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Data-driven neighborhood selection of a Gaussian field

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Abstract: We study the nonparametric covariance estimation of a stationary Gaussian field X observed on a lattice. To tackle this issue, a neighborhood selection procedure has been recently introduced. This procedure amounts to selecting a neighborhood $\widehat{m}$ by a penalization method and estimating the covariance of X in the space of Gaussian Markov random fields (GMRFs) with neighborhood $\widehat{m}$. Such a strategy is shown to satisfy oracle inequalities as well as minimax adaptive properties. However, it suffers several drawbacks which make the method difficult to apply in practice. On the one hand, the penalty depends on some unknown quantities. On the other hand, the procedure is only defined for toroidal lattices. The present contribution is threefold. A data-driven algorithm is proposed for tuning the penalty function. Moreover, the procedure is extended to non-toroidal lattices. Finally, numerical study illustrate the performances of the method on simulated examples. These simulations suggest that Gaussian Markov random field selection is often a good alternative to variogram estimation.

Key-words: Gaussian field, Gaussian Markov random field, Data-driven calibration, model selection, pseudolikelihood.

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Sélection automatique de voisinage d'un champ gaussien

Résumé : Nous étudions l'estimation non-paramétrique d'un champ gaussien stationnaire X observé sur un réseau régulier. Dans ce cadre, nous avons précédemment introduit une procédure de sélection de modèle [Ver09]. Cette procédure revient à sélectionner un voisinage $\widehat{m}$ grâce une technique de pénalisation puis à estimer la covariance du champ X dans l'espace des champs de Markov gaussiens de voisinage $\widehat{m}$. Une telle stratégie satisfait des inégalités oracles et des propriétés d'apdaptation au sens minimax. En pratique, elle présente néanmoins quelques inconvénients. D'une part, la pénalité dépend de quantités inconnues. D'autre part, la procédure est uniquement définie pour des réseaux toriques. La contribution de cet article est triple. Nous proposons un algorithme automatique pour calibrer la pénalité. De plus, nous introduisons une extension à des réseaux non-toriques. Enfin, nous étudions les performances pratiques de la procédure sur des données simulées. Ces simulations suggèrent que la sélection de champs de Markov gaussiens est souvent une bonne alternative à l'estimation de variogramme.

Mots-clés : Champ gaussien, champ de Markov gaussien, calibration automatique, sélection de modèle, pseudo-vraisemblance.

1 Introduction

We study the estimation of the distribution of a stationary Gaussian field $(X_{[i,j]})_{(i,j)\in\Lambda}$ indexed by the nodes of a rectangular lattice Λ of size $p_1 \times p_2$. This problem is often encountered in spatial statistics or in image analysis. Classical statistical procedures allow to estimate and subtract the trend. Henceforth, we assume that the field X is centered. Given a n-sample of the field X, the challenge is to infer the correlation. In practice, the number n of observations often equals one. Different methods have been proposed to tackle this problem.

A traditional approach amounts to computing an empirical variogram and then fitting a suitable parametric variogram model such as the exponential or Matérn model (see [Cre93] Ch.2 or [Ste99]). The main disadvantage with this method is that the practitioner is required to select a *good* variogram model. When the field exhibits long range dependence, specific procedures have been introduced (e.g. Frías *et al.* [FARMA08]). In the sequel, we focus on small range dependences. Most of the nonparametric (Hall *et al.* [HFH94]) and semiparametric (Im *et al.* [ISZ07]) methods are based on the spectral representation of the field. To our knowledge, these procedures have not yet been shown to achieve adaptiveness, i.e. their rate of convergence does not adapt to the *complexity* of the correlation functions.

In this paper, we define and study a nonparametric estimation procedure relying on Gaussian Markov random fields (GMRF). This procedure is computationally fast and satisfies adaptive properties. Let us fix a node $(0,0)$ at the center of Λ and let m be a subset of $\Lambda \setminus \{(0,0)\}$. The field X is a GMRF with respect to the neighborhood m if conditionally to $(X_{[k,l]})_{(k,l)\in m}$, the variable $X_{[0,0]}$ is independent from all the remaining variables in Λ. We refer to Rue and Held [RH05] for a comprehensive introduction on GMRFs. If we know that X is a GMRF with respect to the neighborhood m, then we can estimate the covariance by applying likelihood or pseudolikelihood maximization. Such parametric procedures are well understood, at least from an asymptotic point of view (see for instance [Guy95] Sect.4). However, we do not know in practice what is the "good" neighborhood m. For instance, choosing the empty neighborhood amounts to assuming that all the components of X are independent. Alternatively, if we choose the complete neighborhood, which contains all the nodes of Λ except $(0,0)$, then the number of parameters is huge and estimation performances are poor.

We tackle in this paper the problem of neighborhood selection from a practical point of view. The purpose is to define a data-driven procedure that picks a suitable neighborhood $\widehat{m}$ and then estimates the distribution of X in the space of GMRFs with neighborhood $\widehat{m}$. This procedure neither requires any knowledge on the correlation of X, nor assumes that the field X satisfies a Markov condition. Indeed, the procedure selects a neighborhood $\widehat{m}$ that achieves a trade-off between an *approximation* error (distance between the true correlation and GMRFs with neighborhood m) and an *estimation* error (variance of the estimator). If X is a GMRF with respect to a small neighborhood, then the procedure achieves a parametric rate of convergence. Alternatively, if X is not a GMRF then the rate of convergence of the procedure depends on the rate of approximation of the true covariance by GMRFs with growing neighborhood. In short, the procedure is nonparametric and adaptive.

Besag and Kooperberg [BK95], Rue and Tjelmeland [RT02], Song *et al.* [SFG08], and Cressie and Verzelen [CV08] have considered the problem of *approximating* the correlation of a Gaussian field by a GMRF, but this approach requires the knowledge of the true distribution. Guyon and Yao have stated in [GY99] necessary conditions and sufficient conditions for a model selection pro-

cedure to choose asymptotically the true neighborhood of a GMRF with probability one. Our point of view is slightly different. We do not assume that the field X is a GMRF with respect to a sparse neighborhood. We do not aim at estimating the true neighborhood, we rather want to select a neighborhood that allows to estimate *well* the distribution of X (i.e. to minimize a risk). The distinction between these two points of view has been nicely described in the first chapter of MacQuarrie and Tsai [MT98].

In [Ver09], we have introduced a neighborhood selection procedure based on pseudolikelihood maximization and penalization. Under mild assumptions, the procedure achieves optimal neighborhood selection. More precisely, it satisfies an oracle inequality and it is minimax adaptive to the sparsity of the neighborhood. To our knowledge, these are the first results of neighborhood selection in this spatial setting.

If the procedure exhibits appealing theoretical properties, it suffers several drawbacks from a practical perspective. First, the method constrains the largest eigenvalue of the estimated covariance to be smaller than some parameter ρ. In practice, it is difficult to choose ρ since we do not know the largest eigenvalue of the true covariance. Second, the penalty function pen(.) introduced in Sect.3 of the previous paper depends on the largest eigenvalue of the covariance of the field X. Hence, we need a practical method for tuning the penalty. Third, the procedure has only been defined when the lattice Λ is a square torus.

Our contribution is twofold. On the one hand, we propose practical versions of our neighborhood selection procedure that overcome the previously-mentioned drawbacks:

- The procedure is extended to rectangular lattices.
- We do not constrain anymore the largest eigenvalue of the covariance.
- We provide an algorithm based on the so-called *slope heuristics* of Birgé and Massart [BM07] for tuning the penalty. Theoretical justifications for its use are also given.
- Finally, we extend the procedure to the case where the lattice Λ is not a torus.

On the other hand, we illustrate the performances of this new procedure on numerical examples. When Λ is a torus, we compare it with likelihood-based methods like AIC [Aka73] and BIC [Sch78], even if they were not studied in this setting. When Λ is not toroidal, likelihood methods become intractable. Nevertheless, our procedure still applies and often outperforms variogram-based methods.

The paper is organized as follows. In Section 2, we define a new version of the estimation procedure of [Ver09] that does not require anymore the choice of the constant ρ. We also discuss the computational complexity of the procedure. In Section 3, we connect this new procedure to the original method and we recall some theoretical results. We provide an algorithm for tuning the penalty in practice in Section 4. In Section 5, we extend our procedure for handling non-toroidal lattices. The simulation studies are provided in Section 6. Section 7 summarizes our findings, while the proofs are postponed to Section 8.

Let us introduce some notations. In the sequel, X^v refers to the vectorialized version of X with the convention $X_{[i,j]} = X^v_{[(i-1)\times p_2+j]}$ for any $1 \leq i \leq p_1$ and $1 \leq j \leq p_2$. Using this new notation amounts to "forgetting" the spatial structure of X and allows to get into a more classical statistical framework. We note $\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_n$ the n observations of the field X. The matrix Σ stands for

the covariance matrix of X^v. For any matrix A, $\varphi_{\max}(A)$ and $\varphi_{\min}(A)$ respectively refer the largest eigenvalue and the smallest eigenvalues of A. Finally, I_r denotes the identity matrix of size r.

2 Neighborhood selection on a torus

In this section, we introduce the main concepts and notations for GMRFs on a torus. Afterwards, we describe our procedure based on pseudolikelihood maximization. Finally, we discuss some computational aspects. Throughout this section and the two following sections, the lattice Λ is assumed to be toroidal. Consequently, the components of the matrices X are taken modulo p_1 and p_2.

2.1 GMRFs on the torus

The notion of conditional distribution is underlying the definition of GMRFs. By standard Gaussian derivations (see for instance [Lau96] App.C), there exists a unique $p_1 \times p_2$ matrix θ such that $\theta_{[0,0]} = 0$ and

$$X_{[0,0]} = \sum_{(i,j)\in\Lambda\setminus\{(0,0)\}} \theta_{[i,j]} X_{[i,j]} + \epsilon_{[0,0]} \ , \tag{1}$$

where the random variable $\epsilon_{[0,0]}$ follows a zero-mean normal distribution and is independent from the covariates $(X_{[i,j]})_{(i,j)\in\Lambda\setminus\{(0,0)\}}$. The linear combination $\sum_{(i,j)\in\Lambda\setminus\{(0,0)\}} \theta_{[i,j]} X_{[i,j]}$ is the kriging predictor of $X_{[0,0]}$ given the remaining variables. In the sequel, we note σ^2 the variance of $\epsilon_{[0,0]}$ and we call it the conditional variance of $X_{[0,0]}$.

Equation (1) describes the conditional distribution of $X_{[0,0]}$ given the remaining variables. By stationarity of the field X, it holds that that $\theta_{[i,j]} = \theta_{[-i,-j]}$. The covariance matrix Σ is closely related to θ through the following equation:

$$\Sigma = \sigma^2 \left[I_{p_1 p_2} - C(\theta) \right]^{-1} \ , \tag{2}$$

where the $p_1 p_2 \times p_1 p_2$ matrix $C(\theta)$ is defined by $C(\theta)_{[(i_1-1)p_2+j_1,(i_2-1)p_2+j_2]} := \theta_{[i_2-i_1,j_2-j_1]}$ for any $1 \le i_1, i_2 \le p_1$ and $1 \le j_1, j_2 \le p_2$. The matrix $(I_{p_1 p_2} - C(\theta))$ is called the partial correlation matrix of the field X. The so-defined matrix $C(\theta)$ is symmetric block circulant with $p_2 \times p_2$ blocks. We refer to [RH05] Sect.2.6 or the book of Gray [Gra06] for definitions and main properties on circulant and block circulant matrices.

