximated covariance is smoother than the truth. Numerical results show that the MLOE and MMOM are better in assessing the prediction efficiency than the commonly used MSPE criterion. As an application of our suggested criteria, we use them to give a practical suggestion for selecting the tuning inputs in the TLR method, for which we investigate the performance of prediction and computation, using different tuning inputs from extensive simulation studies. For illustration of the validity of our suggested TLR tuning inputs, we fit a Gaussian-process model with a Matérn covariance function to a large spatial dataset of soil moisture in the area of the Mississippi basin; we then apply the TLR approximation method to obtain the MLEs and perform predictions with the suggested tuning inputs. Our results show that the TLR has a better prediction efficiency compared with most the popular low-rank based method, the Gaussian predictive process ([Banerjee et al., 2008](http://example.com)).

The remainder of this article is organized as follows: Section 2 gives a brief background on the TLR approximation method and its tuning inputs. Section 3 introduces the MLOE and MMOM criteria. In Section 4, we perform a simulation of the validity and sensitivity of the suggested criteria. In Section 5, we explain the simulation design to assess the TLR method, using different tuning inputs settings for which, the MLOE and MMOM criteria are used to measure the prediction accuracy and select the best specification of those tuning
inputs. Section 6 shows the effectiveness of the TLR method with suggested tuning inputs, compared with the exact MLE and the Gaussian predictive process method, using the real soil moisture dataset. Conclusions and discussions are provided in Section 7. More detailed numerical results about the specification of tuning inputs for the TLR method can be found in the Supplementary Material.

2 Tile Low-Rank (TLR) Approximation

In this section, we give a brief background on the TLR approximation method, together with the tuning inputs associated with it in parallel hardware environments.

Tile-based algorithms have been developed on parallel architectures to speedup matrix-linear solver algorithms, for instance, PLASMA \cite{Agullo:2009} and Chameleon \cite{Chameleon} libraries. The given matrix is split into a set of tiles to allow the use of parallel execution, to a maximum degree, by weakening the synchronization points and bringing the parallelism in multithreaded BLAS (Basic Linear Algebra Subprograms) to maximize the hardware utilization.

Since maximizing the log-likelihood in (2) and obtaining the MLE involves applying a set of linear-solver operations to the geospatial covariance matrix $\Sigma$, Abdulah et al. \cite{ExaGeoStat} have developed ExaGeoStat \cite{ExaGeoStat} a framework that uses tile-based linear algebra algorithms to parallelize the MLE operations on existing parallel hardware architecture, on a large scale. This framework has also been extended in Abdulah et al. \cite{ExaGeoStat-2} to apply a TLR approximation to the covariance matrix. The new approximation technique aims at exploiting the data sparsity of the dense covariance matrix by compressing the off-diagonal tiles up to a user-defined accuracy threshold. The TLR method differs from existing low-rank approximation techniques, e.g., Banerjee et al. \cite{Banerjee:2008}, as the low-rank approximation is applied.

\footnote{\url{https://project.inria.fr/chameleon}}
\footnote{\url{https://github.com/ecrc/exageostat}}
separately on each tile, instead of the whole matrix.

![Diagram of TLR structure](image)

Figure 1: An illustrative example of a $8 \times 8$ covariance matrix TLR structure.

Figure 1 gives an illustrative example of the TLR approximation method to a $8 \times 8$ covariance matrix, e.g., $\Sigma(\theta)$, where $\theta$ represents the parameter vector (i.e., variance, range, and smoothness parameters in the Matérn covariance function). Assuming a square positive-definite covariance matrix, the spatial covariance matrix with size $n \times n$ is divided into several tiles $D_{i,j}(\theta)$, where the size of each tile is $nb \times nb$. The Singular Value Decomposition (SVD) is used to approximate the off-diagonal tiles to a user-defined accuracy (i.e., $tlr_{acc}$, the tuning input argument used in ExaGeoStat as indicated in Table 1). In this case, the approximated tiles are the multiplication of two low-rank matrices, e.g., $D_{i,j}(\theta)$ is approximated by $\tilde{D}_{i,j}(\theta) = U_{i,j}(\theta)V_{i,j}(\theta)$, which can be deduced from the most $k$ significant singular values and their associated left and right singular vectors.

This approximation gives a data compression format that requires less memory and offers a faster computational speed of the matrix algebra. In the ExaGeoStat software (Abdulah et al., 2018b), the TLR approximation is performed by the Hierarchical Computations on Manycore Architectures (HiCMA) numerical library (Akbudak et al., 2017), which allows to run the approximation on parallel systems with the help of StarPU (Augonnet et al., 2011).

Applying the TLR approximation to the log-likelihood function requires tuning several inputs to control the performance and accuracy of the approximation, namely, $nb$.
Table 1: Arguments for the tuning inputs of the TLR method in the ExaGeoStat framework

| Name                     | Symbol        |
|--------------------------|---------------|
| Matrix tile size         | nb            |
| TLR maximum rank         | tlr_max_rank  |
| TLR numerical accuracy   | tlr_acc       |
| Optimization tolerance   | opt_tol       |

$tlr\_{\text{max\_rank}}, tlr\_{\text{acc}}, \text{and opt\_tol}$ as shown in Table 1. $nb$ controls the size of each tile $D_{i,j}(\theta)$, and $tlr\_{\text{max\_rank}}$ determines the maximum possible rank of the approximated tiles, which affects the memory allocation process of the approximating low-rank matrices $U_{i,j}(\theta)$ and $V_{i,j}(\theta)$ in the HiCMA library. By adopting the suggested criteria when assessing the prediction efficiency, we herein determine the best combination of the four TLR inputs by tuning these inputs, and by evaluating the performance and the accuracy of the approximated MLE compared with the exact MLE solution.

The effectiveness of the TLR approximation method can be improved by well tuning these four inputs. For instance, the current implementation of TLR in HiCMA uses a fixed-rank method to allocate and process all the given matrix tiles, although different approximated tiles have different ranks. A value of $tlr\_{\text{max\_rank}}$ that is too large causes unnecessary memory usage and more data movements in the case of distributed memory architectures, whereas a too small value may cause a failure in approximating the tile. Thus, the best value of $tlr\_{\text{max\_rank}}$ should be the smallest possible value that makes the approximation feasible for all the off-diagonal tiles. The accuracy threshold $tlr\_{\text{acc}}$ is also important to control the approximation accuracy, such that the approximation $\tilde{D}_{i,j}(\theta)$ of each tile satisfies $\|\tilde{D}_{i,j}(\theta) - D_{i,j}(\theta)\|_2 \leq tlr\_{\text{acc}}$, where $\|\cdot\|_2$ is the $L_2$-norm of a matrix. A lower accuracy (larger $tlr\_{\text{acc}}$) brings the arithmetic intensity of the approximation close to the memory-bound regime, whereas a higher accuracy makes the approximation run in the compute-bound regime (Abdulah et al., 2018b). Thus, the accuracy threshold is an application-specific value. Furthermore, the optimization tolerance $opt\_tol$ is the minimum difference between two log-
likelihood values at different iterations to control the optimization convergence condition. More specifically, the iteration process of computing the maximum point stops when \( |l(\theta_{opt}) - l(\theta_{sub})| \leq opt\_tol \), where \( l(\theta_{opt}) \) is the largest value of the log-likelihood function over all iterations and \( l(\theta_{sub}) \) is the second largest one.

We hope the tuning inputs in the TLR can save as much computational time as possible, without losing too much in estimating the accuracy of the prediction. Abdulah et al. (2018b) investigated the impact of tlr\_acc by showing the box-plots of the estimated parameters and the MSPEs. Here, our work uses the more informative MLOE and MMOM criteria for assessing the spatial prediction efficiency, which we describe in more details in Section 3.

In this study, we use the ExaGeoStatR package\(^6\) to perform the experiments relating to the TLR approximation. ExaGeoStatR is the R-wrapper interface of ExaGeoStat developed to facilitate the exploitation of large-scale capabilities in the R environment. The package provides parallel computation for the evaluation of the Gaussian maximum likelihood function using shared memory, GPUs, and distributed systems, by mitigating its memory space and computing restrictions. This package provides three ways of computing MLE on a large scale: exact, Diagonal Super Tile (DST) approximation (i.e., covariance tapering), and TLR approximation. We are targeting the R functions related to the TLR approximation. The function tlr\_mle() in the ExaGeoStatR package allows the computation of the TLR approximation of the MLE for the Matérn covariance model. This function computes the estimation by substituting the covariance matrix with its TLR approximation in the exact MLE framework.

\(^6\)https://github.com/ecrc/exageostatR
3 Efficiency Criteria for Approximated Spatial Predictions

In this section, we construct two criteria for assessing the accuracy of the spatial prediction, when the covariance matrix in the log-likelihood in (2) is approximated. Our criteria are of the averaged form of the criteria called the Loss of Efficiency (LOE) and the Misspecification of the MSE (MOM), proposed by Stein (1999), in the context of spatial prediction with a misspecified covariance model.

We consider a zero-mean Gaussian random field \( Z(\mathbf{s}) \), where the observations are \( Z = \{ Z(s_1), \ldots, Z(s_n) \}^\top \). When the covariance model is true, the kriging prediction of \( Z(s_0) \) at a point \( s_0 \) is \( \hat{Z}_t(s_0) = \mathbf{k}_t^\top K_t^{-1} \mathbf{Z} \), with MSE given by \( \text{MSE}(s_0) = \mathbb{E}_t \{ e_t^2(s_0) \} = k_{0t} - \mathbf{k}_t^\top K_t^{-1} \mathbf{k}_t \), where \( e_t(s_0) = \hat{Z}_t(s_0) - Z(s_0) \) is the error of the kriging predictor, \( k_{0t} = \text{Var}_t \{ Z(s_0) \} \), \( \mathbb{E}_t \) and \( \text{Var}_t \) mean the expectation and variance with respect to the true covariance model.

