Comparing composite likelihood methods based on pairs for spatial Gaussian random fields

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Abstract

In the last years there has been a growing interest in proposing methods for estimating covariance functions for geostatistical data. Among these, maximum likelihood estimators have nice features when we deal with a Gaussian model. However maximum likelihood becomes impractical when the number of observations is very large. In this work we review some solutions and we contrast them in terms of loss of statistical efficiency and computational burden. Specifically we focus on three types of weighted composite likelihood functions based on pairs and we compare them with the method of covariance tapering. Asymptotics properties of the three estimation methods are derived. We illustrate the effectiveness of the methods through theoretical examples, simulation experiments and by analysing a data set on yearly total precipitation anomalies at weather stations in the United States.

Keywords: Covariance estimation, Geostatistics, Large datasets, Tapering.
# Introduction

The geostatistical approach models data coming from a limited number of monitoring stations as a partial realization from a spatial random field defined on the continuum space. The literature persistently emphasises the importance of the estimation of the covariance function for several reasons. For instance, the best linear unbiased prediction at an unobserved site depends on the knowledge of the covariance function of the process (Cressie, 1993). Since a covariance function must be positive definite, practical estimation generally requires the selection of some parametric classes of covariances and the corresponding estimation of these parameters.

The maximum likelihood method is generally considered the best method for estimating the parameters of covariance models. However, for a Gaussian random field with a given parametric covariance function, exact computation of the likelihood requires calculation of the inverse and determinant of the covariance matrix, and this evaluation is slow when the number of observations is large.

More precisely, let \( \{Z(s), s \in \mathbb{R}^d\} \) be a stationary Gaussian random field with zero mean and covariance function

\[
\text{cov}(Z(s), Z(s')) = \sigma^2 \rho(s - s'; \phi), \quad s, s' \in \mathbb{R}^d, \quad \sigma^2 > 0, \quad \phi \in \Phi \subset \mathbb{R}^p.
\]

The unknown parameters \( \theta = (\sigma^2, \phi)^\top \) must be estimated on the basis of a finite number of \( n \) observations \( Z = (Z(s_1), \ldots, Z(s_n))^\top \).

The log-likelihood function for a the Gaussian random field can be written as

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

where \( \Sigma(\theta)_{ij} = \sigma^2 \rho(s_i - s_j; \phi) \).

The most critical part when evaluating (1) is to evaluate the determinant and inverse of \( \Sigma(\theta) \). This evaluation could be theoretically carried out in \( O(n^{2.81}) \) steps (see, e.g., Aho et al. (1974)), although the most widely used algorithms such as Cholesky decomposition require up to \( O(n^3) \) steps. This can be prohibitive if \( n \) is large. This motivated to look for either approximations to the likelihood function or different minimum-contrast-type methods that require less than \( O(n^3) \) steps to evaluate (Whittle 1954; Vecchia 1988; Curriero and Lele 1999; Stein et al. 2004; Cressie and Johannesson 2008; Stein 2008; Lindgren et al. 2011).
Significant computational gain is achieved when the sampling locations form a regular lattice. In this case, the covariance matrix has a special structure (Whittle, 1954) that can be exploited by using spectral methods, reducing the computational burden. For irregularly spaced data, Fuentes (2007) extended the Whittle’s idea and suggested to integrate the spatial process over grid cells, obtaining an approximation to the likelihood on a lattice structure. The method requires $O(n \log_2 n)$ operations and does not involve calculating determinants.

Rue and Tjelmeland (2002) approximated the inverse of covariance matrix to be the precision matrix of a Gaussian Markov random field wrapped on a torus. In this case the numerical factorization of the precision matrix can be done at a cost of $O(n^{3/2})$ for a two-dimensional Gaussian Markov random field. Recently Lindgren et al. (2011) exploited the representations of certain Gaussian random fields with Matérn covariance structure by the solution of a stochastic partial differential equation and derived an approximation based on a Markov Gaussian random field with sparse precision matrix. The main drawback of this approach is that we can only find the explicit form for those Gaussian random fields that have a Matérn covariance structure at certain degree of smoothness (see the discussion to Lindgren et al., 2011).

Another idea (Banerjee et al., 2008; Cressie and Johannesson, 2008; Stein, 2008) is putting a low rank structure on the covariance matrix, namely

$$\Sigma(\theta) = SK(\theta_0)S^T + \theta_1V$$

where $S$ is a known $n \times r$ matrix, $K(\theta_0)$ a $r \times r$ positive definite matrix depending on the unknown parameter $\theta_0$, $V$ a known diagonal matrix, $\theta_1 \geq 0$ an unknown scalar, and $\theta = (\theta_0, \theta_1)$. This allows to calculate the inverse and the determinant of a large covariance by inverting and calculating the determinant of a matrix of lower dimension ($r \ll n$) according to the Woodbury formula (see, Cressie and Johannesson, 2008, for instance).

All these methods have their relative strengths but they can lead to making unnatural assumptions about the random fields giving a less appropriate model. Instead in the sequel we will concentrate on two estimation methods that preserve the starting model, and, with some adjustments, allow us to perform standard inference as in the case of classical likelihood estimation.
In the tapering approach (Kaufman et al., 2008) certain elements of the covariance matrix that correspond to pairs with large distance are set to zero. This is done, see Section 2, in a way to preserve the property of positive definiteness in the resulting ‘tapered’ matrix. Then sparse matrix algorithms can be used to evaluate efficiently an approximate likelihood where the original covariance has been replaced by the ‘tapered’ matrix. The intuition behind this approach is that correlations between pairs of distant sampling locations are often nearly zero, so little information is lost in taking them to be independent.