Identities (1) and (2) have two main consequences. First, estimating the $p_1 \times p_2$ matrix θ amounts to estimating the covariance matrix Σ up to a multiplicative constant. We shall therefore focus on θ. Second, by Equation (1), the field X is a GMRF with respect to the neighborhood defined by the support θ. The adaptive estimation issue of the distribution of X by neighborhood selection therefore reformulates as an adaptive estimation problem of the matrix θ via support selection.

Let us now precise the set of possible values for θ. The set Θ denotes the vector space of the $p_1 \times p_2$ matrices that satisfy $\theta_{[0,0]} = 0$ and $\theta_{[i,j]} = \theta_{[-i,-j]}$, for any $(i,j) \in \Lambda$. Hence, a matrix $\theta \in \Theta$ corresponds to the distribution of a stationary Gaussian field if and only if the $p_1 p_2 \times p_1 p_2$ matrix $(I_{p_1 p_2} - C(\theta))$ is positive definite. This is why we define the convex subset Θ^+ of Θ by

$$\Theta^+ := \{\theta \in \Theta \ \text{ s.t. } [I_{p_1 p_2} - C(\theta)] \ \text{ is positive definite}\} \ . \tag{3}$$

The set of covariance matrices of stationary Gaussian fields on Λ with unit conditional variance is in one to one correspondence with the set Θ^+. We sometimes assume that the field X is isotropic. The corresponding sets $\Theta^{\rm iso}$ and $\Theta^{+,\rm iso}$ for isotropic fields are introduced as:

$$\Theta^{\rm iso} := \{\theta \in \Theta \ , \ \ \theta_{[i,j]} = \theta_{[-i,j]} = \theta_{[j,i]} \ , \forall (i,j) \in \Lambda\} \quad \text{and } \Theta^{+,\rm iso} := \Theta^+ \cap \Theta^{\rm iso} \ .$$

2.2 Description of the procedure

Let $|(i,j)|_t$ refer to the toroidal norm defined by

$$|(i,j)|_t^2 := [i \wedge (p_1 - i)]^2 + [j \wedge (p_2 - j)]^2 \ ,$$

for any node $(i,j) \in \Lambda$.

In the sequel, a model m stands for a subset of $\Lambda \setminus \{(0,0)\}$. It is also called a neighborhood. For the sake of simplicity, we shall only use the collection of models $\mathcal{M}_1$ defined below.

Definition 2.1. *A subset $m \subset \Lambda \setminus \{(0,0)\}$ belongs to $\mathcal{M}_1$ if and only if there exists a number $r_m > 1$ such that*

$$m = \{(i,j) \in \Lambda \setminus \{(0,0)\} \quad s.t. \quad |(i,j)|_t \leq r_m\} \ . \tag{4}$$

In other words, the neighborhoods m in $\mathcal{M}_1$ are sets of nodes lying in a disc centered at $(0,0)$. Obviously, $\mathcal{M}_1$ is totally ordered with respect to the inclusion. Consequently, we order the models $m_0 \subset m_1 \subset \ldots \subset m_i \ldots$. For instance, m_0 corresponds to the empty neighborhood, m_1 stands for the neighborhood of size 4, and m_2 refers to the neighborhood with 8 neighbours. See Figure 1 for an illustration.

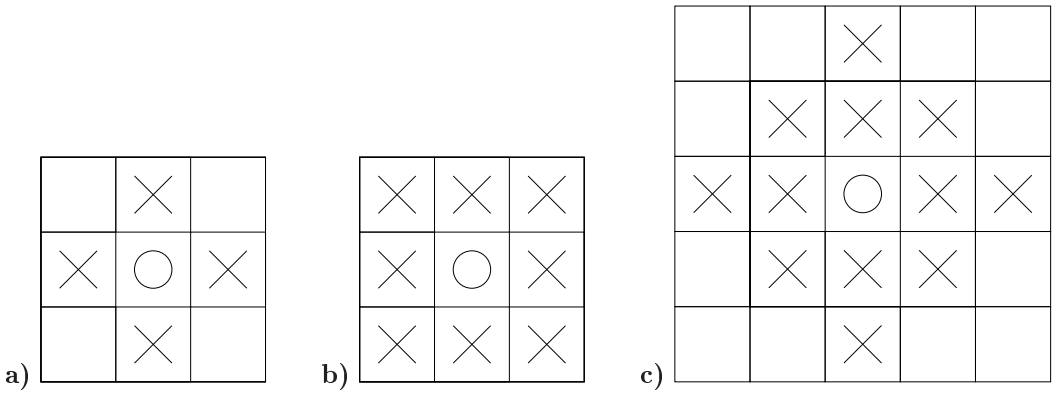

Figure 1: *(a) Model m_1 with first order neighbors. (b) Model m_2 with second order neighbors. (c) Model m_3 with third order neighbors.*

For any model $m \in \mathcal{M}_1$, the vector space Θ_m is the subset of matrices Θ whose support is included in m. Similarly $\Theta_m^{\rm iso}$ is the subset of $\Theta^{\rm iso}$ whose support is included in m. The dimensions of Θ_m and $\Theta_m^{\rm iso}$ are respectively noted d_m and $d_m^{\rm iso}$. Since we aim at estimating the positive matrix $(I_{p_1 p_2} - C(\theta))$, we also consider the convex subsets of Θ_m^+ and $\Theta_m^{+,\rm iso}$ which correspond to non-negative precision matrices.

$$\Theta_m^+ := \Theta_m \cap \Theta^+ \qquad \text{and} \qquad \Theta_m^{+,\rm iso} := \Theta_m^{\rm iso} \cap \Theta^{+,\rm iso} \ . \tag{5}$$

For any $\theta' \in \Theta^+$, the conditional least-squares (CLS) criterion $\gamma_{n,p_1,p_2}(\theta')$ [Guy87] is defined by

$$\gamma_{n,p_1,p_2}(\theta') \;:=\; \frac{1}{np_1p_2}\sum_{i=1}^{n}\sum_{(j_1,j_2)\in\Lambda}\left(\mathbf{X}_{i[j_1,j_2]} - \sum_{(l_1,l_2)\in\Lambda\setminus\{(0,0)\}} \theta'_{[l_1,l_2]}\mathbf{X}_{i[j_1+l_1,j_2+l_2]}\right)^2 . \quad (6)$$

The function $\gamma_{n,p_1,p_2}(.)$ is a least-squares criterion that allows us to perform the simultaneous linear regression of all $\mathbf{X}_{i[j_1,j_2]}$ with respect to the covariates $(\mathbf{X}_{i[l_1,l_2]})_{(l_1,l_2)\neq(k_1,k_2)}$. This criterion is closely connected with the pseudolikelihood introduced by Besag [Bes75]. The associated estimator is slightly less efficient estimator than maximum likelihood estimation ([Guy95] Sect.4.3). Nevertheless, its computation is much faster since it does not involve determinants as for the likelihood. See [Ver09] Sect. 7.1, for a more complete comparison between CLS and maximum likelihood estimators in this setting. For any model $m \in \mathcal{M}_1$, the estimators are defined as the unique minimizers of $\gamma_{n,p_1,p_2}(.)$ on the sets Θ_m^+ and $\Theta_m^{+,\mathrm{iso}}$.

$$\widehat{\theta}_m := \arg\min_{\theta'\in\overline{\Theta_m^+}} \gamma_{n,p_1,p_2}(\theta') \qquad \text{and} \qquad \widehat{\theta}_m^{\mathrm{iso}} := \arg\min_{\theta'\in\overline{\Theta_m^{+,\mathrm{iso}}}} \gamma_{n,p_1,p_2}(\theta') \;, \quad (7)$$

where $\overline{A}$ stands for the closure of A. We further discuss the connection between $\widehat{\theta}_m$ and $\widehat{\theta}_{m,\rho_1}$ in Section 3.

Given a subcollection of models $\mathcal{M}$ of $\mathcal{M}_1$ and a positive function pen : $\mathcal{M} \to \mathbb{R}^+$ called a penalty, we select a model as follows:

$$\widehat{m} := \arg\min_{m\in\mathcal{M}}\left[\gamma_{n,p_1,p_2}\left(\widehat{\theta}_m\right) + \mathrm{pen}(m)\right] \quad \text{and} \quad \widehat{m}^{\mathrm{iso}} := \arg\min_{m\in\mathcal{M}}\left[\gamma_{n,p_1,p_2}\left(\widehat{\theta}_m^{\mathrm{iso}}\right) + \mathrm{pen}(m)\right] . \quad (8)$$

For short, we write $\widetilde{\theta}$ and $\widetilde{\theta}^{\mathrm{iso}}$ for $\widehat{\theta}_{\widehat{m}}$ and $\widehat{\theta}^{\mathrm{iso}}_{\widehat{m}^{\mathrm{iso}}}$. We discuss the choice of the penalty function in Section 4.

2.3 Computational aspects

Since the lattice Λ is a torus, the computation of the estimators $\widehat{\theta}_m$ is performed efficiently thanks to the following lemma.

Lemma 2.1. *For any $p \times p$ matrix A and for any $1 \le i \le p_1$ and $1 \le j \le p_2$, let $\lambda_{[i,j]}(A)$ be the (i,j)-th term of two-dimensional discrete Fourier transform of the matrix A, i.e.*

$$\lambda_{[i,j]}(A) \;:=\; \sum_{k=1}^{p_1}\sum_{l=1}^{p_2} A_{[i,j]} \exp\left[2\iota\pi\left(\frac{ki}{p_1}+\frac{jl}{p_2}\right)\right] , \quad (9)$$

where $\iota^2 = -1$. The conditional least-squares criterion $\gamma_{n,p_1,p_2}(\theta')$ simplifies as

$$\gamma_{n,p_1,p_2}(\theta') \;=\; \frac{1}{np_1^2p_2^2}\left\{\sum_{i=1}^{p_1}\sum_{j=1}^{p_2}\left[1-\lambda_{[i,j]}(\theta)\right]^2\left[\sum_{k=1}^{n}\lambda_{[i,j]}\left(\mathbf{X}_k\right)\overline{\lambda_{[i,j]}\left(\mathbf{X}_k\right)}\right]\right\} .$$

A proof is given in Section 8. Optimization of $\gamma_{n,p_1,p_2}(.)$ over the set Θ_m^+ is performed fastly using the fast Fourier transform (FFT). Nevertheless, this is not the privilege of CLS estimators, since maximum likelihood estimators are also computed fastly by FFT when Λ is a torus.

In Section 5, we mention that the computation of the CLS estimators $\widehat{\theta}_m$ remains quite easy when Λ is not a torus whereas likelihood maximization becomes intractable.