However, when the covariance is approximated, the kriging predictor is \( \hat{Z}_a(s_0) = \mathbf{k}_a^\top K_a^{-1} \mathbf{Z} \) instead, where \( K_a = \text{Cov}_a \{ Z, Z^\top \}, \mathbf{k}_a = \text{Cov}_a \{ Z, Z(s_0) \} \), and \( \text{Cov}_a \) means the covariance is computed under the approximated covariance model. Denoting the error of this predictor by \( e_a(s_0) = \hat{Z}_a(s_0) - Z(s_0) \), then the MSE of this prediction is actually \( \mathbb{E}_a \{ e_a^2(s_0) \} = k_{0a} - 2\mathbf{k}_a^\top K_a^{-1} \mathbf{k}_a + \mathbf{k}_a^\top K_a^{-1} K_a K_a^{-1} \mathbf{k}_a \), and the calculated result of MSE is \( \text{E}_a \{ e_a^2(s_0) \} = k_{0a} - \mathbf{k}_a^\top K_a^{-1} \mathbf{k}_a, \) where \( k_{0a} = \text{Var}_a \{ Z(s_0) \} \), \( \mathbb{E}_a \) and \( \text{Var}_a \) mean that the expectation and variance are computed using the approximated covariance model. Thus, following Stein (1999), the Loss of Efficiency of the prediction is defined as

\[
\text{LOE}(s_0) = \frac{\mathbb{E}_t \{ e_a^2(s_0) \}}{\mathbb{E}_t \{ e_t^2(s_0) \}} - 1, \tag{4}
\]

and the Misspecification of the MSE is defined as

\[
\text{MOM}(s_0) = \frac{\mathbb{E}_a \{ e_a^2(s_0) \}}{\mathbb{E}_t \{ e_a^2(s_0) \}} - 1. \tag{5}
\]

Our criteria are defined as the mean value of the Loss of Efficiency (4) and Misspecification of the MSE (5) over multiple prediction locations. More specifically, when the prediction
locations are $s_{01}, \ldots, s_{0m}$, the Mean Loss of Efficiency is defined as

$$\text{MLOE} = \frac{1}{m} \sum_{i=1}^{m} \text{LOE}(s_{0i}),$$

and the Mean Misspecification of the MSE is defined as

$$\text{MMOM} = \frac{1}{m} \sum_{i=1}^{m} \text{MOM}(s_{0i}).$$

We choose the prediction locations of a regular grid in the observation region, so the value of MLOE and MMOM can describe the average prediction performance over the whole observation region. For instance, when the observation region is $[0, 1]^2$, the prediction locations can be $(i/5, j/5)$ for $i, j = 1, 2, 3, 4$. The MLOE describes the average efficiency loss of the prediction when the approximated covariance model is used instead of the true one, whereas the MMOM describes the average misspecification between the computed and true MSEs.

4 Simulation on the Validity of the Suggested Criteria

We perform a numerical simulation to illustrate the validity and sensitivity of the suggested criteria, compared with the popular Mean Square Prediction Error (MSPE) criterion. Similar to the settings in Stein (1999), we focus on the case where the covariance model is misspecified.

In this simulation, we consider a zero-mean stationary Gaussian random field $\{Z(s), s \in [0, 1]^2\}$ with Matérn covariance function $[1]$. We set the true covariance model as the exponential model, with covariance function $C(h; \theta = (\sigma^2, \alpha, 0.5)^\top)$, and consider two cases of model misspecification. In the first case, the covariance model is correctly specified, but the parameters $\sigma^2$ and $\alpha$ are misspecified as their maximum likelihood estimate. Under this kind of misspecification, the corresponding kriging prediction is called ‘empirical best linear unbiased prediction’ (EBLUP); the EBLUP does not significantly affect the prediction efficiency, according to the intuition and simulation results in the literature (Stein, 1999). In the second case, the covariance model is misspecified as a smoother (Whittle)
covariance model plus a nugget effect term. In this case, the misspecified covariance function is 
\[ C(h; \theta = (\sigma^2, \alpha, 1.0)^\top) + \tau^2 I_{h=0}(h), \]
where \( \tau^2 \) is the nugget variance and \( I_{h=0} \) is the indicator function. In the \( \text{R} \) package \texttt{fields}, the function for fitting covariance model \texttt{MLESpatialProcess()} chooses the smoothness parameter \( \nu = 1 \) as the default value, which is smoother than usual settings \( \nu = 0.5 \). This motivates us to investigate the loss of prediction efficiency for this case.

The observation locations are set to be 
\[ s_{r,l} = n^{-1/2}(r - 0.5 + U_{r,l}, l - 0.5 + V_{r,l}), \]
where \( n \) is the number of observations, \( U_{r,l} \) and \( V_{r,l} \) are i.i.d. samples from the uniform distribution \( U[-0.4, 0.4] \). By ordering \( r, l \) lexicographically, these locations are also denoted by \( s_1, \ldots, s_n \).

We take \( n = 12^2, 24^2, \) or \( 48^2 \). The true covariance function is set as 
\[ C(h; \theta = (\sigma^2, \alpha, 0.5)^\top), \]
where \( \sigma^2 = 1, \alpha = 0.2/(-\log(0.05)) \), such that the true effective range of the model is 0.2. For each parameter setting, we generate 100 independent replications from the random field with the true covariance model at the same observation locations. First, we compute the MLE for the correctly specified and misspecified covariance models, then, we compute the plug-in kriging predictions for both covariance functions at the point \((i/5, j/5)\), for \( i, j = 1, 2, 3, 4 \), denoted by \( s_{01}, \ldots, s_{0p} \) for \( p = 16 \), and compare the results with the kriging results from the exact covariance functions. Lastly, the performance of the prediction is comparatively assessed, using our suggested MLOE in (6) and MMOM in (7), as well as MSPE in (3).

The simulation results are shown in Figures 2 and 3. These figures show that, when the covariance model is correctly specified, the MLOE is very small in comparison with the exact model and has a decreasing trend when the number of observations \( n \) increases. The MMOM is larger, but concentrates near zero and shrinks when \( n \) increases. This shows that the plug-in kriging prediction does not lead to a significant loss of prediction efficiency, which is in agreement with the intuition and the simulation results introduced in [Stein (1999)]. When the model is misspecified, the MLOE is clearly larger than that of the case where the model
is correctly specified. The MMOM may likely have a mean value larger than zero. Thus, when a rougher covariance model is misspecified as a smoother model with nugget effect, the plug-in prediction is suboptimal and the MSE can be overestimated. In Figure 3, the difference of boxplots between the case where the model is correctly specified or misspecified is not apparent, showing that our suggested MLOE and MMOM are more sensitive criteria for prediction accuracy. In conclusion, our suggested MLOE and MMOM criteria are a more valid and sensitive tool to detect the loss of prediction efficiency caused by spatial model approximations in simulation studies.

5 Simulation Experiments on the Tuning Inputs

As an application of the suggested MLOE and MMOM criteria in Section 3, we aim at assessing the performance of the TLR approximation method based on these criteria. We define how to tune the TLR associated inputs based on the target data and the application requirements, using simulation experiments. All experiments being carried out are conducted on a dual-socket 16-core Intel Sandy Bridge Intel Xeon CPU E5-2670 running at 2.60GHz.
5.1 Simulation Settings

Here, we provide an outline of our simulation settings. Similar to the settings in Sun and Stein (2016), our simulation experiments are performed on a set of synthetic datasets generated using the built-in data generator tool in ExaGeoStatR at irregular locations in a 2D space (i.e., simulate_data_exact() function). The generation process assumes a zero-mean stationary Gaussian random field \( \{ Z(s), s \in [0, 1]^2 \} \). The observation locations \( s_1, \ldots, s_n \) are generated by the same settings as those detailed in Section 4. Given the set of \( n \) locations, the covariance matrix \( \Sigma \) is constructed using the Matérn covariance function.

The simulation is to illustrate the effectiveness of using the TLR approximation method for the MLE estimation. The assessments include the total execution time, estimation accuracy, and prediction accuracy. The prediction accuracy is investigated by MLOE and MMOM. The assessment includes the kriging performance obtained by using the estimated parameters to predict unknown sets of values at various specific locations. All the symbols in this section follow the abbreviations illustrated in Table 1.

In the simulation experiments conducted by Abdullah et al. (2018b), both the estimation
and the prediction accuracy of the TLR method were shown by a set of boxplots representing
the estimation accuracy of different model parameters and the MSPE, and compared with the
exact method. The simulation performed in [Abdulah et al. (2018b)] also assessed the impact
of using different TLR accuracy levels $tlr_{acc}$ for both the accuracy and the execution time.
Here, we use the MLOE and MMOM and not only consider $tlr_{acc}$, but also consider the
impact of other tuning inputs, i.e., the tile size, maximum rank, and optimization tolerance
to the overall execution time, estimation accuracy, and prediction accuracy. Moreover, we
consider two different smoothness levels of the underlying random field, i.e., $\nu = 0.5$ and $1$,
whereas the simulations of [Abdulah et al. (2018b)] only considered $\nu = 0.5$.