With composite likelihood (CL) we will indicate a general class of estimating functions based on the likelihood of marginal or conditional events (Lindsay (1988), Varin et al. (2011)). This kind of estimation method can be helpful when it is difficult to evaluate or to specify the full likelihood. In our case the evaluation of the likelihood of the whole set of the observations is too expensive and composing likelihoods with a smaller number of observations is computationally appealing.

Different types of CL functions have been proposed in literature for estimating the covariance model of spatial and spatio-temporal Gaussian random fields. For instance Stein et al. (2004) proposed a CL based on conditional events improving a previous proposal of Vecchia (1988). More recently, Bevilacqua et al. (2012) considered a weighted CL based on difference of Gaussian pairs in the space time context and Eidsvik et al. (2013) developed a pairwise Gaussian block composite likelihood in the same vein of Caragea and Smith (2006).

As outlined in Lindsay et al. (2011), for a given estimation problem the choice of a suitable CL function should be driven by statistical and computational considerations. In particular, for Gaussian random fields, there is a clear computational advantage when we consider only CL based on pairs of observations.

Therefore in this paper we contrast CL functions based on the marginal distribution of a pair or the distribution of an observation conditionally to another observation or the distribution of the difference between two observations. Since the three CL functions are equivalent from computational point of view, the main purpose of the paper is to compare them from statistical efficiency point of view. Moreover we establish the asymptotic properties of the associated estimators. Lastly we argue that the CL approach based on pairs
is a valuable competitor of the tapering approach with respect to the efficiency when the computational burden is heavy. This is done through theoretical examples and simulations.

The paper is organized as follows. In Section 2 we present in more detail the tapering method while Section 3 describes the three CL estimating methods based on Gaussian pairs. In Section 4 we compare the methods described in Section 2 and 3 through theoretical examples and numerical results. As a real data example, in Section 5 we apply CL and tapering methods on a real data set of yearly total precipitation anomalies already analyzed in Kaufman et al. (2008). Finally, in Section 6 we give some conclusions.

2 Tapered likelihood

In the tapering approach, pioneered by Kaufman et al. (2008), certain elements of the covariance matrix $\Sigma(\theta)$ are set to zero multiplying $\Sigma(\theta)$ element by element by a correlation matrix coming from a compactly supported isotropic correlation function. More precisely, we consider a correlation function $r(s - s'; d)$ that is identically 0 whenever $\|s - s'\| \geq d > 0$. The ‘tapered’ matrix $\Sigma_T(\theta) = \Sigma(\theta) \circ R(d)$, where $[R(d)]_{ij} = r(s_i - s_j; d)$ and $\circ$ is the Schur product, is still positive definite and sparse matrix algorithms can be used to evaluate an approximated log-likelihood efficiently (Furrer and Sain, 2010). There are several ways to construct compactly supported correlation function (Gneiting, 2002) and an example that we consider in the sequel is given by a specific type of Wendland function

$$r(h; d) = \left(1 - \frac{\|h\|_d}{d}\right)^4 \left(1 + 4 \frac{\|h\|_d}{d}\right)$$

with $(a)_+ = \max\{0, a\}$. Our choice is supported by the asymptotic results in Kaufman et al. (2008) and Du et al. (2009).

Kaufman et al. (2008) proposed two approximations of the log-likelihood (1), namely

$$l_{T,1}(\theta, d) = -\frac{1}{2} \log |\Sigma_T(\theta)| - \frac{1}{2} Z^\top [\Sigma_T(\theta)]^{-1} Z,$$

and

$$l_T(\theta, d) = -\frac{1}{2} \log |\Sigma_T(\theta)| - \frac{1}{2} Z^\top ([\Sigma_T(\theta)]^{-1} \circ R(d)) Z.$$

In (3) the covariance matrix $\Sigma(\theta)$ is tapered, instead in (4) the $\Sigma(\theta)$ as well as the empirical covariance matrix $ZZ^\top$ are tapered. So the first approximation is computationally more
efficient nevertheless the derivative of \( (4) \) leads to an unbiased estimating equation. For this reason the recent literature (Shaby and Ruppert, 2012; Stein, 2013) has been focused on \( (4) \).

Shaby and Ruppert (2012) show that, under increasing domain asymptotics (Cressie, 1993), the maximizer of \( (4) \) has asymptotic Gaussian distribution and the asymptotic variance is given by the inverse of the Godambe information matrix

\[
G_T(\theta, d) = H_T(\theta, d) J_T(\theta, d)^{-1} H_T(\theta, d)^T, \tag{5}
\]

where

\[
H_T(\theta, d) = -E[\nabla^2 l_T(\theta, d)], \quad J_T(\theta, d) = E[\nabla l_T(\theta, d) \nabla l_T(\theta, d)^T]. \tag{6}
\]

The generic entries of the \( H_T(\theta, d) \) and \( J_T(\theta, d) \) matrices are respectively:

\[
[H_T(\theta, d)]_{ij} = \frac{1}{2} \text{tr} \left\{ B_i \left( \frac{\partial \Sigma(\theta)}{\partial \theta_j} \circ R(d) \right) \right\}
\]

\[
[J_T(\theta, d)]_{ij} = \frac{1}{2} \text{tr} \left\{ [B_i \circ R(d)] \Sigma(\theta) [B_j \circ R(d)] \Sigma(\theta) \right\}
\]

where

\[
B_i = [\Sigma_T(\theta)]^{-1} \left( \frac{\partial \Sigma(\theta)}{\partial \theta_i} \circ R(d) \right) [\Sigma_T(\theta)]^{-1}.
\]