3 Theoretical results

Throughout this section, Λ is assumed to be a toroidal square lattice and we note p its size. Let us mention that the restriction to square lattices made in [Ver09] allows to simplify the proofs but is not necessary so that the theoretical results hold. In this section, we first recall the original procedure and we emphasize the differences with the one defined in the previous section. We also mention a result of optimality. This will provide some insights for calibrating the penalty pen(.) in Section 4.

Given $\rho > 2$ be a positive constant, we define the subsets $\Theta^+_{m,\rho}$ and $\Theta^{+,\mathrm{iso}}_{m,\rho}$ by

$$\begin{aligned} \Theta^+_{m,\rho} &:= \left\{\theta \in \Theta^+_m \ , \ \varphi_{\max}\left[I_{p_1p_2} - C(\theta)\right] < \rho\right\} \\ \Theta^{+,\mathrm{iso}}_{m,\rho} &:= \left\{\theta \in \Theta^{+,\mathrm{iso}}_m \ , \ \varphi_{\max}\left[I_{p_1p_2} - C(\theta)\right] < \rho\right\} \ . \end{aligned} \tag{10}$$

Then, the corresponding estimators $\widehat{\theta}_{m,\rho}$ and $\widehat{\theta}^{\mathrm{iso}}_{m,\rho}$ are defined as in (7), except that we now consider $\Theta^+_{m,\rho}$ instead of Θ^+_m. Let us mention that the estimator $\widehat{\theta}_m$ corresponds to the estimator $\widehat{\theta}_{m,\rho_1}$ defined in [Ver09] Sect.2.2 with $\rho_1 = +\infty$.

$$\widehat{\theta}_{m,\rho} := \arg \min_{\theta' \in \overline{\Theta^+_{m,\rho}}} \gamma_{n,p,p}(\theta') \qquad \text{and} \qquad \widehat{\theta}^{\mathrm{iso}}_{m,\rho} := \arg \min_{\theta' \in \overline{\Theta^{+,\mathrm{iso}}_{m,\rho}}} \gamma_{n,p,p}(\theta') \ .$$

Given a subcollection $\mathcal{M}$ of $\mathcal{M}_1$ and a penalty function pen(.), we select the models $\widehat{m}_\rho$ and $\widehat{m}^{\mathrm{iso}}_\rho$ as in (8) except that we use $\widehat{\theta}_{m,\rho}$ and $\widehat{\theta}^{\mathrm{iso}}_{m,\rho}$ instead of $\widehat{\theta}_m$ and $\widehat{\theta}^{\mathrm{iso}}_m$. We also note $\widetilde{\theta}_\rho$ and $\widetilde{\theta}^{\mathrm{iso}}_\rho$ for $\widehat{\theta}_{\widehat{m}_\rho,\rho}$ and $\widehat{\theta}^{\mathrm{iso}}_{\widehat{m}^{\mathrm{iso}}_\rho,\rho}$.

The only difference between the estimators $\widetilde{\theta}$ and $\widetilde{\theta}_\rho$ is that the largest eigenvalue of the precision matrix $(I_{p^2} - C(\widetilde{\theta}))$ is restricted to be smaller than ρ. We make this restriction in [Ver09] to facilitate the analysis.

In order to assess the performance of the penalized estimator $\widetilde{\theta}_\rho$ and $\widetilde{\theta}^{\mathrm{iso}}_\rho$, we use the prediction loss function $l(\theta_1, \theta_2)$ defined by

$$l(\theta_1, \theta_2) := \frac{1}{p^2} tr\left[(C(\theta_1) - C(\theta_2))\Sigma(C(\theta_1) - C(\theta_2))\right] \ . \tag{11}$$

As explained in [Ver09] Sect.1.3, the loss $l(\theta_1, \theta_2)$ expresses in terms of conditional expectation

$$l(\theta_1, \theta_2) = \mathbb{E}_\theta\left\{\left[\mathbb{E}_{\theta_1}\left(X_{[0,0]}|X_{\Lambda\setminus\{0,0\}}\right) - \mathbb{E}_{\theta_2}\left(X_{[0,0]}|X_{\Lambda\setminus\{0,0\}}\right)\right]^2\right\} \ , \tag{12}$$

where $\mathbb{E}_\theta(.)$ stands for the expectation with respect to the distribution $\mathcal{N}(0, \sigma^2(I_{p_1p_2} - C(\theta))^{-1})$. Hence, $l(\widehat{\theta}, \theta)$ corresponds the mean squared prediction loss of $X_{[0,0]}$ given the other covariates. A similar loss function is also used by Song *et al.* [SFG08], when approximation Gaussian fields by GMRFs. For any neighborhood $m \in \mathcal{M}$, we define the *projection* $\theta_{m,\rho}$ as the closest element of θ in $\Theta^+_{m,\rho}$ with respect to the loss $l(.,.)$.

$$\theta_{m,\rho} := \arg \min_{\theta' \in \overline{\Theta^+_{m,\rho}}} l(\theta', \theta) \qquad \text{and} \qquad \theta^{\mathrm{iso}}_{m,\rho} := \arg \min_{\theta' \in \overline{\Theta^{+,\mathrm{iso}}_{m,\rho}}} l(\theta', \theta) \ .$$

We call the loss $l(\theta_{m,\rho},\theta)$ the bias of the set $\Theta^+_{m,\rho}$. This implies that $\widehat{\theta}_{m,\rho}$ cannot perform better than this loss.

Theorem 3.1. *Let $\rho > 2$, K be a positive number larger than an universal constant K_0 and $\mathcal{M}$ be a subcollection of $\mathcal{M}_1$. If for every model $m \in \mathcal{M}$, it holds that*

$$pen(m) \geq K\rho^2\varphi_{max}(\Sigma)\frac{d_m+1}{np^2} \ , \tag{13}$$

then for any $\theta \in \Theta^+$, the estimator $\widetilde{\theta}_\rho$ satisfies

$$\mathbb{E}_\theta[l(\widetilde{\theta}_\rho,\theta)] \leq L(K) \inf_{m\in\mathcal{M}} [l(\theta_{m,\rho},\theta) + pen(m)] \ , \tag{14}$$

where $L(K)$ only depends on K. A similar bound holds if one replaces $\widetilde{\theta}_\rho$ by $\widetilde{\theta}^{\rm iso}_\rho$, Θ^+ by $\Theta^{+,iso}$, $\theta_{m,\rho}$ by $\theta^{\rm iso}_{m,\rho}$, and d_m by $d^{\rm iso}_m$.

Although we have assumed the correlation is non-singular, the theorem still holds if the spatial field is constant. The nonasymptotic bound is provided in a slightly different version in [Ver09]. It states that $\widetilde{\theta}_\rho$ achieves a trade-off between the bias and a variance term if the penalty is suitable chosen. In Theorem 3.1, we use the penalty $K\rho^2\varphi_{\max}(\Sigma)(d_m+1)/(np^2)$ instead of the penalty $K\rho^2\varphi_{\max}(\Sigma)d_m/(np^2)$ stated in the previous paper. This makes the bound (14) simpler. Observe that these two penalties yield the same model selection since they only differ by a constant. Let us further discuss two points.

- In this paper, we use the estimator $\widetilde{\theta}$ rather than $\widetilde{\theta}_\rho$. Given a collection of models $\mathcal{M}$, there exists some finite $\rho > 2$, such that these two estimators coincide. Take for instance $\rho = \sup_{m\in\mathcal{M}} \sup_{\theta\in\Theta^+_m} \varphi_{\max}(I_{p_1p_2} - C(\theta))$. Admittedly, the so-obtained ρ may be large, especially if there are large models in $\mathcal{M}$. The upper bound (14) on the risk therefore becomes worse. Nevertheless, we do not think that the dependency of (14) on ρ is sharp. Indeed , we illustrate in Section 6 that the risk of $\widetilde{\theta}$ exhibits good statistical performances.
- Theorem 3.1 provides a suitable form of the penalty for obtaining oracle inequalities. However, this penalty depends on $\varphi_{\max}(\Sigma)$ which is not known in practice. This is why we develop a data-driven penalization method in the next section.

4 Slope Heuristics

Let us introduce a data-driven method for calibrating the penalty function pen(.). It is based on the so-called *slope heuristic* introduced by Birgé and Massart [BM07] in the fixed design Gaussian regression framework (see also [Mas07] Sect.8.5.2). This heuristic relies on the notion of minimal penalty. In short, assume that one knows that a good penalty has a form $\text{pen}(m) = NF(d_m)$ (where d_m is the dimension of the model and N is a tuning parameter). Let us define $\widehat{m}(N)$ the selected model as a function of N. There exists a quantity $\widehat{N}_{\min}$ satisfying the following property: If $N > \widehat{N}_{\min}$, the dimension of the selected model $d_{\widehat{m}(N)}$ is reasonable and if $N < \widehat{N}_{\min}$, the dimension of the selected model is huge. The function $pen_{\min}(.) := \widehat{N}_{\min}F(.)$ is called the minimal penalty. In fact, a *dimension jump* occurs for $d_{\widehat{m}(N)}$ at the point $\widehat{N}_{\min}$. Thus, the quantity $\widehat{N}_{\min}$ is clearly

observable for real data sets. In their Gaussian framework, Birgé and Massart have shown that twice the minimal penalty is nearly the optimal penalty. In other words, the model $\widehat{m} := \widehat{m}(2\widehat{N}_{\min})$ yields an efficient estimator.

The slope heuristic method has been successfully applied for multiple change-point detection [Leb05]. Applications are also being developed in other frameworks such as mixture models [MM08], clustering [BCM08], estimation of oil reserves [Lep02], and genomic [Vil07].

If this method was originally introduced for fixed design Gaussian regression, Arlot and Massart [AM09] have proved more recently that a similar phenomenon occurs in the heteroscedastic random-design case. In the GMRF setting, we are only able to partially justify this heuristic. For the sake of simplicity, let us assume in the next proposition that the lattice Λ is a square of size p.

Proposition 4.1. *Consider $\rho > 2$, and $\eta < 1$ and suppose that p is larger than some numerical constant p_0. Let m' be the largest model in $\mathcal{M}_1$ that satisfies $d_{m'} \leq \sqrt{np^2}$. For any model $m \in \mathcal{M}_1$, we assume that*

$$pen(m') - pen(m) \leq K_1(1-\eta)\sigma^2 \left\{ \varphi_{min}\left(I_{p^2} - C(\theta)\right) \wedge \left[\rho - \varphi_{max}\left(I_{p^2} - C(\theta)\right)\right] \right\} \frac{d_{m'} - d_m}{np^2} \ , \quad (15)$$

where K_1 is a universal (constant defined in the proof). Then, for any $\theta \in \Theta^+_{m',\rho}$, it holds that

$$\mathbb{P}\left\{ d_{\widehat{m}_\rho} > L\left[\sqrt{np^2} \wedge p^2\right] \right\} \geq \frac{1}{2} \ ,$$

where L only depends on η, ρ, $\varphi_{min}\left(I_{p^2} - C(\theta)\right)$, and $\varphi_{max}\left(I_{p^2} - C(\theta)\right)$.