All the experiments in this section use spatial data where the number of locations is
$n = 3,600$. For the true values of the parameters in (1), we consider $\sigma^2 = 1$, $\nu = 0.5$ or
$1$, and $\alpha$ is chosen such that the effective range of the model can be $h_{eff} = 0.2, 0.4, 0.8,$
or $1.6$. First, a set of the following experiments aim at comparing the performance of
the TLR approximation under different tile size $nb$ with suitable value of maximum rank
$tlr_{max\_rank}$, while the other tuning inputs $tlr_{acc}$ and $opt_{tol}$ are fixed at a moderate value
which does not affect the estimation accuracy of the approximations. Second, we compare
the performance under different accuracy levels $tlr_{acc}$ and optimization tolerance $opt_{tol}$,
where the tile size $nb$ and maximum rank $tlr_{max\_rank}$ are fixed at the suggested value
obtained in the previous step.

5.2 Performance using Different Tile Sizes

The parallel TLR approximation computation depends on dividing the matrix into a set of
tiles where the tile size is $nb \times nb$. Here $nb$ should be tuned on different hardware platforms to
obtain the best performance that corresponds to the trade-off between the arithmetic intensity and the degree of parallelism. We illustrate the performance and accuracy using different
values of $nb$, i.e., $nb = 400, 450, 600$, and $900$. We fix $tlr_{acc} = 10^{-9}$ and $opt_{tol} = 10^{-6}$ since
these values have little impact on the estimation performance. The \textit{tlr\_max\_rank} is fixed to the smallest feasible value for TLR computation obtained before the simulation. The \textit{tlr\_max\_rank} actually affects the memory allocation process. A value of \textit{tlr\_max\_rank} that is too large can slow down the computation due to the unnecessary allocations, whereas a too small value may cause the failure of the SVD approximation of each off-diagonal tile. Thus, for each value of \textit{nb}, we try to compute TLR approximations for \textit{tlr\_max\_rank} = 10, 20, \ldots, until the value of \textit{tlr\_max\_rank} can make the approximation feasible for all replicates.

For each parameter settings, we generate 100 independent replicates of the observed random field. The synthetic datasets are generated using the \texttt{simulate\_data\_exact()} function in the \texttt{ExaGeoStatR} package. The estimation performed uses both the exact and TLR methods, by the \texttt{exact\_mle()} and the \texttt{tlr\_mle()} functions in the same package, respectively, and estimate both the execution time and the estimation accuracy of each method, for different \textit{nb} values. The last step is to compute the MLOE and MMOM on prediction locations \((i/5, j/5)\), where \(i, j = 1, 2, 3, 4\). The prediction performance is then evaluated by the mean and standard deviations for both the MLOE and MMOM values. In our estimation, the value of \(\nu\) is fixed at its true value and the optimization bound for estimating \(\sigma^2\) and \(\alpha\) is [0.01, 5]. The optimization tolerance of the exact MLE is set as \(10^{-9}\) in order to get more accurate estimation results for comparison.

Selecting the smallest \textit{tlr\_max\_rank} value for each tile size is important to obtain the best performance. Thus, we perform a set of experiments to select the \textit{tlr\_max\_rank} value corresponding to each \textit{nb} when \(n = 3,600\) (Table 2). The reported values show that the feasible \textit{tlr\_max\_rank} does not simply increase when the tile size \textit{nb} increases. In fact, when the number of tiles is divisible by the number of underlying CPUs, i.e., \(nb = 450\) or \(900\), the maximum rank of each tile \textit{tlr\_max\_rank} is relatively small compared to the \textit{nb}. The required \textit{tlr\_max\_rank} is significantly smaller when the model is relatively smoother. Thus, when the number of locations is \(n = 3,600\), we recommend to choose the \textit{tlr\_max\_rank} as
Table 2: Smallest $tlr_{\text{max.rank}}$ that makes the TLR approximation applicable to different values of $nb$, and the parameters of the Matérn covariance. The number of locations is $n = 3,600$.

| $\nu$ | Eff.range | Tile size ($nb$) |
|-------|-----------|------------------|
|       |           | 400 450 600 900  |
| 0.5   | 0.2       | 260 210 310 270  |
|       | 0.4       | 250 210 310 270  |
|       | 0.8       | 250 210 300 260  |
|       | 1.6       | 250 210 300 260  |
| 1.0   | 0.2       | 220 170 250 210  |
|       | 0.4       | 220 170 250 210  |
|       | 0.8       | 210 170 250 210  |
|       | 1.6       | 210 180 250 210  |

the largest values shown in Table 2 for the corresponding values of $\nu$ and $nb$.

For the MLE and different TLR approximations, we only show typical results with $\nu = 0.5$, $h_{\text{eff}} = 0.2$ and $\nu = 1$, $h_{\text{eff}} = 1.6$, shown in Table 3. This table shows that the TLR approximation has a similar estimation and prediction performance for different tile sizes $nb$, whereas the fastest computational time is obtained when $nb = 450$.

Table 3: Estimation and prediction performances of MLE and TLR approximation estimates for different values of $nb$. Bias(·) means the estimate of the parameter minus its true value, whereas the estimation time means the computational time of the corresponding estimation. The value of MLOE is multiplied by $10^6$.

| Mean (sd) | $\nu = 0.5$, $h_{\text{eff}} = 0.2$ | $\nu = 1.0$, $h_{\text{eff}} = 1.6$ |
|-----------|----------------------------------|----------------------------------|
|           | MLE                              | TLR approximations ($nb$)        | MLE                              | TLR approximations ($nb$)        |
|           | 400 450 600 900                  | 400 450 600 900                  | 400 450 600 900                  | 400 450 600 900                  |
| Bias($\sigma^2$) | −0.0080 (0.0908) | −0.0079 (0.0908) | −0.0079 (0.0908) | 0.0163 (0.6546) |
|           | −0.0066 (0.0063) | −0.0066 (0.0063) | −0.0066 (0.0063) | 0.0144 (0.1186) |
| Bias($\alpha$)   | 3.3945 (5.9474) | 3.3756 (5.9474) | 3.3758 (5.9474) | 0.0273 (0.0243) |
|           | 3.3756 (5.9474) | 3.3756 (5.9474) | 3.3756 (5.9474) | 0.0109 (0.0243) |
| MLOE ($\times 10^6$) | 0.0110 (0.0232) | 0.0110 (0.0232) | 0.0110 (0.0232) | 0.0109 (0.0242) |
| MMOM      | 0.0017 (0.0232) | 0.0011 (0.0232) | 0.0011 (0.0232) | 0.0144 (0.0222) |
|           | 0.0111 (0.0232) | 0.0011 (0.0232) | 0.0011 (0.0232) | −0.1428 (0.0223) |
| Estimation| 146.5 (20.2) | 110.2 (15.3) | 90.3 (13.5) | 277.5 (75.6) |
| time (sec) | 146.4 (19.5) | 146.6 (19.5) | 146.6 (19.5) | 122.3 (35.6) |
|           | 108.1 (31.6) | 143.5 (46.6) | 186.5 (63.0) | 108.1 (31.6) |
5.3 Performance using Different TLR Accuracy Levels

We investigate the effect of \texttt{tlr\_acc} and \texttt{opt\_tol} for the TLR approximations, where \( nb = 450 \) and \( tlr\_max\_rank \) is chosen from Table 2. To compare the effect of different values of \( tlr\_acc \), we fix \( opt\_tol = 10^{-6} \) and choose \( tlr\_acc = 10^{-5}, 10^{-7}, 10^{-9}, \) or \( 10^{-11} \). We also compare the effect of different \( opt\_tol \) values; to do so, we fix \( tlr\_acc = 10^{-9} \) and choose \( opt\_tol = 10^{-3}, 10^{-6}, 10^{-9}, \) or \( 10^{-12} \).

The parameter settings and the simulation procedures are similar to those given in Section 5.2. When \( tlr\_acc = 10^{-11} \), the \( tlr\_max\_rank \) value in Table 2 is not large enough. Thus, we use increased values of \( tlr\_max\_rank \) in this case, namely, when \( \nu = 0.5 \), we set \( tlr\_max\_rank = 270 \) for \( h\_eff = 0.2 \) and \( tlr\_max\_rank = 260 \) for other cases; when \( \nu = 1 \), we set \( tlr\_max\_rank = 200 \). We only provide the estimation and prediction performances for two typical cases, when \( \nu = 0.5, h\_eff = 0.2 \), and when \( \nu = 1, h\_eff = 1.6 \). Table 4 shows the results obtained with different values of \( tlr\_acc \), and Table 5 presents the results for different \( opt\_tol \) values. For more detail, please refer to the Supplementary Material.