Note that \( \lim_{d \to \infty} l_T^2(\theta, d) = l(\theta) \), that is when increasing the taper range an improvement of the statistical efficiency is expected. At the limit the asymptotic variance is given by the Fisher information matrix (Mardia and Marshall, 1984)) whose generic entries are:

\[
[I_{ML}(\theta)]_{ij} = \frac{1}{2} \text{tr} \left( [\Sigma(\theta)]^{-1} \frac{d \Sigma}{d \theta_i} [\Sigma(\theta)]^{-1} \frac{d \Sigma}{d \theta_j} \right). \tag{7}
\]

### 3 Composite likelihood estimation based on pairs

Let \( A_k \) be a marginal or conditional set of the data, the composite likelihood (CL) (Lindsay, 1988) is an objective function defined as a product of \( K \) sub-likelihoods

\[
CL(\theta) = \prod_{k=1}^{K} L(\theta; A_k)^{w_k}, \tag{8}
\]

where \( L(\theta; A_k) \) is the likelihood generated from \( f(z; \theta) \) by considering only the random variables in \( A_k \) and \( w_k \) are suitable non negative weights that do not depend on \( \theta \). The maximum CL estimate is given by \( \hat{\theta} = \text{argmax}_\theta CL(\theta) \).
The choice of which and how many factors in (8) can be related to the computational and statistical efficiency (Lindsay et al., 2011). Setting $A_k = (Z(s_i), Z(s_j))$, we obtain the pairwise marginal Gaussian likelihood $L_{ij}$. If we let $A_k = (Z(s_i)|Z(s_j))$ we obtain the pairwise conditional Gaussian likelihood $L_{ij|j}$ and finally setting $A_k = (Z(s_i) - Z(s_j))$ we obtain the pairwise difference Gaussian likelihood $L_{i-j}$. The computational cost for considering all possible pairs is of order $O(n^2)$ while it is of order $O(n^3)$ in considering all possible three-wise i.e. the same order of the evaluation of the likelihood for Gaussian random fields. Thus from a computational point of view only the pairwise CL is opportune.

The expression for the logarithm of the sub-likelihoods are

$$l_{ij}(\theta) = \frac{1}{2} \left\{ 2 \log \sigma^2 + \log(1 - \rho_{ij}^2) + \frac{B_{ij}}{\sigma^2(1 - \rho_{ij}^2)} \right\}$$

(9)

$$l_{ij}(\theta) = \frac{1}{2} \left\{ \log \sigma^2 + \log(1 - \rho_{ij}^2) + \frac{G_{ij}}{\sigma^2(1 - \rho_{ij}^2)} \right\}$$

(10)

$$l_{i-j}(\theta) = \frac{1}{2} \left\{ \log \sigma^2 + \log(1 - \rho_{ij}) + \frac{U_{ij}^2}{2\sigma^2(1 - \rho_{ij})} \right\}$$

(11)

where $\rho_{ij} = \rho(s_i - s_j; \phi)$, $B_{ij} = Z(s_i)^2 + Z(s_j)^2 - 2\rho_{ij}Z(s_i)Z(s_j)$, $G_{ij} = Z(s_i) - 2\rho_{ij}Z(s_j)$, $U_{ij} = Z(s_i) - Z(s_j)$. The corresponding weighted composite log-likelihoods are:

$$pl_M(\theta) = \sum_{i=1}^{n} \sum_{j>i}^{n} l_{ij}(\theta)w_{ij},$$

(12)

$$pl_C(\theta) = \sum_{i=1}^{n} \sum_{j\neq i}^{n} l_{ij}(\theta)w_{ij} - \sum_{i=1}^{n} \sum_{j>i}^{n} (2l_{ij}(\theta) - l_i(\sigma^2) - l_j(\sigma^2))w_{ij},$$

(13)

$$pl_D(\theta) = \sum_{i=1}^{n} \sum_{j>i}^{n} l_{i-j}(\theta)w_{ij},$$

(14)

where

$$l_i(\sigma^2) = -\frac{\log \sigma^2}{2} - \frac{Z(s_i)^2}{2\sigma^2}$$

is the likelihood of one observation. Here we assume that the weights are symmetric, i.e. $w_{ij} = w_{ji}$. Note that if the marginal parameter $\sigma^2$ is known, then marginal and the conditional pairwise likelihood have the same efficiency. Otherwise it is not obvious which kind of estimation is more efficient.

A distinctive feature of $pl_a$, $a = C, D, M$, is that the associated estimating function, $\nabla cl_a(\theta)$, is unbiased, irrespective of the distributional assumptions on the pairs. In Appendix A we will show that the maximum composite likelihood estimators are consistent.
and asymptotically normal. Note that the above results have been derived in a more
general settings than those in Bevilacqua et al. (2012) for strictly increasing sequence on
evenly-spaced lattices. In contrast here we do not impose any particular restrictions on
the geometry and growth behavior of the lattice, allowing unevenly spaced locations. This
framework is more suited for real data analysis.

Under these results, again the inverse of the Godambe information matrix

\[ G_a(\theta) = H_a(\theta) J_a(\theta)^{-1} H_a(\theta)^\top, \quad a = C, D, M \]  

(15)

where

\[ H_a(\theta) = -E[\nabla^2 p_{la}(\theta)], \quad J_a(\theta) = E[\nabla p_{la}(\theta) \nabla p_{la}(\theta)^\top] \]  

(16)

is an approximation of the asymptotic variance of the CL estimator. In the Appendix B
we can find closed form expressions for the Godambe information.