The proof is postponed to Section 8. Let us define

$$N_1 := K_1\sigma^2 \left\{ \varphi_{\min}\left(I_{p_1p_2} - C(\theta)\right) \wedge \left[\rho - \varphi_{\max}\left(I_{p_1p_2} - C(\theta)\right)\right] \right\} \ ,$$

and let us consider penalty functions $\mathrm{pen}(m) = N\frac{d_m}{np_1p_2}$ for some $N > 0$. The proposition states that if N is smaller than N_1, then the procedure selects a model of huge dimension with large probability, i.e $d_{\widehat{m}(N)}$ is huge. Alternatively, let us define

$$N_2 := K_0 \frac{\sigma^2\rho^2}{\varphi_{\min}\left(I_{p_1p_2} - C(\theta)\right)} \frac{d_m}{np_1p_2} \ ,$$

where the numerical constant K_0 is introduced in Theorem 3.1 in [Ver09]. By Theorem 3.1, choosing $N > N_2$ ensures that the risk of $\widetilde{\theta}_\rho$ achieves a type-oracle inequality and the dimension $d_{\widehat{m}_\rho(N)}$ is reasonable. The quantities N_1 and N_2 are different especially when the eigenvalues of $(I_{p_1p_2} - C(\theta))$ are far from 1. Since we do not know the behavior of the selected model $\widehat{m}_\rho(N)$ when N is between N_1 and N_2, we are not able to really prove a dimension jump as the fixed design Gaussian regression framework. Besides, we have mentioned in the preceding section that we are more interested in the estimator $\widetilde{\theta}$ than $\widetilde{\theta}_\rho$. Nevertheless, we clearly observe in simulation studies a dimension jump for some N between N_1 and N_2 even if we use the estimators $\widehat{\theta}_m$ instead of $\widehat{\theta}_{m,\rho}$. This suggests that the slope heuristic is still valid in the GMRF framework.

Algorithm 4.1. *(Data-driven penalization with slope heuristic). Let $\mathcal{M}$ be a subcollection of $\mathcal{M}_1$.*

1. *Compute the selected model $\widehat{m}(N)$ as a function of $N > 0$*

$$\widehat{m}(N) \in \arg\min_{m\in\mathcal{M}} \left\{ \gamma_{n,p_1,p_2}\left(\widehat{\theta}_m\right) + N\frac{d_m}{np_1p_2} \right\} \ .$$

2. *Find* $\widehat{N}_{\min} > 0$ *such that the jump* $d_{\widehat{m}\left(\left[\widehat{N}_{\min}\right]_-\right)} - d_{\widehat{m}\left(\left[\widehat{N}_{\min}\right]_+\right)}$ *is maximal.*

3. *Select the model* $\widehat{m} = \widehat{m}(2\widehat{N}_{\min})$.

The difference $f(x_-) - f(x_+)$ measures the discontinuity of a function f at the point x. Step 2 may need to introduce huge models in the collection $\mathcal{M}$ all the other ones being considered as "reasonably small". As the function $\widehat{m}(.)$ is piecewise linear with at most $\mathrm{Card}(\mathcal{M})$ jumps, so that steps 1-2 have a complexity $\mathcal{O}\left(\mathrm{Card}(\mathcal{M})\right)^2$. We refer to App.A.1 of [AM09] for more details on the computational aspects of steps 1 and 2. Let us mention that there are other ways of estimating $\widehat{N}_{\min}$ than choosing the largest jump as described in [AM09] App.A.2. Finally, the methodology described in this section straightforwardly extends to the case of isotropic GMRFs estimation by replacing $\widehat{m}(N)$ by $\widehat{m}^{\mathrm{iso}}(N)$ and d_m by d_m^{iso}.

In conclusion, the neighborhood selection procedure described in Algorithm 4.1 is completely data-driven and does not require any prior knowledge on the matrix Σ. Moreover, its computational burden remains small. We illustrate its efficiency in Section 6.

5 Extension to non-toroidal lattices

It is often artificial to consider the field X as stationary on a torus. However, we needed this hypothesis for deriving nonasymptotic properties of the estimator $\widetilde{\theta}$ in [Ver09]. In many applications, it is more realistic to assume that we observe a small window of a Gaussian field defined on the plane $\mathbb{Z}^2$. If we are unable to prove nonasymptotic risk bounds in this new setting. Nevertheless, Lakshman and Derin have shown in [LD93] that there is no phase transition within the valid parameter space for GMRFs defined on the plane $\mathbb{Z}^2$. Let us briefly explain what this means: consider a GMRF defined on a square lattice of size p, but only observed on a square lattice of size p'. The absence of phase transition implies the distribution of this field observed on this fixed window of size p' does not asymptotically depend on the bound conditions when p goes to infinity. Consequently, it is reasonable to think that our estimation procedure still performs well to the price of slight modifications. In the sequel, we assume that the field X is defined on $\mathbb{Z}^2$, but the data $\mathbf{X}$ still correspond to n independent observations of the field X on the window Λ of size $p_1 \times p_2$. The conditional distribution of $X_{[0,0]}$ given the remaining covariates now decomposes as

$$X_{[0,0]} = \sum_{(i,j)\in\mathbb{Z}^2\setminus\{(0,0)\}} \theta_{[i,j]} X_{[i,j]} + \epsilon_{[0,0]} \ , \tag{16}$$

where $\theta_{[.,.]}$ is an "infinite" matrix defined on $\mathbb{Z}^2$ and where $\epsilon_{[0,0]}$ is a centered Gaussian variable of variance σ^2 independent of $(X_{[i,j]})_{(i,j)\in\Lambda\setminus\{(0,0)\}}$. The distribution of the field X is uniquely defined by the function θ and positive number σ^2. The set $\Theta^{+,\infty}$ of valid parameter for θ is now defined using the spectral density function. We refer to Rue and Held [RH05] Sect.2.7 for more details.

Definition 5.1. *A function* $\theta : \mathbb{Z}^2 \to \mathbb{R}$ *belongs to the set* $\Theta^{+,\infty}$ *if it satisfies the three following conditions:*

1. $\theta_{[0,0]} = 0$.

2. *For any* $(i,j) \in \mathbb{Z}^2$, $\theta_{[i,j]} = \theta_{[-i,-j]}$.

3. For any $(\omega_1, \omega_2) \in [0, 2\pi)^2$, $1 - \sum_{(i,j)\in\mathbb{Z}^2} \theta_{[i,j]} \cos(i\omega_1 + j\omega_2) > 0$.

Similarly, we define the set $\Theta^{+,\infty,\text{iso}}$ for the isotropic GMRFs on the lattices. As done in Section 2 for toroidal lattices, we now introduce the parametric parameter sets. For any model $m \in \mathcal{M}_1$, the set $\Theta_m^{+,\infty}$ refers to the subset of matrices θ in $\Theta^{+,\infty}$ whose support is included in m. Analogously, we define the parameter set $\Theta_m^{+,\infty,\text{iso}}$ corresponding to isotropic GMRFs.

We cannot directly extend the CLS empirical contrast $\gamma_{n,p_1,p_2}(.)$ defined in (6) in this new setting because we have to take the edge effect into account. Indeed, if we want to compute the conditional regression of $\mathbf{X}_{i[j_1,j_2]}$, we have to observe *all* its neighbors with respect to m, i.e. $\{\mathbf{X}_{i[j_1+l_1,j_2+l_2]},\ (l_1,l_2) \in m\}$. In this regard, we define the sublattice Λ_m for any model $m \in \mathcal{M}_1$.

$$\Lambda_m := \{(i_1,i_2) \in \Lambda\,,\ (m + (i_1,i_2)) \subset \Lambda\}\ ,$$

where $(m + (i,j))$ denotes the set m of nodes translated by (i,j). For instance, if we consider the model m_1 with four nearest neighbors, the edge effect size is one and Λ_m contains all the nodes that do not lie on the border. The model m_3 with 12 nearest neighbors yields an edge effect of size 2 and Λ_m contains all the nodes in Λ, except those which are at a (euclidean) distance strictly smaller than 2 from the border.

For any model $m \in \mathcal{M}_1$, any $\theta' \in \Theta_m^{+,\infty}$, and any sublattice $\Lambda' \subset \Lambda_m$, we define $\gamma_{n,p_1,p_2}^{\Lambda'}(.)$ as an analogous of $\gamma_{n,p_1,p_2}(.)$ except that it only relies on the conditional regression of the nodes in Λ'.

$$\gamma_{n,p_1,p_2}^{\Lambda'}(\theta') \quad := \quad \frac{1}{n\text{Card}(\Lambda')} \sum_{i=1}^{n} \sum_{(j_1,j_2)\in\Lambda'} \left(\mathbf{X}_{i[j_1,j_2]} - \sum_{(l_1,l_2)\in m} \theta'_{[l_1,l_2]} \mathbf{X}_{i[j_1+l_1,j_2+l_2]} \right)^2 .$$

Then, the *CLS* estimators $\widehat{\theta}_m^{\Lambda'}$ and $\widehat{\theta}_m^{\Lambda',\text{iso}}$ are defined by

$$\widehat{\theta}_m^{\Lambda'} \in \arg\min_{\theta'\in\Theta_m^{+,\infty}} \gamma_{n,p_1,p_2}^{\Lambda'}(\theta') \qquad \text{and} \qquad \widehat{\theta}_m^{\Lambda',\text{iso}} \in \arg\min_{\theta'\in\Theta_m^{+,\infty,\text{iso}}} \gamma_{n,p_1,p_2}^{\Lambda'}(\theta')\ .$$

Contrary to $\widehat{\theta}_m$, the estimator $\widehat{\theta}_m^{\Lambda_m}$ is not necessarily unique especially if the size of Λ_m is smaller than d_m. Let us mention that it is quite classical in the literature to remove nodes to take edge effects or missing data into account (see e.g. [Guy95] Sect.4.3). We cannot use anymore fast Fourier transform for computing the parametric estimator. Nevertheless, the estimators $\widehat{\theta}_m^{\Lambda'}$ are still computationally amenable, since they minimizes a quadratic function on the closed convex set $\Theta_m^{+,\infty}$.

Suppose we are given a subcollection $\mathcal{M}$ of $\mathcal{M}_1$. We note $\Lambda_{\mathcal{M}}$ the smallest sublattice among the collection of lattices Λ_m with $m \in \mathcal{M}$. In order to select the neighborhood $\widehat{m}$, we compute the estimators $\widehat{\theta}_m^{\Lambda_{\mathcal{M}}}$ and minimize the criteria $\gamma_{n,p_1,p_2}^{\Lambda_{\mathcal{M}}}(\widehat{\theta}_m^{\Lambda_{\mathcal{M}}})$ penalized by a quantity of the order $d_m/(n\text{Card}(\Lambda_{\mathcal{M}}))$. We compute the quantities $\gamma_{n,p_1,p_2}^{\Lambda_{\mathcal{M}}}(\widehat{\theta}_m^{\Lambda_{\mathcal{M}}})$ instead of $\gamma_{n,p_1,p_2}^{\Lambda_m}(\widehat{\theta}_m^{\Lambda_m})$ since we want to compare the adequation of the models using the *same* data set.