Table 4: Estimation and prediction performances of the exact MLE and TLR approximation estimates for different \( tlr\_acc \) values. Bias(\( \cdot \)) means the estimate of the parameter minus its true value, and the estimation time means the computational time of the corresponding estimation. The value of MLOE is multiplied by \( 10^6 \). The missing part in the table (-) corresponds to a computational error (Error in LAPACK portf).

| Mean (sd) | \( \nu = 0.5, h\_eff = 0.2 \) | \( \nu = 1.0, h\_eff = 1.6 \) |
| --- | --- | --- |
| | MLE | TLR accuracy (\( tlr\_acc \)) | MLE | TLR accuracy (\( tlr\_acc \)) |
| | \( 10^{-5} \) | \( 10^{-7} \) | \( 10^{-9} \) | \( 10^{-11} \) | \( 10^{-5} \) | \( 10^{-7} \) | \( 10^{-9} \) | \( 10^{-11} \) |
| Bias(\( \sigma^2 \)) | -0.0080 (0.0908) | -0.0023 (0.1095) | -0.0079 (0.0908) | -0.0079 (0.0908) | 0.0163 (0.6546) | -0.3800 (0.3154) | 0.2236 (0.7793) | 0.2276 (0.7927) |
| Bias(\( \alpha \)) | -0.0006 (0.0063) | -0.00002 (0.0077) | -0.0006 (0.0063) | -0.0006 (0.0063) | -0.0144 (0.1186) | -0.1033 (0.0686) | 0.0577 (0.1394) | 0.0581 (0.1408) |
| MLOE (\( \times 10^6 \)) | 3.3945 (5.9931) | 3.5691 (6.4517) | 3.3756 (5.9476) | 3.3756 (5.9474) | 0.0273 (0.0669) | -0.0079 (0.0167) | 0.0110 (0.0243) | 0.0109 (0.0242) |
| MMOM | 0.0017 (0.0232) | 0.0009 (0.0233) | 0.0011 (0.0232) | 0.0011 (0.0232) | 0.0014 (0.0227) | -0.1436 (0.0222) | -0.1428 (0.0222) | -0.1428 (0.0222) |
| Estimation time (sec) | 168.1 (22.3) | 69.8 (11.9) | 77.8 (9.5) | 90.4 (13.5) | 112.1 (15.5) | 274.3 (74.6) | 62.7 (26.7) | 106.7 (31.2) | 111.6 (33.7) |

Tables 4 and 5 indicate that the exact MLE and the TLR approximations can provide...
Table 5: Estimation and prediction performances of the exact MLE and TLR approximation estimates for different opt\_tol values. Bias(\cdot) means the estimate of the parameter minus its true value, and the estimation time means the computational time of the corresponding estimation. The value of MLOE is multiplied by $10^6$.

| V | MLE | Optimization tolerance (opt\_tol) | MLE | Optimization tolerance (opt\_tol) |
|---|-----|---------------------------------|-----|---------------------------------|
|   |     | $10^{-3}$ | $10^{-6}$ | $10^{-9}$ | $10^{-12}$   |     | $10^{-3}$ | $10^{-6}$ | $10^{-9}$ | $10^{-12}$   |
|   | Mean (sd) |   |   |   |   |   |   |   |   |   |
|   | V = 0.5, h\_eff = 0.2 |   |   |   |   |   |   |   |   |   |
| V | Bias($\sigma^2$) | -0.0080 (0.0008) | 0.3654 (0.3017) | -0.0079 (0.0908) | -0.0079 (0.0908) | 0.0163 (0.6546) | 0.3263 (0.4421) | 0.2230 (0.7793) | 0.2234 (0.7787) | 0.2234 (0.7787) |
| V | Bias($\alpha$) | -0.0006 (0.0063) | 0.0253 (0.0210) | -0.0006 (0.0063) | -0.0006 (0.0063) | -0.0144 (0.1186) | 0.0896 (0.0904) | 0.0577 (0.1394) | 0.0577 (0.1393) | 0.0577 (0.1393) |
| V | MLOE ($\times 10^6$) | 3.3945 (5.9931) | 19.3107 (13.9768) | 3.3756 (5.9474) | 3.3756 (5.9475) | 0.0273 (0.0669) | 0.0150 (0.0708) | 0.0110 (0.0243) | 0.0110 (0.0243) | 0.0110 (0.0243) |
| V | MMOM | 0.0017 (0.0232) | -0.0061 (0.0234) | 0.0011 (0.0232) | 0.0011 (0.0232) | 0.0014 (0.0227) | -0.1432 (0.0222) | -0.1428 (0.0222) | -0.1428 (0.0222) | -0.1428 (0.0222) |
| V | Estimation time (sec) | 168.1 (22.3) | 33.8 (13.6) | 90.4 (13.5) | 102.2 (13.2) | 113.0 (13.0) | 274.3 (74.6) | 29.4 (21.7) | 106.7 (31.2) | 124.1 (34.8) | 136.2 (36.0) |

accurate prediction results since the small MLOE values suggest that the loss of prediction efficiency is very small. The MMOM results indicate that the computed MSEs are also accurate, except when $\nu = 1$ and $h\_eff = 1.6$, which shows that the plug-in kriging based on TLR approximations may underestimate the prediction MSEs for a smoother random field with a larger effective range. The plug-in kriging based on the exact MLE works well for all cases.

Table 4 shows that the TLR approximations give similar and relatively satisfactory performances of the estimation when tlr\_acc $\leq 10^{-9}$, and that the prediction performs well when tlr\_acc $\leq 10^{-7}$. The computational time increases when tlr\_acc decreases, so we suggest tlr\_acc $= 10^{-9}$ for maintaining estimation performance and tlr\_acc $= 10^{-7}$ for maintaining prediction performance.

Table 5 shows that the estimation performs relatively well when opt\_tol $\leq 10^{-6}$. For prediction performances, the case of opt\_tol $= 10^{-3}$ performs well enough, though the MLOE values are larger compared with other cases. So we suggest opt\_tol $= 10^{-6}$ for keeping estimation performances and opt\_tol $= 10^{-3}$ for keeping prediction performances because of the significantly faster computational speed in this case.
To further investigate the impact of different combinations of \( tlr\_acc \) and \( opt\_tol \) for prediction performances, we also try the cases where \( tlr\_acc \) can be \( 10^{-7}, \ 10^{-9} \) and \( opt\_tol \) can be \( 10^{-3}, \ 10^{-6} \). Table 6 shows that choosing \( tlr\_acc = 10^{-7} \) and \( opt\_tol = 10^{-3} \) can provide a faster computation without losing too much prediction efficiency; we therefore suggest to select \( tlr\_acc = 10^{-7} \) and \( opt\_tol = 10^{-3} \) for keeping the prediction performances.

Table 6: Prediction performance and the computational time for TLR approximations with different combinations of \( tlr\_acc \) and \( opt\_tol \). The estimation time means the computational time of the corresponding estimation. The value of MLOE is multiplied by \( 10^6 \).

| Mean (sd) \((tlr\_acc, opt\_tol)\), \( \nu = 0.5, \ h_{eff} = 0.2 \) | \((tlr\_acc, opt\_tol)\), \( \nu = 1.0, \ h_{eff} = 1.6 \) |
|---|---|
| MLOE \((\times 10^6)\) | 19.0060 (13.6484) | 19.3107 (13.9768) | 3.3756 (5.9476) | 3.3756 (5.9474) |
| MMOM | 0.0138 (0.0688) | 0.0150 (0.0708) | 0.0079 (0.0167) | 0.0110 (0.0243) |
| Estimation time (sec) | 28.8 (11.4) | 33.1 (13.3) | 76.6 (9.4) | 88.5 (13.2) |
| | 19.4 (8.8) | 29.8 (22.1) | 63.5 (27.1) | 108.1 (31.3) |

In conclusion, the TLR approximation method can significantly reduce the computational time and maintain the prediction efficiency. The only problematic aspect of the TLR method is that, when \( \nu = 1 \) and the effective range is large, the prediction MSE may be underestimated. For tuning the inputs in the TLR approximation, we recommend a moderate value of \( nb \) that makes the number of tiles divisible by the total number of CPUs, and a smallest feasible \( tlr\_max\_rank \), which can be obtained by our simulations or by some simple trials. We suggest \( tlr\_acc = 10^{-9}, \ opt\_tol = 10^{-6} \) for maintaining estimation performances; and we suggest \( tlr\_acc = 10^{-7}, \ opt\_tol = 10^{-3} \), when only the prediction performances are necessary to maintain. Our suggested MLOE and MMOM criteria can successfully assess the loss of spatial prediction efficiency of the TLR method with different tuning inputs.

Remark 1. Table 4 shows that the TLR method with \( tlr\_acc = 10^{-5} \) can maintain the prediction performance for the exponential covariance model, but cannot for the Whittle covariance model, suggesting that one may need a lower \( tlr\_acc \) value for a smoother process. Thus, if the process is smoother than the Whittle covariance model and \( tlr\_acc = 10^{-7} \) is
not applicable, then one can choose smaller \( tlr_{\text{acc}} \) such as \( 10^{-9} \).

6 Application to Soil Moisture Data

To show the effectiveness of the TLR approximation with our suggested settings of the tuning inputs for real datasets, we compare the estimation and prediction performance of this approximation to the exact MLE for the soil moisture dataset, with Intel Sandy Bridge Intel Xeon CPU E5-2670 running at 2.60GHz, allowing the computation of the exact MLE by the ExaGeoStat framework. We use 4 nodes, each node has 16 underlying CPUs, so the number of tiles is divisible by the total number of CPUs.

This dataset describes the daily soil moisture percentage at the top layer of the Mississippi basin, U.S., on January 1st, 2004, including the observation locations and the residual of the fitted linear model in Huang and Sun (2018), and can be obtained from the website \url{https://ecrc.github.io/exageostat/md_docs__examples.html}, containing the example data of the ExaGeoStat package. The full dataset consists of about 2 million locations, however, we select a region of \( N = 64,648 \) locations that can be considered as representative regions for the whole area. For our computational experiment, we consider a subset of this dataset, where the latitude and longitude of the locations lie within \([33.0, 35.2] \times [-106.1, -103.9]\), as shown in Figure 4. We use the latitude and longitude as the coordinates of the observation locations in our computation.