The role of the weights in CL function is to save computational time and improve
the statistical efficiency. In principle we can derive them using the theory on the optimal
estimating functions (Heyde, 1997). Another possible strategy is to consider different weight
functions for different estimating equations coming from the CL function. Bevilacqua et al.
(2012) showed that this kind of weights can improve the statistical efficiency of the method.
A cut-off weight function namely \( w_{ij}(d) = 1 \) if \( \|s_i - s_j\| \leq d \), and 0 otherwise, has evident
computational advantages with respect to a smooth one. Moreover it can improve the
efficiency as it has been shown in Joe and Lee (2009), Davis and Yau (2011) and Bevilacqua
et al. (2012). The intuition behind this approach is that the correlations between pairs of
distant sampling locations are often nearly zero. Therefore the use of the whole pairs may
lose efficiency since too many redundant pairs of observations can skew the information
confined in pairs of near observations. Hereafter we use \( p_{la}(\theta, d) \) to denote CL function
based on pairs using simple cut-off weight function and \( G_a(\theta, d) \) the associated Godambe
information matrix.

4 Numerical examples

We have considered four models:
1. the exponential covariance function

\[ C(h; \theta) = \sigma^2 \exp(-3\|h\|/\phi) \]  \hspace{1cm} (17)

2. the Cauchy covariance function

\[ C(h; \theta) = \frac{\sigma^2}{1 + (\sqrt{19}\|h\|/\phi)^2} \]  \hspace{1cm} (18)

3. the spherical covariance function

\[ C(h; \theta) = \begin{cases} 
\sigma^2(1 - 1.5(\|h\|/\phi) + 0.5(\|h\|/\phi)^3) & \text{if } \|h\| < \phi \\
0 & \text{otherwise} 
\end{cases} \]  \hspace{1cm} (19)

4. the wave or cardinal sine covariance function

\[ C(h; \theta) = \sigma^2(20.371 \|h\|/\phi)^{-1} \sin(20.371 \|h\|/\phi) \]  \hspace{1cm} (20)

The covariance models (17), (18) and (20) are parametrized in terms of practical range that is the correlation is lower than 0.05 when \( \|h\| \geq \phi \). The aforementioned models cover a wide spectrum of situations that can arise in geostatistics. The first model probably is the most commonly used model in geostatistics and it is a special case of the Matérn model when \( \nu = 1/2 \). Model (18) is polynomially decreasing and hence more suitable than the exponential model for modeling of a slowly decaying covariance. Model (19) is an example of compactly supported covariance function, i.e. \( C(h; \theta) = 0 \) for \( \|h\| > \phi \). In principle if the taper range \( d \) is greater than \( \phi \) taper is not necessary. Model (20) allows for negative correlations (see Figure 1).

For the data locations we use the same setup as in Kaufman et al. (2008). We have considered a regular grid with increments 0.03 over \( W_k \) where \( W_k = [0, 2^{k/2}] \times [0, 2^{k/2}] \), \( k = 0, \ldots, 5 \). The grid points have been perturbed adding a uniform random value on \([-0.01, 0.01]\) to each coordinates and, finally, we have randomly chosen \( n_k = 500 \cdot 2^k \) points without replacement.

First of all we compare the computational time required for one evaluation of the likelihood (1), the tapered likelihood (4), the weighted marginal pairwise likelihood (12) and its unweighted version using the exponential covariance function, with \( \phi = 0.4 \). As taper we
Figure 1: (a) Covariance functions with equivalent practical range, where $\sigma^2 = 1$, $\phi = 0.4$, (b) the tapered covariance functions using (2), with $d = \phi$

consider the Wendland function (2). As taper range and cut-off distance for the weighted composite likelihood estimator we have set $d = \phi$, i.e. the practical range. Figure 1 illustrates the behaviour of the tapered correlation functions.

Table 1 depicts the saving in terms of computational burden for large datasets for the marginal pairwise likelihood estimates (all calculations were carried out on a 2.27 GHz processor with 6 GB of memory). In particular, the saving is quite remarkable when we consider the weighted version of the marginal pairwise likelihood. Increasing $k$ and consequently the number $n$ of observations, the fraction of nonzero elements in the resulting tapered covariance matrix decreases (see the last column of Table 1). Note also that for large taper range, i.e. small $n$, the overhead required for the sparse matrix overwhelms the expected computational advantages of the tapering estimator.

Now we compare the asymptotic relative efficiency of the estimates $\hat{\sigma}^2$ and $\hat{\phi}$ for the covariance models (17), (18), (19) and (20). As overall measure we consider:

$$ARE_{a}(d) = \left( \frac{|G_{a}(\theta; d)|}{|I_{ML}(\theta)|} \right)^{1/p}, \quad a = C, D, M, T$$

(21)

where $I_{ML}(\theta)$ is the Fisher information matrix (7) and $p = 2$ is the number of unknown components in $\theta$. We have considered the case $k = 0$ that is 500 locations sites over $[0, 1] \times [0, 1]$, $\phi = 0.4$ and several increasing values of the taper range $d$, corresponding to increasing values of the percentage of non zero values in the tapered covariance matrix. Specifically we consider the sequence 0.01, 0.02, . . . , 0.2 of percentages of non zero values. The reason for considering this sequence is that, as outlined in Stein et al. (2013), the
Table 1: Time in seconds when evaluating ML, $TAP(d)$, $PL_M$ and $PL_M(d)$ functions increasing the spatial domain of observation and the associated percentages of non zero values in the tapered matrix.

| $n$  | ML  | $TAP(d)$ | $PL_M$ | $PL_M(d)$ | %    |
|------|-----|----------|--------|-----------|------|
| 500  | 0.38 | 0.34     | 0.03   | 0.00      | 0.33 |
| 1000 | 0.95 | 1.27     | 0.11   | 0.03      | 0.19 |
| 2000 | 3.21 | 4.77     | 0.40   | 0.05      | 0.11 |
| 4000 | 17.58| 23.38    | 1.63   | 0.12      | 0.06 |
| 8000 | 129.83| 120.02  | 6.53   | 0.29      | 0.03 |
| 16000| 2388.16| 789.69  | 26.82  | 0.78      | 0.01 |

tapered covariance matrix must be very sparse to help a great deal with calculating the log determinant of the covariance matrix.