We now describe a data-driven model selection procedure for choosing the neighborhood. It is based on the slope heuristic developed in the previous section.

Algorithm 5.1. *(Data-driven penalization for non-toroidal lattice).*

1. Compute the selected model $\widehat{m}(N)$ *as a function of* $N > 0$

$$\widehat{m}(N) \in \arg\min_{m\in\mathcal{M}} \left\{ \gamma_{n,p_1,p_2}^{\Lambda_{\mathcal{M}}}(\widehat{\theta}_m^{\Lambda_{\mathcal{M}}}) + N \frac{d_m}{n\,Card(\Lambda_{\mathcal{M}})} \right\}\ .$$

2. *Find* $\widehat{N}_{\min} > 0$ *such that the jump* $d_{\widehat{m}\left([\widehat{N}_{\min}]_-\right)} - d_{\widehat{m}\left([\widehat{N}_{\min}]_+\right)}$ *is maximal.*

3. *Select the model* $\widehat{m} = \widehat{m}(2\widehat{N}_{\min})$.

4. *Compute the estimator* $\widehat{\theta}^{\Lambda_{\widehat{m}}}_{\widehat{m}}$.

This procedure straightforwardly extends to the case of isotropic GMRFs estimation by replacing $\widehat{m}(N)$ by $\widehat{m}^{\text{iso}}(N)$ and d_m by d^{iso}_m. For short, we write $\widetilde{\theta}$ (resp. $\widetilde{\theta}^{\text{iso}}$) for $\widehat{\theta}^{\Lambda_{\widehat{m}}}_{\widehat{m}}$ (resp. $\widehat{\theta}^{\Lambda_{\widehat{m}},\text{iso}}_{\widehat{m}}$). As for Algorithm 4.1, it is advised to introduce huge models in the collection $\mathcal{M}$ in order to better detect the dimension jump. However, when the dimension of the models increases the size of Λ_m decreases and the estimator $\widehat{\theta}^{\Lambda_m}_m$ may become unreliable. The method therefore requires a reasonable number of data. In practice, Λ should not contain less than 100 nodes.

6 Simulation study

In the first simulation experiment, we compare the efficiency of our procedure with penalized maximum likelihood methods when the field is a torus. In the second and third studies, we consider the estimation of a Gaussian field observed on a rectangle. The calculations are made with *R* [R D08]. Throughout these simulations, we only consider isotropic estimators.

6.1 Isotropic GMRF on a torus

First, we consider X an isotropic GMRF on the torus Λ of size $p = p_1 = p_2 = 20$. There are therefore 400 points in the lattice. The number of observations n equals one and the conditional variance σ^2 is one. We introduce a radius $r := \sqrt{17}$. Then, for any number $\phi > 0$, we define the $p \times p$ matrix θ^ϕ as:

$$\left\{ \begin{array}{lcll} {\theta^\phi}_{[0,0]} & := & 0 \ , & \\ {\theta^\phi}_{[i,j]} & := & \phi & \text{if } |(i,j)|_t \leq r \text{ and } (i,j) \neq (0,0) \ , \\ {\theta^\phi}_{[i,j]} & := & 0 & \text{if } |(i,j)|_t > r \ . \end{array} \right.$$

In practice, we set ϕ to 0, 0.0125, 0.015, and 0.0175. Observe that these choices constrain $\|\theta^\phi\|_1 < 1$. The matrix θ^ϕ therefore belongs to the set $\Theta^{+,\text{iso}}_{m_{10}}$ of dimension 10 introduced in Definition 2.1.

First simulation experiment. In Section 3, we have advocated the use of the estimator $\widetilde{\theta}$ instead of $\widetilde{\theta}_\rho$, although theoretical results are only available for $\widetilde{\theta}_\rho$ with $\rho < \infty$. We recall that $\widetilde{\theta} = \widetilde{\theta}_\rho$ with $\rho = \infty$. We check in this simulation study that the performances of $\widetilde{\theta}$ and $\widetilde{\theta}_\rho$ with different values of ρ are similar.

We consider the collection of neighborhoods $\mathcal{M} := \{m_0, m_1, \ldots, m_{20}\}$ whose maximal dimension $d^{\text{iso}}_{m_{20}}$ is 21. The estimator $\widetilde{\theta}^{\text{iso}}$ is built using the CLS model selection procedure introduced in Algorithm 4.1. The estimators $\widetilde{\theta}^{\text{iso}}_\rho$ are computed similarly, except that they are based on the parametric estimators $\widehat{\theta}^{\text{iso}}_{m,\rho}$ (Sect. 3) instead of $\widehat{\theta}^{\text{iso}}_m$.

The Gaussian field X with $\phi = 0.015$ is simulated by using the fast Fourier transform. The quality of the estimations is assessed by the prediction loss function $l(.,.)$ defined in (11). The experiments are repeated 1000 times. For $\rho = 2,\ 4,\ 8$, we evaluate the risks $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\text{iso}}, \theta^\phi)]$ and $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\text{iso}}_\rho, \theta^\phi)]$ as well as the corresponding empirical 95% confidence intervals by a Monte-Carlo

method. We also estimate the risks of $\widehat{\theta}^{\rm iso}_m$ and $\widehat{\theta}^{\rm iso}_{m,\rho}$ for each model $m \in \mathcal{M}$. It then allows to evaluate the oracle risks $\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\rm iso}_{m^*,\rho}, \theta^\phi)]$ and the risk ratios $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\rm iso}_\rho, \theta^\phi)]/\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\rm iso}_{m^*,\rho}, \theta^\phi)]$. The risk ratio measures how well the selected model $\widehat{m}^{\rm iso}$ performs in comparison to the "best" model m^*. Moreover, the risk ratio roughly illustrates the oracle type inequality presented in Theorem 3.1. Indeed, the infimum $\inf_{m\in\mathcal{M}}[l(\theta_{m,\rho}, \theta) + {\rm pen}(m)]$ in (14) is a good measure of the risk $\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\rm iso}_{m^*,\rho}, \theta^\phi)]$ as explained in [Ver09] Sect.4. The results are given in Table 1. They corroborate that the estimators $\widetilde{\theta}^{\rm iso}$ and $\widetilde{\theta}^{\rm iso}_\rho$ perform similarly. Moreover, the risk ratios $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\rm iso}_\rho, \theta^\phi)]/\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\rm iso}_{m^*,\rho}, \theta^\phi)]$ correspond to the ratios

ρ	2	4	8	∞
$\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\rm iso}_\rho, \theta^\phi)] \times 10^2$	4.1 ± 0.1	4.2 ± 0.2	4.2 ± 0.1	4.2 ± 0.3
$\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\rm iso}_\rho, \theta^\phi)]/\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\rm iso}_{m^*,\rho}, \theta^\phi)]$	1.3 ± 0.1	1.3 ± 0.1	1.3 ± 0.1	1.3 ± 0.2

Table 1: First simulation study. Estimates and 95% confidence intervals of the risks $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\rm iso}, \theta^\phi)]$, $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\rm iso}_\rho, \theta^\phi)]$, and of the ratios $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\rm iso}, \theta^\phi)]/\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\rm iso}_{m^*}, \theta^\phi)]$ and $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\rm iso}_\rho, \theta^\phi)]/\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\rm iso}_{m^*,\rho}, \theta^\phi)]$ with $\phi = 0.015$ and $\rho = 2,\ 4,\ 8$.

Second simulation experiment. We compare the efficiency of the method with two alternative model selection procedures. For each of them, we use the collection $\mathcal{M}$ as in the previous experiment. The two alternative procedures are based on likelihood maximization. In this regard, we first define the parametric maximum likelihood estimator $\widehat{\theta}^{\rm mle}_m$ for any model $m \in \mathcal{M}$,

$$\left(\widehat{\theta}^{\rm mle}_m, \widehat{\sigma}^{\rm mle}_m\right) := \arg \min_{\theta' \in \Theta^{+,{\rm iso}}_m, \sigma'} -\mathcal{L}_p(\theta', \sigma', \mathbf{X}) \ ,$$

where $\mathcal{L}_p(\theta', \mathbf{X})$ stands for the log-likelihood at the parameter θ'. We then select a model m applying either an AIC-type criterion [Aka73] or a BIC-type criterion [Sch78]:

$$\begin{aligned} \widehat{m}^{\rm AIC} &:= \arg \min_{m\in\mathcal{M}} \left\{ -2\mathcal{L}_p(\widehat{\theta}^{\rm mle}_m, \widehat{\sigma}^{\rm mle}_m, \mathbf{X}) + 2d^{\rm iso}_m \right\} \ , \\ \widehat{m}^{\rm BIC} &:= \arg \min_{m\in\mathcal{M}} \left\{ -2\mathcal{L}_p(\widehat{\theta}^{\rm mle}_m, \widehat{\sigma}^{\rm mle}_m, \mathbf{X}) + \log(p^2) d^{\rm iso}_m \right\} \ . \end{aligned}$$

For short, we write $\widehat{\theta}^{\rm AIC}$ and $\widehat{\theta}^{\rm BIC}$ for the two obtained estimators $\widehat{\theta}^{\rm mle}_{\widehat{m}^{\rm AIC}}$ and $\widehat{\theta}^{\rm mle}_{\widehat{m}^{\rm BIC}}$. Although AIC and BIC procedures are not justified in this setting, we still apply them as they are widely used in many frameworks. Their computation is performed efficiently using the fast Fourier transform described in Section 2.3.

The experiments are repeated 1000 times. The Gaussian field is simulated using the fast Fourier transform. The quality of the estimations is assessed by the prediction loss function $l(.,.)$. For any ϕ and any of these three estimators, we evaluate the risks $\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\rm AIC}, \theta^\phi)]$, $\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\rm BIC}, \theta^\phi)]$, and $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\rm iso}, \theta^\phi)]$ as well as the corresponding empirical 95% confidence intervals by a Monte-Carlo method. We also estimate the risk ratios $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\rm iso}, \theta^\phi)]/\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\rm iso}_{m^*}, \theta^\phi)]$ The results are given in Table 2.

$\phi \times 10^2$	0	1.25	1.5	1.75
$\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\mathrm{AIC}}, \theta^\phi)] \times 10^2$	1.2 ± 0.2	3.1 ± 0.2	4.3 ± 0.2	6.4 ± 0.2
$\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\mathrm{BIC}}, \theta^\phi)] \times 10^2$	0.01 ± 0.01	1.9 ± 0.1	3.7 ± 0.1	9.7 ± 0.3
$\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\mathrm{iso}}, \theta^\phi)] \times 10^2$	1.6 ± 0.2	3.2 ± 0.2	4.2 ± 0.1	7.2 ± 0.3
$\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\mathrm{iso}}, \theta^\phi)] / \mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\mathrm{iso}}_{m^*}, \theta^\phi)]$	$+\infty$	1.9 ± 0.7	1.3 ± 0.2	1.5 ± 0.3

Table 2: Second simulation study. Estimates and 95% confidence intervals of the risks $\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\mathrm{AIC}}, \theta^\phi)]$, $\mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\mathrm{BIC}}, \theta^\phi)]$, and $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\mathrm{iso}}, \theta^\phi)]$ and of the ratio $\mathbb{E}_{\theta^\phi}[l(\widetilde{\theta}^{\mathrm{iso}}, \theta^\phi)] / \mathbb{E}_{\theta^\phi}[l(\widehat{\theta}^{\mathrm{iso}}_{m^*}, \theta^\phi)]$.