In this numerical experiment, we randomly choose \( n = 3,600, 14,400, 32,400, \) or 57,600 points for the estimation, and use the remaining points for assessing the prediction performance. For estimation, the smoothness parameter \( \nu \) is either treated as unknown or fixed at \( \nu = 0.5 \). The searching intervals for optimizing the likelihood function are \( \sigma^2 \in [0.01, 5] \), \( \alpha \in [0.01, 5] \), and \( \nu \in [0.01, 5] \) for the unknown case. In TLR approximations, we choose \( tlr_{\text{acc}} = 10^{-9}, \text{opt}_\text{tol} = 10^{-6} \) and \( tlr_{\text{acc}} = 10^{-7}, \text{opt}_\text{tol} = 10^{-3} \), which are our recommendations for keeping the estimation and prediction performances, respectively. The
Figure 4: Image plot of the soil moisture dataset residuals for the real case study.

$tlr_{\text{max.rank}}$ value is determined using the procedure presented in Section 5.2. The settings of $nb$ and $tlr_{\text{max.rank}}$ are shown in Table 7, and results are given in Table 8.

Table 7: The value of $nb$ and the corresponding $tlr_{\text{max.rank}}$ used in the estimation of the soil moisture data.

| $n$  | $nb$  | $tlr_{\text{max.rank}}$ ($\nu$ unknown) | $tlr_{\text{max.rank}}$ ($\nu$ known) |
|------|-------|----------------------------------------|----------------------------------------|
| 3,600| 450   | 210                                    | 210                                    |
| 14,400| 900   | 310                                    | 320                                    |
| 32,400| 1350  | 490                                    | 500                                    |
| 57,600| 1800  | 430                                    | 430                                    |

Table 8 indicates that, when $tlr_{\text{acc}} = 10^{-9}$ and $opt_{\text{tol}} = 10^{-6}$, the TLR approximation can provide parameter estimates that are very close to the exact MLE, with a significantly shorter computational time. The computational times are further shortened when $tlr_{\text{acc}} = 10^{-7}$ and $opt_{\text{tol}} = 10^{-3}$. In this case, the prediction performances are similar to the exact MLE, though the estimates are no longer similar. Thus, our proposed tuning input suggestions work well, and the TLR approximation clearly appears as an efficient method.
Table 8: Estimation results, computational time and MSPE of the MLE and TLR estimation for soil moisture data, where $\nu$ is unknown or fixed at 0.5.

| n   | tlr, acc | opt_tol | $\nu$ is unknown | $\nu$ is fixed at 0.5 |
|-----|---------|---------|------------------|----------------------|
|     | $\sigma^2$ | $\alpha$ | $\nu$ | Times (sec) | MSPE | $\sigma^2$ | $\alpha$ | Times (sec) | MSPE |
| 3,600 | Exact MLE | 1.2488 | 0.4590 | 0.2970 | 3355.1 | 0.2283 | 1.0970 | 0.1105 | 819.0 | 0.2335 |
|      | $10^{-5}$ | 1.1107 | 0.3918 | 0.2934 | 35.8 | 0.2283 | 1.1842 | 0.1191 | 19.4 | 0.2337 |
|      | $10^{-9}$ | 1.2486 | 0.4587 | 0.2971 | 240.7 | 0.2283 | 1.0969 | 0.1106 | 69.5 | 0.2335 |
| 14,400 | Exact MLE | 1.1412 | 0.2358 | 0.3566 | 21491.6 | 0.1461 | 1.0478 | 0.1263 | 10984.3 | 0.1457 |
|      | $10^{-5}$ | 0.8784 | 0.1740 | 0.3488 | 670.4 | 0.1462 | 1.2210 | 0.1054 | 177.5 | 0.1458 |
|      | $10^{-9}$ | 1.1410 | 0.2356 | 0.3568 | 1898.9 | 0.1461 | 1.0046 | 0.0865 | 733.7 | 0.1457 |
| 32,400 | Exact MLE | 1.0478 | 0.1263 | 0.4282 | 561009.3 | 0.1067 | 0.9870 | 0.0774 | 52128.7 | 0.1060 |
|      | $10^{-5}$ | 1.4342 | 0.1898 | 0.4229 | 5342.0 | 0.1068 | 1.1183 | 0.0913 | 1201.9 | 0.1060 |
|      | $10^{-9}$ | 1.0475 | 0.1261 | 0.4285 | 13023.0 | 0.1067 | 0.9935 | 0.0798 | 5556.4 | 0.1060 |
| 57,600 | Exact MLE | 0.9870 | 0.0774 | 0.5066 | 1898.9 | 0.1067 | 0.9868 | 0.0773 | 52965.1 | 0.1061 |
|      | $10^{-5}$ | 1.3356 | 0.2347 | 0.3928 | 13023.0 | 0.1067 | 0.9937 | 0.0806 | 13023.0 | 0.1060 |

Remark 2. When the smoothness parameter $\nu$ is fixed, the MLE and TLR approximations have a significantly faster computational time than when $\nu$ is unknown, without losing too much prediction performance in terms of the MSPE. Thus, we can set the $\nu$ value to be a value suggested by the exploratory analysis or from another source of information.

We also compare the TLR with the most popular low-rank based approximation method, the Gaussian predictive process (GPP) method proposed by Banerjee et al. (2008). For some predetermined knots $s_1^\star, \ldots, s_m^\star$, the GPP method approximates the observed value $Z(s)$ by its kriging prediction value with respect to the observations on the knots plus a nugget term. Denote the observations on the knots by $Z^\star := \{Z(s_1^\star), \ldots, Z(s_m^\star)\}^\top$. The kriging prediction, which is treated as an approximation of $Z(s)$, is

$$E\{Z(s)|Z(s_1^\star), \ldots, Z(s_m^\star)\} = c^\top(s, \theta)(C^\star)^{-1}(\theta)Z^\star,$$

so the Gaussian predictive process model is

$$\tilde{Z}(s) = c^\top(s, \theta)(C^\star)^{-1}(\theta)Z^\star + \epsilon(s),$$

where $c(s, \theta) = [C(s, s_j^\star; \theta)]_{j=1}^m, C^\star(\theta) = [C(s_i^\star, s_j^\star; \theta)]_{i,j=1}^m, C(s_1, s_2; \theta) = \text{Cov}\{Z(s_1), Z(s_2)\}$, and $\epsilon(s)$ is the nugget effect term which has a normal distribution with mean zero and vari-
ance $\tau^2$. The approximated kriging prediction is computed with the covariance matrix of the approximated random field $\tilde{Z}(s)$. For the Gaussian predictive process model, the computation of the inverse covariance matrix only involves the inversion of the matrix of order $m$, so the computational time can be saved, compared with directly inverting a matrix of order $n$.

We still consider $n = 3,600, 14,400, 32,400, 57,600$ and use the same soil moisture dataset stated above. First, we fit the Gaussian predictive process model (8) by maximum likelihood estimation, where the covariance function $C(s_1, s_2; \theta)$ is the Matérn covariance (1). The smoothness parameter $\nu$ is either treated as unknown, or fixed at $\nu = 0.5$. Next, we compute the plug-in kriging prediction, based on the GPP model on the same prediction points as stated above, together with the MSPE. We choose the knots as the $23 \times 23$ regular grid, which is evenly distributed on the observed range $[33.0, 35.2] \times [-106.1, -103.9]$.

The optimization of the log-likelihood function is computed using the function `optim()` of the R software, where the initial value is $(\sigma^2, \alpha, \nu, \tau) = (1, 0.1, 0.5, 0.2)$. Our code for Gaussian predictive process estimation does not involve multi-core computation, so the computational time is not comparable with the aforementioned computational times of the MLE and TLR approximations. The computation results, including the estimates, MSPEs, and the computational times, can be found in Table 9.

Table 9 indicates that when $\nu$ is unknown, the estimation results of $\nu$ are larger than 0.5, and also larger than the corresponding exact maximum likelihood estimate given in Table 8. The MSPE of the GPP model is significantly larger than the corresponding results of the prediction based on exact MLE. Moreover, the value of MSPE has no apparent change when the number of observations $n$ increases. Thus, for kriging prediction, the Gaussian predictive process method is less efficient than the exact MLE and the TLR approximations.

To evaluate the performance of the Gaussian predictive process method, with respect to different numbers of knots $m$, we also perform the estimation and prediction for $m = 900, 1,600, 2,500$, and 3,600, for the case where $n = 3,600$. The knots used in this
Table 9: Maximum likelihood estimation results of the approximated Gaussian predictive process model for the soil moisture data, including the parameter estimate, MSPE and the computational time. The MSPE value is compared with the corresponding kriging results from the MLE of the correct Matérn covariance model (Exact). The number of knots in the Gaussian predictive process is $m = 529$.

| $n$  | $\sigma^2$ | $\alpha$ | $\nu$ | $\tau$ | MSPE (Exact) | MSPE (Exact) | Time (sec) |
|------|------------|----------|-------|--------|--------------|--------------|------------|
| 3,600| 0.7910     | 0.1743   | 2.5082| 1.7807 | 0.4292       | 0.2283       | 5126       |
| 14,400| 0.8822   | 0.1665  | 2.8800| 3.5698 | 0.4328       | 0.1461       | 8380       |
| 32,400| 0.8703   | 0.3467  | 1.2688| 5.3881 | 0.4298       | 0.1067       | 20552      |
| 57,600| 0.8403   | 0.1861  | 2.5100| 7.2297 | 0.4268       | 0.0811       | 89817      |

| $n$  | $\sigma^2$ | $\alpha$ | $\nu$ (fixed) | $\tau$ | MSPE (Exact) | MSPE (Exact) | Time (sec) |
|------|------------|----------|----------------|-------|--------------|--------------|------------|
| 3,600| 0.9533     | 0.9423   | 0.5000         | 1.7720| 0.4095       | 0.2335       | 1687       |
| 14,400| 1.0155    | 1.0865  | 0.5000         | 3.5710| 0.4137       | 0.1457       | 34461      |
| 32,400| 1.0033   | 1.0969  | 0.5000         | 5.3784| 0.4178       | 0.1060       | 159889     |
| 57,600| 0.9877   | 1.0937  | 0.5000         | 7.2308| 0.4158       | 0.0812       | 488795     |

Computation are chosen as the $\sqrt{m} \times \sqrt{m}$ regular grids, evenly distributed on the observed range $[33.0, 35.2] \times [-106.1, -103.9]$. The other computational settings are similar. The computation results, including the estimates, MSPEs, and the computational times, can be found in Table 10.