In Figure 2 we depict the measure (21) as a function of the considered percentages of non zero values. As general remark for the taper method, the asymptotic relative efficiency is a monotonic increasing function of the percentages of non zero values as expected.

Moreover, for these examples, there is no practical difference in considering marginal and conditional likelihood estimates, so that a preference should be given to the first one because requires less computation. On the other hand, for small percentages of non zero values, where the maximum tapered likelihood estimates takes advantage from the sparsity of the covariance matrix, the maximum marginal and conditional pairwise likelihood estimates outperform the maximum tapered likelihood and the maximum difference pairwise likelihood estimates.

Note also that asymptotic efficiency of the maximum CL estimates is not a increasing function of the distance considered in the weight function with the exception of the wave model. These examples suggest that a proper choice of the distance $d$ can improve significantly the statistical efficiency of maximum CL estimates under specific models. Our findings add more evidence to previous results reported in the literature [Joe and Lee, 2009; Davis and Yau, 2011; Bevilacqua et al., 2012]. Moreover such distance, i.e. the number of pairs, in the marginal and conditional pairwise CL should be different with respect to the
Figure 2: ARE of the $TAP(d)$, and $PL_a(d), a = C, M, D$ estimators with respect of the percentage
distance of the difference CL. For instance in the exponential model the ‘good’ distance for the marginal and conditional pairwise CL is approximately 0.06 while for difference CL is 0.165.

Looking at the behaviour for the different models, we see that the the maximum tapered likelihood estimate performs reasonably well under the exponential and the Cauchy model, but requires a large taper range for outperforming the maximum pairwise likelihood estimates, vanishing the computational advantage of the sparsity of the covariance matrix. Note that for the spherical and wave models the maximum tapered likelihood estimate perform worse than the CL methods bases on pairs at least for the sequence of percentages of the tapered matrix considered.

Finally we simulate 1000 random samples drawn from a Gaussian random fields under the same setting, to compare numerically the performance of CL methods based on pairs and tapering method with respect to ML one. All the estimates have been carried out using the R package CompRandFld (Padoan and Bevilacqua 2012), avaible on CRAN (http://cran.r-project.org/). In that package all the estimation methods described here are fully implemented both in the spatial and spatio temporal case. In particular the covariance tapering methods use the collection of R/Fortran functions for sparse matrix algebra provided by the package spam (Furrer and Sain 2010).

In the maximizing the objective functions for the spherical models, we have found some numerical difficulties. In such case (Mardia and Watkins 1989) reported that the log-likelihood may be multimodal for sample of finite size. An example of these is given in Figure 3 where we plot the profile functions with respect to $\phi$, obtained in a simulation where the optimization procedure failed.

Note that the marginal pairwise likelihood is unimodal with a well-identified maximum value. This is an example where, as outlined by Varin et al. (2011), the composite likelihood surface can be much smoother than the full joint likelihood, and thus easier to maximize. The tapering approach outperforms the CL methods (see Figure 4) in the case of exponential and Cauchy model, but shows the same performances for the other models. Note also that the CL functions based on the differences yield to estimates with large variability.
Figure 3: Profile log functions with respect to $\phi$ for the likelihood, tapering and CL based on pairs functions for a particular simulation from a spherical model. In the plots vertical solid lines correspond to the true value and dashed lines are located to the maxima.
Figure 4: Boxplots of the estimates [(a) \( \phi \), (b) \( \sigma^2 \)]. From the top, each row refers to the exponential, Cauchy, spherical and wave covariance model, respectively. In the boxplots the dashed lines represent the true values.
Figure 5: Yearly total precipitation anomalies registered at 7,352 USA weather stations in 1962.

5 A real data example

As data example we consider the data-set in [Kaufman et al. (2008)] that can be retrieved from [www.image.ucar.edu/Data/precip_tapering/]. We consider yearly total precipitation anomalies registered at 7,352 location sites in the USA from 1895 to 1997 (see Figure 5). The yearly totals have been standardized by the long-run mean and standard deviation for each station from 1962. The data-set can be considered of medium size allowing ML estimation although it is very slow to compute.

[Kaufman et al. (2008)] adapted a zero mean Gaussian random field with an exponential covariance model using the maximum likelihood and the tapering method. Here we choose an exponential covariance model plus a nugget effect, i.e.

\[
C(h; \theta) = \tau^2 I(||h|| = 0) + \sigma^2 \exp \left\{-\frac{||h||}{\phi}\right\},
\]

as suggested by inspecting the empirical variogram (Figure 6).
The parameter $\theta = (\tau^2, \sigma^2, \phi)'$ is estimated with maximum likelihood, tapering and $pl_a(\theta; d), a = C, D, M$ methods. The distance between two sites are measured using the great-circle distance and the exponential function is still positive definite for this distance (Huang et al., 2011). As taper function we use the Wendland function where the taper range is fixed to $d = 112.654$ Km, the same value as in Kaufman et al. (2008). Moreover we use the same distance in $pl_a(\theta; d), a = C, D, M$.