The BIC criterion outperforms the other procedures when $\phi = 0$, 0.0125, or 0.015 but behaves bad for a large ϕ. Indeed, the BIC criterion has a tendency to overpenalize the models. For the two first values of ϕ the oracle model in $\mathcal{M}$ is m_0. Hence, overpenalizing increases the performance of estimation in this case. However, when ϕ increases, the dimension of the oracle model is larger and BIC therefore selects too small models.

In contrast, AIC and the CLS estimator exhibit similar behaviors. If we forget the case $\phi = 0$ for which the oracle risk is 0, the risk of $\widetilde{\theta}^{\mathrm{iso}}$ is close to the risk of the oracle model (the ratio is close to one). Hence, the neighborhood choice for $\widetilde{\theta}^{\mathrm{iso}}$ is almost optimal.

In conclusion, $\widetilde{\theta}^{\mathrm{iso}}$ or $\widehat{\theta}^{\mathrm{AIC}}$ both exhibit good performances for estimating the distribution of a regular Gaussian field on a torus. The strength of our neighborhood selection procedure lies in the fact it easily generalizes to non-toroidal lattices as illustrated in the next section.

6.2 Isotropic Gaussian fields on $\mathbb{Z}^2$

First simulation experiment. We now consider X an isotropic Gaussian field defined on $\mathbb{Z}^2$ but only observed on a square Λ of sizes $p = p_1 = p_2 = 20$ or $p = p_1 = p_2 = 100$. This corresponds to the setting described in Section 5. The variance of $X_{[0,0]}$ is set to one and the distribution of the field is therefore uniquely defined by its correlation function $\rho(k,l) := \mathrm{corr}(X_{[k,l]}, X_{[0,0]})$. Again, the number of replications n is chosen to be one. In the first experiment, we use four classical correlation functions: exponential, spherical, circular, and Matérn (e.g. [Cre93] Sect.2.3.1 and [Mat86]).

$$\text{Exponential:} \quad \rho(k,l) = \exp\left(-\frac{d(k,l)}{r}\right)$$

$$\text{Circular:} \quad \rho(k,l) = \begin{cases} 1 - \frac{2}{\pi}\left[\frac{d(k,l)}{r}\sqrt{1-\left(\frac{d(k,l)}{r}\right)^2} + \sin^{-1}\left(\sqrt{\frac{d(k,l)}{r}}\right)\right] & \text{if} \quad d(k,l) \le r \\ 0 & \text{else} \end{cases}$$

$$\text{Spherical:} \quad \rho(k,l) = \begin{cases} 1 - 1.5\frac{d(k,l)}{r} + 0.5\left(\frac{d(k,l)}{r}\right)^3 & \text{if} \quad d(k,l) \le r \\ 0 & \text{else} \end{cases}$$

$$\text{Matérn:} \quad \rho(k,l) = \frac{1}{2^{\kappa-1}\Gamma(\kappa)}\left(\frac{d(k,l)}{r}\right)^\kappa \mathcal{K}_\kappa\left(\frac{d(k,l)}{r}\right),$$

where $d(k,l)$ denotes the euclidean distance from (k,l) to $(0,0)$ and $\mathcal{K}_\kappa(.)$ is the modified Bessel function of order κ. In a nutshell, the parameter r represents the range of correlation, whereas κ

may be regarded as a smoothness parameter for the Matérn function. In this simulation experiment, we set r to 3. When considering the Matérn model, we take κ equal to 0.05, 0.25, 0.5, 1, 2, and 4.

The Gaussian fields are simulated using the function *GaussRF* in the library *RandomFields* [Sch09]. For each of experiments, we compute the estimator $\widetilde{\theta}^{\text{iso}}$ based on Algorithm 5.1 with the collection $\mathcal{M} := \{m \in \mathcal{M}_1 \, , \, d_m^{\text{iso}} \leq 18\}$. Since the lattice Λ is not a torus, methods based on likelihood maximization exhibit a prohibitive computational burden. Consequently, we do not use MLE in this experiment. We shall compare the efficiency of $\widetilde{\theta}^{\text{iso}}$ with a variogram-based estimation method.

We recall that the linear combination $\sum_{(i,j)\in\Lambda\setminus\{(0,0)\}} \theta_{[i,j]} X_{[i,j]}$ is the kriging predictor of $X_{[0,0]}$ given the remaining variables (Equation (1)). A natural method to estimate θ in this spatial setting amounts to estimating the variogram of the observed Gaussian field and then performing ordinary kriging at the node $(0,0)$. More precisely, we first estimate the empirical variogram by applying the modulus estimator of Hawkes and Cressie (e.g. [Cre93] Eq.(2.2.8)) to the observed field of 400 points. Afterwards, we fit this empirical variogram to a variogram model using the reweighted least-squares suggested by Cressie [Cre85]. This procedure therefore requires the choice of a particular variogram model. In the first simulation study, we choose *the model* that has generated the data. Observe that this method is *not* adaptive since it requires the knowledge of the variogram model. In practice, we use Library *geoR* [RJD01] implemented in *R* [R D08] to estimate the parameters r, $\text{var}(X_{[0,0]})$ and eventually κ of the variogram model. Then, we compute the estimator $\widehat{\theta}^V$ by performing ordinary kriging at the center node of Λ. For each of these estimations, we assume that the variogram model is known. For computational reasons, we use a kriging neighborhood of size 11×11 that contains 120 points. Previous simulations have indicated that this neighborhood choice does not decrease the precision of the estimation. For the Matèrn model with $\kappa = 2$ and 4, the covariance is almost singular. There are sometimes inversion difficulties and we therefore use kriging neighborhood of respective size 7×7 and 3×3.

We again assess the performances of the procedures using the loss $l(.,.)$. Even if this loss is defined in (11) for a torus, the alternative definition (12) clearly extends to this non-toroidal setting. Consequently, the loss $l(\widehat{\theta}, \theta)$ measures the difference between the prediction error of $X_{[0,0]}$ when using $\sum_{(i,j)\in\Lambda\setminus\{(0,0)\}} \widehat{\theta}_{[i,j]} X_{[i,j]}$ and the prediction error of $X_{[0,0]}$ when using the best predictor $\mathbb{E}[X_{[0,0]}|(X_{[i,j]})_{(i,j)\in\Lambda\setminus\{(0,0)\}}]$. In other words, $l(\widehat{\theta}, \theta)$ is the difference of the kriging error made with the estimated parameters $\widehat{\theta}$ and the kriging error made with the true parameter θ.

The experiments are repeated 1000 times. For any of the four correlation models previously mentioned, we evaluate the risks $\mathbb{E}_\theta[l(\widetilde{\theta}^{\text{iso}}, \theta)]$ and $\mathbb{E}_\theta[l(\widehat{\theta}^V, \theta)]$ by Monte-Carlo. In order to assess the efficiency of the selection procedure, we also evaluate the risk ratio

$$Risk.ratio = \frac{\mathbb{E}_\theta[l(\widehat{\theta}^{\Lambda_{\mathcal{M}},\text{iso}}_{\widehat{m}}, \theta)]}{\mathbb{E}_\theta[l(\widehat{\theta}^{\Lambda_{\mathcal{M}},\text{iso}}_{m^*}, \theta)]} \, .$$

As in Section 6.1, the oracle risk $\mathbb{E}[l(\widehat{\theta}^{\Lambda_{\mathcal{M}},\text{iso}}_{m^*}, \theta)]$ is evaluated by taking the minimum of the evaluations of the risks $\mathbb{E}[l(\widehat{\theta}^{\Lambda_{\mathcal{M}},\text{iso}}_{m}, \theta)]$ over all models $m \in \mathcal{M}$. Results of the simulation experiment are given in Table 3 and 4.

Observe that none of the fields considered in this study are GMRFs. Here, the GMRF models should only be viewed as a collection of approximation sets of the true distribution. This simulation experiment is in the spirit of Rue and Tjelmeland's study [RT02]. However, there are some major differences. Contrary to them, we perform estimation and not only approximation. Moreover, our

lattice is not a torus. Finally, we use our prediction loss $l(.,.)$ to assess the performance, whereas they compare the correlation functions.

Model	Exponential	Circular	Spherical
$\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta]\times 10^2$	0.08 ± 0.01	9.1 ± 0.5	2.9 ± 0.1
$\mathbb{E}_\theta[l(\widetilde{\theta}^{\rm iso},\theta)]\times 10^2$	1.08 ± 0.01	6.5 ± 0.1	3.4 ± 0.1
Risk.ratio	3.6 ± 0.4	1.4 ± 0.1	1.6 ± 0.1

Table 3: Estimates and 95% confidence intervals of the risks $\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]$ and $\mathbb{E}_\theta[l(\widetilde{\theta}^{\rm iso},\theta)]$ and of *Risk.ratio* for the exponential, circular and spherical models with $p=20$.

κ	0.05	0.25	0.5	1
$\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]\times 10^3$	91.8 ± 0.7	80.0 ± 0.2	18.0 ± 0.1	2.5 ± 0.1
$\mathbb{E}_\theta[l(\widetilde{\theta}^{\rm iso},\theta)]\times 10^3$	2.24 ± 0.01	0.62 ± 0.01	0.33 ± 0.01	0.08 ± 0.01
Risk.ratio	1.3 ± 0.1	1.7 ± 0.2	1.5 ± 0.2	1.3 ± 0.1

κ	2	4
$\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]\times 10^4$	6.3 ± 1.1	0.011 ± 0.001
$\mathbb{E}_\theta[l(\widetilde{\theta}^{\rm iso},\theta)]\times 10^4$	1.9 ± 0.1	0.17 ± 0.01
Risk.ratio	2.6 ± 0.2	1.1 ± 0.1

Table 4: Estimates and 95% confidence intervals of the risks $\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]$ and $\mathbb{E}_\theta[l(\widetilde{\theta}^{\rm iso},\theta)]$ and of *Risk.ratio* for Matérn model with $p=100$.

Comments on Tables 3 and 4. In both tables, the ratio $\mathbb{E}_\theta[l(\widehat{\theta}^{\Lambda_{\mathcal{M}},{\rm iso}}_{\widehat{m}},\theta)]/\mathbb{E}_\theta[l(\widehat{\theta}^{\Lambda_{\mathcal{M}},{\rm iso}}_{m^*},\theta)]$ stays close to one. Hence, the model selection is almost optimal from an efficiency point of view. In most of the cases, the estimator $\widetilde{\theta}^{\rm iso}$ outperforms the estimator $\widehat{\theta}^V$ based on geostatistical methods. This is particularly striking for the Matérn correlation model because in that case the computation of $\widehat{\theta}^V$ requires the estimation of the additional parameter κ. Indeed, let us recall that the exponential model and the Matérn model with $\kappa=0.5$ are equivalent. For $\kappa=0.5$, the risk of $\widehat{\theta}^V$ is 100 times higher when κ has to be estimated than when κ is known.