Table 10 indicates that when $\nu$ is unknown, the estimates of $\sigma^2$ and $\alpha$ slightly increase when $m$ increases, whereas the estimates of $\nu$ and $\tau$ have an apparent decreasing trend when $m$ increases. When $\nu$ is fixed at 0.5, the estimate of $\sigma^2$ also slightly increases when $m$ increases, whereas the estimates of $\alpha$ and $\tau$ significantly decrease when $m$ increases. For these two cases, the MSPE has a decreasing trend when $m$ increases, but the value is still larger than that of the prediction based on exact MLE results or TLR approximation results. In conclusion, the prediction performance of the TLR approximation is better than that of the Gaussian predictive process method on this dataset.

**Remark 3.** When the number of knots $m$ is less than the number of observations, the Gaussian predictive process method gives a larger estimate of $\nu$, compared with the exact MLE. In other words, the GPP method treats the model of the spatial dataset as a smoother
approximation of the Matérn covariance model plus a nugget effect. By the simulation results in Section 4, when the true covariance model is a rougher model, it is not appropriate to approximate the model by a smoother covariance model with nugget term, since this approximation can lose the prediction efficiency. In this case, it may also not be appropriate to approximate the model by an approximation of a smoother covariance model with nugget term, e.g., the Gaussian predictive process model with larger $\nu$. This may be the reason why the prediction performance of GPP method is less favourable.

In conclusion, the TLR approximation is a practicable and effective method to solve the estimation and prediction problem for large spatial datasets; it outperforms the Gaussian predictive process method in the soil moisture data prediction problem. Also, our suggested settings of the tuning inputs for TLR approximation, obtained by using the MLOE and MMOM criteria, can maintain the estimation or prediction performances.
7 Concluding Remarks

In this article, we present the Mean Loss of Efficiency (MLOE) and Mean Misspecification of the MSE (MMOM) criteria as tools to detect the difference of the prediction performance between the true and the approximated covariance models in simulation studies. We find that the suggested criteria are more appropriate than the commonly used Mean Square Prediction Error criterion, as the criteria can detect the efficiency loss when a smoother covariance model is misspecified as a rougher covariance model with a nugget effect in simulation studies, which the MSPE cannot do. Our suggested criteria are valuable tools for understanding the impact of the tuning inputs on the statistical performance of sophisticated approximation methods, which is crucial for selecting these inputs. To illustrate this, we compare the estimation and prediction performances of the Tile Low-Rank approximation with different tuning inputs, and obtain a practical suggestion on how to choose these tuning inputs for different application requirements. With the suggested tuning inputs, we show by a real-case study in which the TLR method outperforms the popular Gaussian predictive process method in prediction efficiency.

It is worth noting that a good knowledge of the smoothness of the covariance model can be helpful for the estimation and prediction. For example, our simulations show that the computational time of the exact MLE and the TLR approximation are significantly shorter when the smoothness parameter $\nu$ is fixed. The smoothness can also affect the effectiveness of adopting the TLR approximation in spatial prediction and the proper value of tuning inputs in this approximation. For instance, if we can ensure that the process is not smoother than the exponential covariance model, then we can further relax $tlr_{acc}$ in the TLR method, say $tlr_{acc} = 10^{-5}$, which can still maintain the prediction performance. Thus, it would be appealing to introduce a suitable method for determining this kind of smoothness, such as determining the range of $\nu$ in the Matérn covariance model, before estimation and prediction. However, as it has been shown by simulations, misspecification
of the smoothness of a random field significantly worsens the spatial prediction performance. Thus the smoothness determination method should be accurate enough. In future work, we will develop suitable smoothness parameter determination methods, such as the hypothesis tests proposed by [Hong et al. (2018)] and the references therein, and apply the method in the parameter estimation process to further improve the computation performance. It would also be interesting to compare the performance of the other tile-based approximation methods with the TLR method, using the suggested MLOE and MMOM criteria, in order to determine the best method for different application cases.

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# Supplementary Material for Efficiency Assessment of Approximated Spatial Predictions for Large Datasets

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In this Supplementary Material, we list the simulation results omitted in Section 5 due to space limitations.

Table 11: Estimation and prediction performances of MLE and TLR approximation estimates for different nb values. Bias(·) means the estimate of the parameter minus its true value, while the estimation time means the computational time of the corresponding estimation. The value of MLOE is multiplied by 10^6.

| nb | Mean (sd) | \( \nu = 0.5 \) | \( \nu = 1.0 \) |
|----|-----------|-----------------|-----------------|
|    | MLE       | Tile size (nb)  | MLE             | Tile size (nb)  |
|    |           | 400 500 600 900 |                 | 400 450 600 900 |
| 0.2 | Bias(\( \sigma^2 \)) | -0.0060 (0.0908) -0.0079 (0.0908) -0.0079 (0.0908) -0.0079 (0.0908) | -0.0085 (0.01054) -0.0085 (0.01058) -0.0085 (0.01058) -0.0085 (0.01057) |
|    | Bias(\( \alpha \))  | -0.0006 (0.0063) -0.0006 (0.0063) -0.0006 (0.0063) -0.0006 (0.0063) | -0.0005 (0.00028) -0.0005 (0.00029) -0.0005 (0.00029) -0.0005 (0.00028) |
|    | MLOE (\( \times 10^6 \)) | 3.3946 (5.9744) 3.3956 (5.9744) 3.3956 (5.9744) 3.3956 (5.9744) | 3.1738 (2.6485) 3.1738 (2.6485) 3.1738 (2.6485) 3.1738 (2.6485) |
|    | MMOM      | 0.0017 (0.0232) 0.0017 (0.0232) 0.0017 (0.0232) 0.0017 (0.0232) | 0.0019 (0.00240) 0.0019 (0.00240) 0.0019 (0.00240) 0.0019 (0.00240) |
|    | Estimation time (sec) | 110.2 (15.3) 90.3 (13.5) 146.1 (21.7) 146.1 (19.5) | 197.4 (30.8) 197.4 (30.8) 197.4 (30.8) 197.4 (30.8) |
| 0.4 | Bias(\( \sigma^2 \)) | -0.0178 (0.1739) -0.0172 (0.1742) -0.0172 (0.1742) -0.0172 (0.1741) | -0.0207 (0.1955) -0.0207 (0.1990) -0.0207 (0.1990) -0.0207 (0.1990) |
|    | Bias(\( \alpha \))  | -0.0026 (0.0234) -0.0023 (0.0234) -0.0023 (0.0234) -0.0023 (0.0234) | -0.0016 (0.00100) -0.0016 (0.00102) -0.0016 (0.00102) -0.0016 (0.00102) |
|    | MLOE (\( \times 10^6 \)) | 0.9790 (2.0581) 0.9681 (2.0581) 0.9682 (2.0581) 0.9682 (2.0581) | 0.8041 (0.5944) 0.9365 (0.5943) 0.9365 (0.5943) 0.9365 (0.5943) |
|    | MMOM      | 0.0018 (0.0228) 0.0018 (0.0228) 0.0018 (0.0228) 0.0018 (0.0228) | 0.0019 (0.0230) 0.0019 (0.0230) 0.0019 (0.0230) 0.0019 (0.0230) |
|    | Estimation time (sec) | 118.5 (18.0) 83.6 (14.2) 114.5 (22.0) 114.5 (22.0) | 115.7 (43.0) 115.7 (43.0) 115.7 (43.0) 115.7 (43.0) |
| 0.8 | Bias(\( \sigma^2 \)) | -0.0147 (0.3474) -0.0143 (0.3482) -0.0143 (0.3482) -0.0143 (0.3482) | -0.0226 (0.3678) 0.0384 (0.3925) 0.0395 (0.3927) 0.0395 (0.3931) |
|    | Bias(\( \alpha \))  | -0.0042 (0.0928) -0.0032 (0.0933) -0.0032 (0.0933) -0.0032 (0.0933) | -0.0057 (0.0361) 0.0050 (0.0383) 0.0050 (0.0383) 0.0050 (0.0383) |
|    | MLOE (\( \times 10^6 \)) | 0.3286 (0.9494) 0.3221 (0.9494) 0.3221 (0.9494) 0.3221 (0.9494) | 0.1051 (0.1429) 0.0759 (0.1429) 0.0759 (0.1427) 0.0759 (0.1426) |
|    | MMOM      | 0.0016 (0.0227) 0.0016 (0.0227) 0.0016 (0.0227) 0.0016 (0.0227) | 0.0027 (0.0225) 0.0027 (0.0225) 0.0027 (0.0225) 0.0027 (0.0225) |
|    | Estimation time (sec) | 145.8 (26.4) 110.3 (19.4) 142.7 (22.0) 142.7 (22.0) | 114.2 (51.9) 114.2 (51.9) 114.2 (51.9) 114.2 (51.9) |
| 1.6 | Bias(\( \sigma^2 \)) | -0.0132 (0.6292) -0.0158 (0.6308) -0.0158 (0.6309) -0.0158 (0.6309) | 0.0163 (0.6546) 0.2173 (0.7339) 0.2236 (0.7793) 0.2236 (0.7924) |
|    | Bias(\( \alpha \))  | 0.0069 (0.3369) 0.0108 (0.3393) 0.0108 (0.3393) 0.0108 (0.3393) | -0.0144 (0.1186) 0.0577 (0.1348) 0.0577 (0.1348) 0.0577 (0.1348) |
|    | MLOE (\( \times 10^6 \)) | 0.1221 (0.4307) 0.1178 (0.4307) 0.1178 (0.4307) 0.1178 (0.4307) | 0.0275 (0.0243) 0.0109 (0.0242) 0.0109 (0.0242) 0.0109 (0.0242) |
|    | MMOM      | 0.0014 (0.0227) 0.0014 (0.0227) 0.0014 (0.0227) 0.0014 (0.0227) | -0.1028 (0.0222) -0.1028 (0.0222) -0.1028 (0.0222) -0.1028 (0.0222) |
|    | Estimation time (sec) | 161.5 (28.2) 111.4 (22.8) 145.3 (20.8) 145.3 (20.8) | 217.5 (75.6) 217.5 (75.6) 217.5 (75.6) 217.5 (75.6) |