Table 2 reports the estimates of maximum likelihood, tapering and $pl_a(\theta; d), a = C, D, M$ methods and the associate standard errors. For maximum likelihood and tapering methods standard errors are computed using the inverse of the Fisher and Godambe information matrices in (7) and (5). The evaluations of the plug-in estimates for $H_a$ and $J_a$ for the CL methods are of order $O(n^2)$ and $O(n^4)$ respectively, and the evaluation of $J_a$ become computationally unfeasible for large data-sets. For this we exploit the spatial subsambling techniques as explained in Bevilacqua et al. (2012). The results confirm the superiority of the tapering techniques in terms of efficiency, however $pl_a(\theta; d), a = C, M$ are good competitors in terms of fitting (see Figure 6).

|       | $ML$  | $TAP(d)$ | $PL_C(d)$ | $PL_M(d)$ | $PL_D(d)$ |
|-------|-------|----------|-----------|-----------|-----------|
| $\tau^2$ | 0.1033 | 0.0586   | 0.1069    | 0.1070    | 0.06019   |
|       | (0.0042) | (0.0088) | (0.0026)  | (0.0033)  | (0.0083)  |
| $a$  | 168.1174 | 119.0561 | 186.2457  | 185.7594  | 62.25251  |
|       | (12.2329) | (9.4117) | (17.3979) | (19.0835) | (13.7225) |
| $\sigma^2$ | 0.6693 | 0.7464   | 0.5890    | 0.5866    | 0.35391   |
|       | (0.0632) | (0.0447) | (0.0182)  | (0.0359)  | (0.0295)  |

Table 2: $ML$, $TAP(d)$ and $PL_a(d), a = C, M, D$ estimates for the exponential covariance model with nugget effect (estimated standard errors are reported between parentheses).

Next, we compare the prediction performance. Assuming that $Z$ is a Gaussian random field, let $f_i$ the conditional density of $Z(s_i)$ given all observations except $Z(s_i)$, i.e.

$$f_i(z) = \sqrt{2\pi\nu_i^2} \exp \left\{-\frac{1}{2} \frac{(z - \hat{Z}_{-i}(s_i))^2}{\nu^2_i}\right\}$$
Figure 6: Empirical variogram and theoretical ones, estimated according to different estimation methods.

where $\hat{Z}_{-i}(s_i)$ and $\nu^2_{-i}$ are the conditional expectation and variance. In calculating these last quantities for large dataset, we make use of the formula in Zhang and Wang (2010).

We have considered three predictive scores (Gneiting and Raftery, 2007), namely

1. the root-mean-square error (RMSE)

$$\text{RMSE} = \left[ n^{-1} \sum_{i=1}^{n} \{Z(s_i) - \hat{Z}_{-i}(s_i)\}^2 \right]^{1/2}$$

2. the logarithmic score (LSCORE)

$$\text{LSCORE} = -n^{-1} \sum_{i=1}^{n} \log f_i(Z(s_i))$$
Table 3: Prediction performance in terms of MSPE for exponential covariance model with and without nugget effect estimated with $ML$, $TAP(d)$ and $PL_a(d), a = C, M, D$ methods.

| Model                      | $ML$   | $TAP(d)$ | $PL_C(d)$ | $PL_M(d)$ | $PL_D(d)$ |
|----------------------------|--------|----------|-----------|-----------|-----------|
| Exponential with nugget    | 0.2178264 | 0.2208672 | 0.2177944 | 0.2177954 | 0.2196979 |
| Exponential without nugget | 0.2293623 | 0.2292307 | 0.2312318 | 0.2312022 | 0.231374  |

Table 4: Prediction performance in terms of LSCORE for exponential covariance model with and without nugget effect estimated with $ML$, $TAP(d)$ and $PL_a(d), a = C, M, D$ methods.

| Model                      | $ML$   | $TAP(d)$ | $PL_C(d)$ | $PL_M(d)$ | $PL_D(d)$ |
|----------------------------|--------|----------|-----------|-----------|-----------|
| Exponential with nugget    | 0.6380736 | 0.6404574 | 0.6422388 | 0.6422617 | 0.6432923 |
| Exponential without nugget | 0.6773373 | 0.6697904 | 0.8676976 | 0.8686335 | 0.696967  |

3. the continuous ranked probability score (CRPS)

$$CRPS = n^{-1} \sum_{i=1}^{n} \int_{-\infty}^{\infty} [F_i(z) - I_{(\infty,z]}(Z(s_i))]^2 dz$$

where $F_i(z)$ is the conditional cumulative distribution function of $Z(s_i)$

In Table 3, 4 and 5 we report RMSE, LSCORE and CRPS for the exponential model and we contrast them with an exponential model without nugget effect, as proposed by Kaufman et al. (2008). Our findings highlight how we have an effective improvement when we consider an additional nugget effect. Moreover $pl_a(\theta; d), a = C, M$ estimates provides comparable results with respect to the tapering method.

6 Concluding remarks

The class of CL functions is very large and for a given estimation problem it is not clear how to choose in this class. In the Gaussian case, if the choice of the CL is driven by computational concerns then the CL based on pairs have clear computational advantages with respect to other type of CL.
Table 5: Prediction performance in terms of CRPS for exponential covariance model with and without nugget effect estimated with $ML$, $TAP(d)$ and $PL_a(d), a = C, M, D$ methods.

In this paper through theoretical and numerical examples we have compared three methods of weighted CL based on pairs (marginal, conditional and difference), using the covariance tapering method as benchmark.

One advantage of the covariance tapering method is that it is possible to control the trade-off between the statistical and computationally efficiency with the taper range while this is not the case for CL based on pairs as explained in the theoretical examples. The choice of the distance in the weight function for the CL based on pairs should be driven by some optimality criterion. Bevilacqua et al. (2012) for instance proposed a method based on the minimization of the trace of the Godambe information matrix. Nevertheless this method could be computationally hard in particular for large data-set.