Second simulation experiment. The kriging estimator $\widehat{\theta}^V$ requires the knowledge or the choice of a correlation model. In the second simulation experiment, the correlation of X is the Matèrn function with range $r=3$ and $\kappa=0.05$. The size p of the lattice is chosen to be 100. We now estimate θ using *different* variogram models, namely the exponential, the circular, the spherical and the Matèrn model. The estimator $\widetilde{\theta}^{\rm iso}$ for such a field was already considered in Table 4. The experiment is repeated 1000 times.

Comments on Table 5. One observes that circular and spherical models yield worse performances than Matèrn model. In contrast, the exponential model behaves better. The choice of the variogram model therefore seems critical to get good performances. The model selection estimator $\widetilde{\theta}^{\rm iso}$ (Table 4) exhibits a smaller risk than the exponential model.

Model	Exponential	Circular	Spherical	Matèrn
$\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]\times 10^3$	48.3 ± 0.4	461 ± 16	293 ± 7	91.8 ± 0.7

Table 5: Estimates and 95% confidence intervals of the risks $\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]$ for Matérn model with $\kappa=0.05$ when using the exponential, circular, spherical, and Matèrn models with $p=100$.

6.3 Anisotropic Gaussian fields on $\mathbb{Z}^2$

We still consider X a Gaussian field observed on a square Λ of size 100×100. Contrary to the previous study, the field is not assumed to be isotropic. To model the geometric anisotropy, we suppose that X is an isotropic field on a deformed lattice Λ'. The transformation consists in multiplying the original coordinates by a rotation R and a shrinking matrix T. For the sake of simplicity, we take the identity for R. The shrinking matrix T is defined by the anisotropy ratio (*Ani.ratio*). It corresponds to the ratio between the directions with smaller and greater continuity in the field X, i.e the ratio between maximum and minimum ranges. In this experiment, X follows a Matèrn correlation with range $r=3$, $\kappa=0.05$, 0.25, 0.5, 1, 2, and 4 and *Ani.ratio*=2 or 5. We compute the anisotropic estimator $\widetilde{\theta}$ based on Algorithm 5.1 with the collection $\mathcal{M}:=\{m\in\mathcal{M}_1, d_m\le 28\}$. As a benchmark, we also compute the variogram-based estimator $\widehat{\theta}^V$ based on the Matèrn model. In order to compute $\widehat{\theta}^V$, we assume that we *know* the anisotropy ratio and the anisotropy directions. Observe that the estimator $\widetilde{\theta}$ does not require any assumption on the form of anisotropy, while $\widehat{\theta}^V$ uses the geometric parameters of the anisotropy.

The experiments are repeated 1000 times. We evaluate the risks $\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]$ and $\mathbb{E}_\theta[l(\widetilde{\theta},\theta)]$ and the risk ratio defined by

$$Risk.ratio=\frac{\mathbb{E}_\theta[l(\widehat{\theta}^{\Lambda,\mathcal{M}}_{\widehat{m}},\theta)]}{\mathbb{E}_\theta[l(\widehat{\theta}^{\Lambda,\mathcal{M}}_{m^*},\theta)]}\ .$$

κ	0.05	0.25	0.5	1
$\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]\times 10^2$	15.8 ± 0.1	13.9 ± 0.1	3.3 ± 0.1	0.30 ± 0.01
$\mathbb{E}_\theta[l(\widetilde{\theta},\theta)]\times 10^2$	0.65 ± 0.01	0.20 ± 0.01	0.089 ± 0.001	0.17 ± 0.01
Risk.ratio	1.2 ± 0.1	1.1 ± 0.1	1.1 ± 0.1	1.7 ± 0.2

κ	2	4
$\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]\times 10^4$	9.8 ± 0.1	0.020 ± 0.001
$\mathbb{E}_\theta[l(\widetilde{\theta}^{\mathrm{iso}},\theta)]\times 10^4$	45.0 ± 0.1	4.3 ± 0.1
Risk.ratio	2.9 ± 0.2	22.3 ± 1.7

Table 6: Estimates and 95% confidence intervals of the risks $\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]$ and $\mathbb{E}_\theta[l(\widetilde{\theta},\theta)]$ and of *Risk.ratio* for Matérn model and *Ani.ratio*= 2.

Comments on Tables 6 and 7. Except for the cases $\kappa=2,4$, the estimator $\widetilde{\theta}$ performs better than the variogram-based estimator $\widehat{\theta}^V$, although $\widehat{\theta}^V$ uses the true anisotropy parameters. For $\kappa=4$, the neighborhood selection is no performed efficiently (the risk ratio is large).

κ	0.05	0.25	0.5	1
$\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]\times 10^2$	11.2 ± 0.1	14.9 ± 0.1	3.7 ± 0.1	2.9 ± 0.1
$\mathbb{E}_\theta[l(\widetilde{\theta},\theta)]\times 10^2$	0.66 ± 0.1	0.40 ± 0.01	0.081 ± 0.001	0.14 ± 0.01
Risk.ratio	1.1 ± 0.1	1.1 ± 0.1	1.2 ± 0.1	3.4 ± 0.8

κ	2	4
$\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]\times 10^4$	30.6 ± 0.1	0.22 ± 0.01
$\mathbb{E}_\theta[l(\widetilde{\theta}^{\mathrm{iso}},\theta)]\times 10^4$	38.0 ± 0.1	39.6 ± 0.1
Risk.ratio	2.1 ± 0.1	9.0 ± 1.4

Table 7: Estimates and 95% confidence intervals of the risks $\mathbb{E}_\theta[l(\widehat{\theta}^V,\theta)]$ and $\mathbb{E}_\theta[l(\widetilde{\theta},\theta)]$ and of *Risk.ratio* for Matérn model and *Ani.ratio*$= 5$.

7 Discussion

In this paper, we have extended a neighborhood selection procedure introduced in [Ver09]. On the one hand, an algorithm is provided for tuning the penalty in practice. On the other hand, the new method also handles non-toroidal lattices. The computational complexity remains reasonable even when the size of the lattice is large.

In the case of stationary fields on a torus, our neighborhood selection procedure exhibits a computational burden and statistical performances analogous to the AIC procedure. Even if AIC has not been analyzed from an efficiency point of view, this suggests that AIC may achieve an oracle inequality in this setting. Moreover, we have empirically checked that $\widetilde{\theta}$ performs almost as well as the oracle model since the oracle ratio $\mathbb{E}[l(\widetilde{\theta},\theta)]/\mathbb{E}[l(\widehat{\theta}_{m^*},\theta)]$ remains close to one.

The strength of this neighborhood selection procedure lies in the fact it easily extends to non-toroidal lattices. We have illustrated that our method often outperforms variogram-based estimation methods in terms of the mean-squared prediction error. Moreover, the procedure behaves almost as well as the oracle. In contrast, variogram-based procedures may perform well for some covariances structure but also yield terrible results for other covariance structures. These results illustrate the *adaptivity* of the neighborhood selection procedure.

In many statistical applications, Gaussian fields (or Gaussian Markov random fields) are not directly observed. For instance, Aykroyd [Ayk98] or Dass and Nair [DN03] use compound Gaussian Markov random fields to account for non stationarity and steep variations. The wavelet transform has emerged as a powerful tool in image analysis. The wavelet coefficients of an image are sometimes modeled using hidden Markov models [CNB98, PSWS03]. More generally, the success of the GMRFs is mainly due to the use of hierarchical models involving latent GMRFs [RMC09]. The study and the implementation of our penalization strategy for selecting the complexity of latent Markov models is an interesting direction of research.

8 Proofs

Let us introduce some notations that shall be used throughout the proofs. For any $1 \leq k \leq n$, the vector $\mathbf{X}_k^v$ denotes the vectorialized version of the k-th sample of X. Moreover, $\mathbf{X}^{\mathbf{v}}$ is the matrix

of size $p_1p_2 \times n$ of the n realisations of the vector $\mathbf{X}_k^v$. Throughout these proofs, L, L_1, L_2 denote constants that may vary from line to line. The notation $L(.)$ specifies the dependency on some quantities. Finally, the $\gamma(.)$ function stands for an infinite sampled version of the CLS criterion $\gamma_{n,p_1,p_2}(.)$: $\gamma(.) := \mathbb{E}[\gamma_{n,p_1,p_2}(.)]$.

8.1 Proof of Lemma 2.1

Let us provide an alternative expression of $\gamma_{n,p_1,p_2}(\theta')$ in term of the factor $C(\theta')$ and the empirical covariance matrix $\overline{\mathbf{X^v}\mathbf{X^{v*}}}$.

$$\gamma_{n,p_1,p_2}(\theta') \quad = \quad \frac{1}{np_1p_2} tr\left[(I_{p_1p_2} - C(\theta'))\overline{\mathbf{X^v}\mathbf{X^{v*}}}(I_{p_1p_2} - C(\theta'))\right] \ . \tag{17}$$

This is justified in [Ver09] Sect.2.2.

Lemma 8.1. *There exists an orthogonal matrix P which simultaneously diagonalizes every $p_1p_2 \times p_1p_2$ symmetric block circulant matrices with $p_2 \times p_2$ blocks. Let θ be a matrix of size $p_1 \times p_2$ such that $C(\theta)$ is symmetric. The matrix $D(\theta) = P^*C(\theta)P$ is diagonal and satisfies*

$$D(\theta)_{[(i-1)p_2+j,(i-1)p_2+j]} = \sum_{k=1}^{p_1}\sum_{l=1}^{p_2} \theta_{[k,l]} \cos\left[2\pi(ki/p_1 + lj/p_2)\right] \ , \tag{18}$$

for any $1 \leq i \leq p_1$ and $1 \leq j \leq p_2$.

This lemma is proved as in [RH05] Sect.2.6.2 to the price of a slight modification that takes into account the fact that P is orthogonal and not unitary. The difference comes from the fact that contrary to Rue and Held we also assume that $C(\theta)$ is symmetric. Lemma 8.1 states that all symmetric block circulant matrices are simultaneously diagonalizable. Observe that for any $1 \leq i \leq p_1$ and $1 \leq j \leq p_2$, it holds that $D(\theta)_{[(i-1)p_2+j,(i-1)p_2+j]} = \lambda_{[i,j]}(\theta)$ since $\theta_{[k,l]} = \theta_{[p_1-k,p_2-l]}$. Hence, Expression (17) becomes

$$\gamma_{n,p_1,p_2}(\theta') \quad = \quad \frac{1}{np_1p_2}\left\{ \sum_{i=1}^{p_1}\sum_{j=1}^{p_2} \left[1 - \lambda_{[i,j]}(\theta)\right]^2 \left[\sum_{k=1}^{n} \left[P^*\mathbf{X}_k^v(\mathbf{X}_k^v)^*P\right]_{[(i-1)p_2+j,(i-1)p_2+j]}\right]\right\} ,$$

where $\mathbf{X}_k^v$ is the vectorialized version of the k-th observation of the field X. Straightforward computations allow us to prove that the quantities

$$\left(P^*\mathbf{X}_k^v(\mathbf{X}_k^v)^*P\right)_{[(i-1)p_2+j,(i-1)p_2+j]} + \left(P^*\mathbf{X}_k^v(\mathbf{X}_k^v)^*P\right)_{[(p_1-i-1)p_2+p_2-j,(p_1-i-1)p_2+p_2-j]}$$

and

$$\frac{1}{\sqrt{p_1p_2}}\lambda_{[i,j]}(\mathbf{X}_k^v)\overline{\lambda_{[i,j]}(\mathbf{X}_k^v)} + \frac{1}{\sqrt{p_1p_2}}\lambda_{[p_1-i,p_2-j]}(\mathbf{X}_k^v)\overline{\lambda_{[p_1-i,p_2-j]}(\mathbf{X}_k^v)}$$

are equal for any $1 \leq i \leq p_1$ and $1 \leq j \leq p_2$. Here, the entries of the matrix $\lambda(.)$ are taken modulo p_1 and p_2 and the entries of $[P^*\mathbf{X}_k^v(\mathbf{X}_k^v)^*P]$ are taken modulo p_1p_2. The result of Lemma 2.1 follows.