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Table 12: Estimation and prediction performances of the exact MLE and TLR approximation estimates for different tlr_acc values. Bias(·) means the estimate of the parameter minus its true value, while the estimation time means the computational time of the corresponding estimation. The value of MLOE is multiplied by 10^6. The missing part in the table (-) corresponds to a computational error (Error in LAPACK portf).

| h_eff | Mean (sd) | ν = 0.5 | TLR accuracy (tlr_acc) | ν = 1.0 | TLR accuracy (tlr_acc) |
|-------|-----------|---------|------------------------|---------|------------------------|
|       |           | MLE     | 10^{-9} | 10^{-7} | 10^{-9} | 10^{-7} | 10^{-9} | 10^{-7} | 10^{-9} | 10^{-7} |
|       | Bias(σ²)  |         |         |         |         |         |         |         |         |         |
| 0.2   | −0.0080 (0.0908) | −0.0023 −0.0079 −0.0079 −0.0079 | −0.0085 (0.1054) | 0.0124 −0.0061 −0.0061 −0.0061 | 0.0124 −0.0061 −0.0061 −0.0061 |
|       | Bias(α)   |         |         |         |         |         |         |         |         |         |
| 0.2   | −0.0006 (0.0063) | −0.0002 −0.0006 −0.0006 −0.0006 | −0.0006 (0.0028) | 0.0004 −0.0002 −0.0002 −0.0002 | 0.0004 −0.0002 −0.0002 −0.0002 |
|       | MLOE (×10^6) | 3.3945 (5.9931) | 3.5691 3.3756 3.3756 3.3756 | 1.7378 (2.7659) | 2.1075 1.6942 1.6938 1.6940 |
|       | MMOM      | 0.0017 (0.0023) | 0.0009 0.0111 0.0111 0.0111 | 0.0019 (0.0024) | −0.0022 −0.0016 −0.0016 −0.0016 |
|       | Estimation time (sec) | 168.1 (22.3) | 68.9 77.8 90.4 112.1 | 211.0 (34.0) | 102.9 108.5 116.3 125.3 |
|       | Bias(σ²)  |         |         |         |         |         |         |         |         |         |
| 0.4   | −0.0178 (0.1379) | −0.0073 −0.0172 −0.0172 −0.0172 | −0.0207 (0.1955) | −0.0047 −0.0070 −0.0070 −0.0070 | −0.0047 −0.0070 −0.0070 −0.0070 |
|       | Bias(α)   |         |         |         |         |         |         |         |         |         |
| 0.4   | −0.0026 (0.0234) | −0.0010 −0.0023 −0.0023 −0.0023 | −0.0016 (0.0100) | −0.0002 −0.0003 −0.0003 −0.0003 | −0.0002 −0.0003 −0.0003 −0.0003 |
|       | MLOE (×10^6) | 0.9790 (2.0811) | 0.9290 0.9679 0.9682 0.9681 | 0.4034 (0.6804) | 0.3665 0.3659 0.3659 0.3659 | 0.3665 0.3659 0.3659 0.3659 |
|       | MMOM      | 0.0018 (0.0028) | 0.0004 0.0005 0.0005 0.0005 | 0.0019 (0.0023) | −0.0107 −0.0107 −0.0107 −0.0107 |
|       | Estimation time (sec) | 126.8 (19.5) | 60.2 65.2 72.4 86.9 | 252.1 (49.2) | 103.0 107.5 117.2 121.7 |
|       | Bias(σ²)  |         |         |         |         |         |         |         |         |         |
| 0.8   | −0.0147 (0.3474) | −0.0171 −0.0133 −0.0133 −0.0133 | −0.0226 (0.3678) | −0.0458 0.0379 0.0379 0.0379 | −0.0458 0.0379 0.0379 0.0379 |
|       | Bias(α)   |         |         |         |         |         |         |         |         |         |
| 0.8   | −0.0042 (0.0928) | 0.0880 −0.0043 −0.0032 −0.0032 | −0.0057 (0.0361) | −0.0068 0.0050 0.0050 0.0050 | −0.0068 0.0050 0.0050 0.0050 |
|       | MLOE (×10^6) | 0.3286 (0.9662) | 0.1459 0.3213 0.3221 0.3220 | 0.1051 (0.2078) | 0.0624 0.0758 0.0759 0.0759 | 0.0624 0.0758 0.0759 0.0759 |
|       | MMOM      | 0.0016 (0.0227) | −0.0028 −0.0007 −0.0007 −0.0007 | 0.0017 (0.0227) | −0.0441 −0.0438 −0.0438 −0.0438 |
|       | Estimation time (sec) | 159.3 (28.4) | 70.1 86.5 96.2 112.9 | 235.5 (54.1) | 106.1 120.4 130.9 130.9 |
|       | Bias(σ²)  |         |         |         |         |         |         |         |         |         |
| 1.6   | 0.0133 (0.6292) | 0.1515 −0.0066 0.0158 0.0159 | 0.0163 (0.6546) | −0.3800 0.2236 0.2276 0.2276 | −0.3800 0.2236 0.2276 0.2276 |
|       | Bias(α)   |         |         |         |         |         |         |         |         |         |
| 1.6   | 0.0069 (0.3369) | 0.0843 −0.0013 0.0108 0.0108 | −0.0144 (0.1186) | −0.1033 0.0577 0.0581 0.0581 | −0.1033 0.0577 0.0581 0.0581 |
|       | MLOE (×10^6) | 0.1221 (0.4450) | 0.0044 0.1174 0.1178 0.1178 | 0.0273 (0.0669) | −0.0079 0.0110 0.0109 0.0109 | −0.0079 0.0110 0.0109 0.0109 |
|       | MMOM      | 0.0014 (0.0227) | −0.0044 −0.0033 −0.0033 −0.0033 | 0.0014 (0.0227) | −0.1436 −0.1428 −0.1428 −0.1428 |
|       | Estimation time (sec) | 177.5 (33.9) | 68.7 93.8 96.3 117.1 | 274.3 (74.6) | 62.7 106.7 111.6 111.6 | 62.7 106.7 111.6 111.6 |

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Table 13: Estimation and prediction performances of the exact MLE and TLR approximation estimates for different \textit{opt\_tol} values. Bias(\cdot) means the estimate of the parameter minus its true value, while the estimation time means the computational time of the corresponding estimation. The value of MLOE is multiplied by $10^6$.