The theoretical and numerical examples highlights a slightly better performance of the weighted conditional and marginal CL with respect to weighted difference CL. Moreover the weighted marginal CL are computationally preferable with respect to the tapering method while the tapering method shows better statistical efficiency when increasing the taper range. Our suggestion for the practitioners is to consider both the methods when it is computationally feasible, as in the real data example proposed. For data sets of large dimension CL based on pairs is preferable since in general a little loss of statistical efficiency is offset by good computational performances. Our findings are consistent with those of Stein (2013) who compares the covariance tapering with a specific type of composite likelihood based on independent blocks.
Appendix A

Asymptotic results can be been proved for spatial processes which are observed at finitely many locations in the sampling region. In this case we deal with an increasing domain setup where the sampling region is unbounded.

We consider a weakly dependent random field \( \{Z(s), s \in S\} \), defined over an arbitrary lattice \( S \) in \( \mathbb{R}^d \) that is not necessarily regular. The lattice \( S \) is equipped with the metric \( \delta(s_k, s_l) = \max_{1 \leq l \leq d} |s_{i,l} - s_{j,l}| \) and the distance between any subsets \( A, B \subset S \) is defined as \( \delta(A, B) = \inf \{\delta(s_k, s_l) : s_k \in A \text{ and } s_l \in B\} \). We denote

\[
\alpha(U, V) = \sup_{A, B} \{ |P(A \cap B) - P(A)P(B)| : A \in \mathcal{F}(U), B \in \mathcal{F}(V) \},
\]

where \( \mathcal{F}(E) \) is the \( \sigma \)-algebra generated by the random variables \( \{Z(s), s \in E\} \). The \( \alpha \)-mixing coefficient [Doukhan 1994] for the random field \( \{Z(s), s \in S\} \) is defined as

\[
\alpha(a, b, m) = \sup_{U, V} \{\alpha(U, V), |U| < a, |V| < b, \delta(U, V) \geq m\}.\]

We make the following assumptions:

C1: \( S \) is infinite, locally finite: for all \( s \in S \) and \( r > 0 \), \( |B(s, r) \cap S| = O(r^d) \), with \( B(s, r) \)
\( d \)-dimensional ball of center \( s \) and radius \( r \); \( D_n = \{s_1, \ldots, s_n\}, n \geq 1 \), is a sequence of arbitrary subsets of \( S \) such that \( d_n = |D_n| \to \infty \) as \( n \to \infty \);

C2: \( Z \) is a Gaussian random field with covariance function \( C(h; \theta) \). It is also \( \alpha \)-mixing with mixing coefficient \( \alpha(m) = \alpha(\infty, \infty, m) \) satisfying:

\( \alpha(m) = \alpha(\infty, \infty, m) \) satisfying:

\[
(C2a) \quad \exists \eta > 0 \text{ s.t. } \sum_{s_k, s_l \in D_n} \alpha(\delta(s_k, s_l)) \frac{7}{27^\eta} = O(d_n),
\]

\[
(C2b) \quad \sum_{m \geq 0} m^{d-1} \alpha(m) < \infty;
\]

C3: \( \theta^* \), the true unknown value of the parameter, is an interior point of a compact set \( \Theta \) of \( \mathbb{R}^p \);

C4: the function \( \theta \mapsto C(h; \theta) \) has continuous second order partial derivatives with respect to \( \theta \in \Theta \), and these functions are continuous with respect to \( h \) and \( \inf_{\theta \in \Theta} C(h; \theta) > 0 \);
C5: the composite likelihood estimator is given by

\[ \hat{\theta}_n = \arg\min_{\theta \in \Theta} Q_n(\theta), \]

where

\[ Q_n(\theta) = \frac{1}{d^d} \sum_{k \in D_n} g_k(Y(k); \theta), \quad \theta \in \Theta, \]

with \( Y(k) = (Z(s), s \in V_k)' \) and \(|V_k| \leq B\) for all \( k \in S\);

C6: the function \( g_k(Y(k); \theta) \) is defined as

\[ g_k(Y(k); \theta) = -\frac{1}{2} \sum_{l \in V_k, l \neq k} l_{(k,l)}(\theta) \]

where \( l_{(k,l)} = l_{kl}, l_{k|l}, l_{k-l} \). The functions \( l_{(k,l)} \) are defined as in (9), (10) and (11);

C7: the function \( \overline{Q}_n(\theta) = E_{\theta^*}[Q_n(\theta)] \) has a unique global minimum over \( \Theta \) at \( \theta^* \).

Remarks

1. The assumption C[2] is satisfied for a stationary Gaussian random field on regular lattice with correlation function \( C(h; \theta) = O(||h||)^{-c} \), for some \( c > d \) and its spectral density bounded below (Doukhan, 1994, Corollary 2, p. 59).

2. The assumption C[7] is an identifiability condition. For each \( s \), the function \( E_{\theta^*}[g_s(Y_s; \theta)] \) has a global minimum at \( \theta^* \) according the Kullback-Leibler inequality but in the multidimensional case \( (p > 1) \) \( \theta^* \) fails, in general, to be the unique minimizer.

3. The assumption C[5] is satisfied if we suppose a cut-off weight function for \( w_{kl} \).

4. Any individual log-likelihood \( l_{(i,j)} \) can be written as

\[ l_{(k,l)} = c_1(\theta, k - l) + c_2(\theta, k - l)Z_k^2 + c_3(\theta, k - l)Z_k^2 + c_4(\theta, k - l)Z_kZ_l, \]

where the functions \( c_i, i = 1, \ldots, 4 \) are \( C^2 \) functions with respect to \( \theta \).

Consistency

Given the previous assumptions C1-C[7], \( \hat{\theta}_n \) is a consistent estimator for \( \theta_0 \) provided that \( \sup_{\theta \in \Theta} |Q_n(\theta) - \overline{Q}_n(\theta)| \to 0 \) in probability, as \( n \to \infty \). According Corollary 2.2 in Newey (1991), we have to prove that
1: for each $\theta \in \Theta$, $Q_n(\theta) - \overline{Q}_n(\theta) \to 0$ in probability, as $n \to \infty$;

2: for $M_n = O_p(1)$,

$$|\overline{Q}_n(\theta') - \overline{Q}_n(\theta)| \leq M_n||\theta' - \theta||.$$ 

We sketch the proof for $l_{(k,l)} = l_{kl}$, the same arguments apply for the other sub-likelihoods, using the fourth remark.

1: We prove that $\sup_{k \in D_n} E[(\sup_{\theta \in \Theta} g_k(Y(k); \theta))^2 + \eta] < \infty$, for $\eta > 0$. In fact, we have

$$g_k(Y(k); \theta) = \frac{1}{2} \sum_{l \in V_k, l \neq k} \left\{ 2 \log \sigma^2 + \log(1 - \rho_{kl}^2) + \frac{Z_k^2 + Z_l^2 - 2 \rho_{kl} Z_k Z_l}{\sigma^2(1 - \rho_{kl}^2)} \right\}$$

$$\leq \sum_{l \in V_k, l \neq k} \log \sigma^2 + \frac{1}{2} \log(1 - \rho_{kl}^2) + \frac{Z_k^2 + Z_l^2}{\sigma^2(1 - \rho_{kl}^2)}$$

$$\leq c_1 |V_k| \log \sigma^2 + c_2 |V_k| Z_k^2 + c_2 \sum_{l \in V_k, l \neq k} Z_l^2$$

and $|V_k|$ is uniformly bounded according the assumption C5. The uniform bounded moments $g_k(Y(k); \theta)$ entail uniform $L^1$ integrability of $g_k$ and with the assumption C2 we obtain (Jenish and Prucha, 2009, Theorem 3)

$$Q_n(\theta) - \overline{Q}_n(\theta) = d_n^{-1} \sum_{k \in D_n} \{g_k(Y(k), \theta) - E[\theta] g_k(Y(k), \theta)]\} \to 0, \text{ in probability}$$

2: We have

$$|g_k(Y(k); \theta') - g_k(Y(k); \theta)| = \frac{1}{2} \sum_{l \in V_k, l \neq k} \left| 2 \log \frac{\sigma_{kl}^2}{\sigma^2} + \log \frac{1 - \rho_{kl}^2}{1 - \rho_{kl}^2} \right.$$

$$+ (Z_k^2 + Z_l^2) \left[ \frac{1}{\sigma^2(1 - \rho_{kl}^2)} - \frac{1}{\sigma^2(1 - \rho_{kl}^2)} \right]$$

$$- 2 \rho_{kl} Z_k Z_l \left[ \frac{\rho_{kl}}{\sigma^2(1 - \rho_{kl}^2)} - \frac{\rho_{kl}}{\sigma^2(1 - \rho_{kl}^2)} \right] \left| \right|$$

$$\leq c_1 |V_k| ||\theta' - \theta|| + c_2 (|V_k| Z_k^2 + \sum_{l \in V_k, l \neq k} Z_l^2) ||\theta' - \theta||$$

$$|\overline{Q}_n(\theta') - \overline{Q}_n(\theta)| \leq d_n^{-1} \sum_{k \in D_n} |q_k(\theta') - q_k(\theta)|$$

$$\leq c_3 d_n^{-1} \sum_{k \in D_n} (1 + Z_k^2 + \sum_{l \in V_k, l \neq k} Z_l^2) ||\theta' - \theta||$$

$$= M_n ||\theta' - \theta||$$
for some positive constants $c_1$, $c_2$ and $c_3$ and $M_n = c_3 d_n^{-1} \sum_{k \in D_n} (1 + Z_k^2 + \sum_{l \in V_k, l \neq k} Z_l^2)$.

Since $E_\theta[M_n] < \infty$, we obtain the desired result.

**Asymptotic normality**

We make the additional assumption:

N1: there exists two symmetric positive definite matrices $I$ and $J$ such that for large $n$:

$$J_n = \text{var}_\theta(\sqrt{d_n} \nabla Q_n(\theta)) \geq J > 0 \quad \text{and} \quad I_n = E_\theta(\nabla^2 Q_n(\theta)) \geq I > 0.$$

We note that because $g_s$ is a $C^2$ and $\Theta$ is a compact space there exists a random variable $h(Y(s))$, $E_\theta(h(Y(s))) < \infty$ satisfying:

$$\left| \frac{\partial^2}{\partial \theta_k \partial \theta_l} g_s(Y(s), \theta) \right|^2 \leq h(Y(s)).$$

Moreover for all $s \in S$, $E_\theta[\frac{\partial}{\partial \theta_k} g_s(\theta)] = 0$, because $g_s$ is a sum of log-likelihoods, and it is easy to show that we have that $\sup_{s \in S, \theta \in \Theta} E_\theta\left[ \left| \frac{\partial}{\partial \theta_k} g_s(\theta) \right|^{2+\eta} \right] < \infty$ and $\sup_{s \in S, \theta \in \Theta} E_\theta\left[ \left| \frac{\partial^2}{\partial \theta_k \partial \theta_l} g_s(\theta) \right|^{2+\eta} \right] < \infty$.

Under the condition C1-C7 and N1, conditions (H1-H2-H3) of Theorem 3.4.5 in Guyon (1995) are satisfied and

$$\sqrt{d_n} J_n^{-1/2} I_n (\hat{\theta}_n - \theta^*) \xrightarrow{d} N(0, J_p).$$

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