| $h_{\text{eff}}$ | Mean (sd) | $\nu = 0.5$ | Optimization tolerance ($\text{opt\_tol}$) | $\nu = 1.0$ | Optimization tolerance ($\text{opt\_tol}$) |
|-----------------|-----------|--------------|------------------------------------------|--------------|------------------------------------------|
|                 |           | MLE          | $10^{-3}$ | $10^{-6}$ | $10^{-9}$ | $10^{-12}$ | MLE          | $10^{-3}$ | $10^{-6}$ | $10^{-9}$ | $10^{-12}$ |
| 0.2             | Bias($\sigma^2$) | $-0.0080$ | 0.3654 | $-0.0079$ | $-0.0079$ | $-0.0079$ | $-0.0085$ | 0.2977 | $-0.0061$ | $-0.0061$ | $-0.0061$ |
|                 | Bias($\alpha$)   | $-0.0006$ | 0.0253 | $-0.0006$ | $-0.0006$ | $-0.0006$ | $-0.0003$ | 0.0073 | $-0.0002$ | $-0.0002$ | $-0.0002$ |
|                 | MLOE ($\times 10^6$) | 3.3945 | (5.9931) | 19.3107 | 3.3756 | 3.3756 | 3.3756 | 1.7378 | (2.7659) | 6.9237 | 1.6938 | 1.6940 | 1.6940 |
|                 | MMOM       | 0.0017 | -0.0016 | 0.0011 | 0.0011 | 0.0011 | 0.0019 | (0.0240) | 0.0019 | $-0.0013$ | $-0.0016$ | $-0.0016$ | $-0.0016$ |
|                 | Estimation time (sec) | 168.1 | (22.3) | 33.8 | 90.4 | 102.2 | 113.0 | 211.0 | (34.0) | 20.7 | 116.3 | 133.3 | 146.9 |
| 0.4             | Bias($\sigma^2$) | $-0.0178$ | 0.0836 | $-0.0172$ | $-0.0172$ | $-0.0172$ | $-0.0207$ | 0.1373 | $-0.0070$ | $-0.0070$ | $-0.0070$ |
|                 | Bias($\alpha$)   | $-0.0026$ | 0.0114 | $-0.0023$ | $-0.0023$ | $-0.0023$ | $-0.0016$ | 0.0072 | $-0.0003$ | $-0.0003$ | $-0.0003$ |
|                 | MLOE ($\times 10^6$) | 0.9790 | (2.0811) | 0.3301 | 0.9682 | 0.9681 | 0.9681 | 0.4034 | (0.6804) | 0.1364 | 0.3659 | 0.3659 | 0.3659 |
|                 | MMOM       | 0.0018 | -0.0009 | 0.0005 | 0.0005 | 0.0005 | 0.0019 | (0.0231) | 0.0019 | $-0.0135$ | $-0.0107$ | $-0.0107$ | $-0.0107$ |
|                 | Estimation time (sec) | 126.8 | (19.5) | 19.8 | 72.4 | 85.6 | 97.8 | 292.1 | (49.2) | 22.4 | 107.5 | 126.4 | 142.2 |
| 0.8             | Bias($\sigma^2$) | $-0.0147$ | 0.2387 | $-0.0033$ | $-0.0033$ | $-0.0033$ | $-0.0226$ | 0.1099 | 0.0379 | 0.0381 | 0.0381 |
|                 | Bias($\alpha$)   | $-0.0042$ | 0.0649 | $-0.0032$ | $-0.0032$ | $-0.0032$ | $-0.0057$ | 0.0156 | 0.0050 | 0.0050 | 0.0050 |
|                 | MLOE ($\times 10^6$) | 0.3286 | (0.9662) | 0.2252 | 0.3221 | 0.3221 | 0.3221 | 0.1051 | (0.2078) | 0.0102 | 0.0758 | 0.0758 | 0.0758 |
|                 | MMOM       | 0.0016 | -0.0018 | $-0.0007$ | $-0.0007$ | $-0.0007$ | 0.0017 | (0.0227) | 0.0017 | $-0.0448$ | $-0.0438$ | $-0.0438$ | $-0.0438$ |
|                 | Estimation time (sec) | 159.3 | (28.4) | 32.3 | 96.2 | 108.6 | 121.3 | 235.5 | (54.1) | 21.4 | 120.4 | 137.1 | 152.3 |
| 1.6             | Bias($\sigma^2$) | 0.0133 | 0.0962 | 0.0158 | 0.0158 | 0.0158 | 0.0163 | 0.3263 | 0.2236 | 0.2234 | 0.2234 |
|                 | Bias($\alpha$)   | 0.0009 | 0.0542 | 0.0108 | 0.0108 | 0.0108 | $-0.0144$ | 0.0896 | 0.0577 | 0.0577 | 0.0577 |
|                 | MLOE ($\times 10^6$) | 0.1221 | (0.4450) | 0.0694 | 0.1178 | 0.1178 | 0.1178 | 0.0273 | (0.0669) | 0.0150 | 0.0110 | 0.0110 | 0.0110 |
|                 | MMOM       | 0.0014 | -0.0038 | $-0.0033$ | $-0.0033$ | $-0.0033$ | 0.0014 | (0.0227) | 0.0014 | $-0.1432$ | $-0.1428$ | $-0.1428$ | $-0.1428$ |
|                 | Estimation time (sec) | 177.5 | (33.9) | 42.0 | 96.3 | 113.2 | 126.8 | 274.3 | (74.6) | 29.4 | 106.7 | 124.1 | 136.2 |
Table 14: Prediction performance and the computational time for Tile Low-Rank approximations with different combinations of $\text{tlr} \_\text{acc}$ and $\text{opt} \_\text{tol}$, where $\nu$ is the smoothness parameter and $h_{\text{eff}}$ is the effective range. The estimation time means the computational time of the corresponding estimation, while value of MLOE is multiplied by $10^6$.

| $h_{\text{eff}}$ | Mean (sd) | $(\text{tlr} \_\text{acc} \_\text{opt} \_\text{tol}), \nu = 0.5$ | $(\text{tlr} \_\text{acc} \_\text{opt} \_\text{tol}), \nu = 1.0$ |
|------------------|-----------|----------------------------------|----------------------------------|
|                  |           | $(10^{-1},10^{-1})$ | $(10^{-1},10^{-6})$ | $(10^{-6},10^{-6})$ | $(10^{-1},10^{-1})$ | $(10^{-1},10^{-6})$ | $(10^{-6},10^{-6})$ | $(10^{-1},10^{-1})$ | $(10^{-1},10^{-6})$ | $(10^{-6},10^{-6})$ |
| **MLOE ($\times 10^6$)** |           |                     |                     |                     |                     |                     |                     |                     |                     |                     |
| 0.2              |           |                     |                     |                     |                     |                     |                     |                     |                     |                     |
| MLOE             | 19.0060   | 19.3107             | 3.3756              | 3.3756              | 7.0268              | 6.9237              | 1.6942              | 1.6938              |                     |                     |
| (13.6484)        | (13.9768) | (5.9476)            | (5.9474)            |                     | (2.8741)            | (2.9270)            | (2.6494)            | (2.6480)            |                     |                     |
| MMOM             | -0.0062   | -0.0061             | 0.0011              | 0.0011              | -0.0106             | -0.0103             | -0.0016             | -0.0016             |                     |                     |
| (0.0232)         | (0.0234)  | (0.0232)            | (0.0232)            |                     | (0.0246)            | (0.0243)            | (0.0240)            | (0.0240)            |                     |                     |
| Estimation       | 28.8      | 33.1                | 76.6                | 88.5                | 19.7                | 20.8                | 108.9               | 117.2               |                     |                     |
| time (sec)       | (11.4)    | (13.3)              | (9.4)               | (13.2)              | (7.0)               | (6.5)               | (16.9)              | (20.0)              |                     |                     |
| 0.4              |           |                     |                     |                     |                     |                     |                     |                     |                     |                     |
| MLOE             | 0.3374    | 0.3301              | 0.9679              | 0.9682              | 0.1348              | 0.1364              | 0.3665              | 0.3659              |                     |                     |
| (1.2055)         | (1.1812)  | (2.0559)            | (2.0581)            |                     | (0.1289)            | (0.1295)            | (0.5937)            | (0.5943)            |                     |                     |
| MMOM             | -0.0011   | -0.0009             | 0.0005              | 0.0005              | -0.0105             | -0.0105             | -0.0107             | -0.0107             |                     |                     |
| (0.0226)         | (0.0225)  | (0.0228)            | (0.0228)            |                     | (0.0221)            | (0.0222)            | (0.0230)            | (0.0230)            |                     |                     |
| Estimation       | 17.8      | 19.7                | 65.1                | 72.6                | 21.0                | 22.5                | 103.3               | 108.1               |                     |                     |
| time (sec)       | (5.2)     | (5.5)               | (13.0)              | (14.2)              | (1.6)               | (2.8)               | (23.6)              | (26.1)              |                     |                     |
| 0.8              |           |                     |                     |                     |                     |                     |                     |                     |                     |                     |
| MLOE             | 0.1703    | 0.2252              | 0.3213              | 0.3221              | 0.0102              | 0.0102              | 0.0624              | 0.0758              |                     |                     |
| (0.3915)         | (0.6756)  | (0.9496)            | (0.9494)            |                     | (0.0070)            | (0.0074)            | (0.1390)            | (0.1427)            |                     |                     |
| MMOM             | -0.0019   | -0.0018             | -0.0007             | -0.0007             | -0.0447             | -0.0448             | -0.0441             | -0.0438             |                     |                     |
| (0.0230)         | (0.0229)  | (0.0227)            | (0.0227)            |                     | (0.0227)            | (0.0226)            | (0.0227)            | (0.0225)            |                     |                     |
| Estimation       | 28.4      | 32.4                | 86.8                | 96.5                | 20.0                | 21.4                | 106.3               | 120.4               |                     |                     |
| time (sec)       | (15.0)    | (16.9)              | (17.8)              | (16.5)              | (5.3)               | (6.4)               | (36.8)              | (33.1)              |                     |                     |
| 1.6              |           |                     |                     |                     |                     |                     |                     |                     |                     |                     |
| MLOE             | 0.0760    | 0.0694              | 0.1174              | 0.1178              | 0.0138              | 0.0150              | 0.0079              | 0.0110              |                     |                     |
| (0.3605)         | (0.3458)  | (0.4307)            | (0.4307)            |                     | (0.0688)            | (0.0708)            | (0.0167)            | (0.0243)            |                     |                     |
| MMOM             | -0.0038   | -0.0038             | -0.0033             | -0.0033             | -0.1436             | -0.1432             | -0.1436             | -0.1428             |                     |                     |
| (0.0227)         | (0.0227)  | (0.0227)            | (0.0227)            |                     | (0.0219)            | (0.0220)            | (0.0222)            | (0.0222)            |                     |                     |
| Estimation       | 36.2      | 41.2                | 92.1                | 95.8                | 19.4                | 29.8                | 63.5                | 108.1               |                     |                     |
| time (sec)       | (16.2)    | (18.2)              | (18.2)              | (20.8)              | (8.8)               | (22.1)              | (27.1)              | (31.3)              |                     |                     |

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