8.2 Proof of Proposition 4.1

Proof of Proposition 4.1. We only consider the anisotropic case, since the proof for isotropic estimation is analogous. For any model $m \in \mathcal{M}_1$, we define

$$\Delta(m,m') := \gamma_{n,p,p}\left(\widehat{\theta}_{m,\rho}\right) + \mathrm{pen}(m) - \gamma_{n,p,p}\left(\widehat{\theta}_{m',\rho}\right) - \mathrm{pen}(m') \ .$$

We aim at showing that with large probability, the quantity $\Delta(m,m')$ is positive for all small dimensional models m. Hence, we would conclude that the dimension of $\widehat{m}$ is large. In this regard, we bound the deviations of the differences

$$\begin{aligned}\gamma_{n,p,p}\left(\widehat{\theta}_{m,\rho}\right) - \gamma_{n,p,p}\left(\widehat{\theta}_{m',\rho}\right) &= \left[\gamma_{n,p,p}\left(\widehat{\theta}_{m,\rho}\right) - \gamma_{n,p,p}\left(\theta_{m,\rho}\right)\right] + \left[\gamma_{n,p,p}\left(\theta_{m,\rho}\right) - \gamma_{n,p,p}\left(\theta\right)\right] \\ &+ \left[\gamma_{n,p,p}(\theta) - \gamma_{n,p,p}\left(\widehat{\theta}_{m',\rho}\right)\right] \ .\end{aligned}$$

Lemma 8.2. *Let K_2 be some universal constant that we shall define in the proof. With probability larger than $3/4$,*

$$\gamma_{n,p,p}(\theta) - \gamma_{n,p,p}(\theta_{m,\rho}) \leq \frac{K_2}{2}\rho^2\varphi_{max}(\Sigma)\frac{d_m \vee 1}{np^2}$$

and

$$\gamma_{n,p,p}\left(\theta_{m,\rho}\right) - \gamma_{n,p,p}\left(\widehat{\theta}_{m,\rho}\right) \leq \frac{K_2}{2}\rho^2\varphi_{max}(\Sigma)\frac{d_m}{np^2}$$

for all models $m \in \mathcal{M}_1$.

Lemma 8.3. *Assume that p is larger than some numerical constant p_0. With probability larger than $3/4$, it holds that*

$$\gamma_{n,p,p}(\theta) - \gamma_{n,p,p}(\widehat{\theta}_{m',\rho}) \geq K_3\sigma^2\left\{\varphi_{min}\left(I_{p^2} - C(\theta)\right) \wedge \left[\rho - \varphi_{max}\left(I_{p^2} - C(\theta)\right)\right]\right\}\frac{d_{m'}}{np^2} \ ,$$

where K_3 is a universal constant defined in the proof.

Let us take K_1 to be exactly K_3. Gathering the two last lemma with Assumption (15), there exists an event Ω of probability larger than $1/2$ such that

$$\Delta(m,m') \geq \frac{\sigma^2}{np^2}\left\{K_1\eta d_{m'}\left[\varphi_{\min}\left(I_{p^2} - C(\theta)\right) \wedge \left[\rho - \varphi_{\max}\left(I_{p^2} - C(\theta)\right)\right]\right] - K_2\frac{(d_m \vee 1)\rho^2}{\varphi_{\min}\left(I_{p^2} - C(\theta)\right)}\right\} \ ,$$

for all models $m \in \mathcal{M}_1$. Thus, conditionally to Ω, $\Delta(m,m')$ is positive for all models $m \in \mathcal{M}_1$ that satisfy

$$\frac{d_m \vee 1}{d_{m'}} \leq \frac{K_3\eta}{K_2\rho^2}\varphi_{\min}\left(I_{p^2} - C(\theta)\right)\left\{\varphi_{\min}\left(I_{p^2} - C(\theta)\right) \wedge \left[\rho - \varphi_{\max}\left(I_{p^2} - C(\theta)\right)\right]\right\} \ .$$

By Lemma 8.7 in [Ver09], the dimension $d_{m'}$ is larger than $0.5[\sqrt{np^2} \wedge (p^2 - 1)]$. We conclude that

$$d_{\widehat{m}_\rho} \vee 1 \geq \left[\sqrt{np^2} \wedge p^2 - 1\right]\frac{K_3\eta}{K_2\rho^2}\varphi_{\min}\left(I_{p^2} - C(\theta)\right)\left\{\varphi_{\min}\left(I_{p^2} - C(\theta)\right) \wedge \left[\rho - \varphi_{\max}\left(I_{p^2} - C(\theta)\right)\right]\right\} \ ,$$

with probability larger than $1/2$. □

Proof of Lemma 8.2. In the sequel, $\overline{\gamma}_{n,p,p}(.)$ denotes the difference $\gamma_{n,p,p}(.)$ -$\gamma(.)$. Given a model m, we consider the difference

$$\gamma_{n,p,p}(\theta) - \gamma_{n,p,p}(\theta_{m,\rho}) \quad = \quad \overline{\gamma}_{n,p,p}(\theta) - \overline{\gamma}_{n,p,p}(\theta_{m,\rho}) - l(\theta_{m,\rho},\theta) \ .$$

Upper bounding the difference of $\gamma_{n,p,p}$ therefore amounts to bounding the difference of $\overline{\gamma}_{n,p,p}$. By definition of $\gamma_{n,p,p}$ and γ, it expresses as

$$\overline{\gamma}_{n,p,p}(\theta) - \overline{\gamma}_{n,p,p}(\theta_{m,\rho}) \quad = \quad \frac{1}{p^2} tr\left\{\left[(I_{p^2} - C(\theta))^2 - (I_{p^2} - C(\theta_{m,\rho}))^2\right]\left(\overline{\mathbf{X^v X^{v*}}} - \Sigma\right)\right\} \ .$$

The matrices Σ, $(I_{p^2} - C(\theta))$, and $(I_{p^2} - C(\theta_{m,\rho}))$ are symmetric block circulant. By Lemma 8.1, they are jointly diagonalizable in the same orthogonal basis. If we note P an orthogonal matrix associated to this basis, then $C(\theta_{m,\rho})$, $C(\theta)$, and Σ respectively decompose in

$$C(\theta_{m,\rho}) = P^* D(\theta_{m,\rho}) P \ , \ C(\theta) = P^* D(\theta) P \ \text{ and } \Sigma = P^* D(\Sigma) P \ ,$$

where the matrices $D(\theta_{m,\rho})$, $D(\theta)$, and $D(\Sigma)$ are diagonal.

$$\begin{aligned} \overline{\gamma}_{n,p,p}(\theta) \quad - \quad & \overline{\gamma}_{n,p,p}(\theta_{m,\rho}) = \\ & \frac{1}{p^2} tr\left\{\left(D(\theta_{m,\rho}) - D(\theta)\right)\left[2I_{p^2} - D(\theta) - D(\theta_{m,\rho})\right] D_\Sigma\left(\overline{\mathbf{YY}^*} - I_{p^2}\right)\right\} \ , \end{aligned} \tag{19}$$

where the matrix $\mathbf{Y}$ is defined as $P\sqrt{\Sigma^{-1}}\mathbf{X}^v P^*$. Its components follow independent standard Gaussian distributions. Since the matrices involved in (19) are diagonal, Expression (19) is a linear combination of centered χ^2 random variables. We apply the following lemma to bound its deviations.

Lemma 8.4. *Let $(Y_1, \ldots, Y_D)$ be i.i.d. standard Gaussian variables. Let $a_1, \ldots, a_D$ be fixed numbers. We set*

$$\|a\|_\infty := \sup_{i=1,\ldots,D} |a_i|, \quad \|a\|_2^2 := \sum_{i=1}^D a_i^2$$

Let T be the random variable defined by

$$T := \sum_{i=1}^D a_i \left(Y_i^2 - 1\right) \ .$$

Then, the following deviation inequality holds for any positive x

$$\mathbb{P}\left[T \geq 2\|a\|_2\sqrt{x} + 2\|a\|_\infty x\right] \leq e^{-x} \ .$$

This result is very close to Lemma 1 of Laurent and Massart in [LM00]. The only difference lies in the fact that they constrain the coefficients a_i to be non-negative. Nevertheless, their proof easily extends to our situation. Let us define the matrix a of size $n \times p^2$ as

$$a^i[j] := \frac{D_{\Sigma[i,i]}\left(D(\theta_{m,\rho})_{[i,i]} - D(\theta)_{[i,i]}\right)\left(2 - D(\theta[i,i] - D(\theta_{m,\rho})[i,i]\right)}{np^2} \ ,$$

for any $1 \leq i \leq n$ and any $1 \leq j \leq p^2$. Since the matrices $I - C(\theta)$ and $I - C(\theta_{m,\rho})$ belong to the set Θ_ρ^+, their largest eigenvalue is smaller than ρ. By Definition (11) of the loss function $l(.,.)$, $\|a\|_2 \leq 2\rho\sqrt{\varphi_{\max}(\Sigma) l(\theta_{m,\rho},\theta)/(np^2)}$ and $\|a\|_\infty \leq 4\rho^2\varphi_{\max}(\Sigma)/(np^2)$. By Applying Lemma 8.4 to Expression (19), we conclude that

$$\mathbb{P}\left[\overline{\gamma}_{n,p,p}(\theta) - \overline{\gamma}_{n,p,p}(\theta_{m,\rho}) \geq l(\theta_{m,\rho},\theta) + 12\rho^2\frac{\varphi_{\max}(\Sigma)}{np^2}x\right] \leq e^{-x} ,$$

for any $x > 0$. Consequently, for any $K > 0$, the difference of $\gamma_{n,p,p}(.)$ satisfies

$$\gamma_{n,p,p}(\theta) - \gamma_{n,p,p}(\theta_{m,\rho}) \leq \frac{K}{2}\rho^2\varphi_{\max}(\Sigma)\frac{d_m \vee 1}{np^2} ,$$

simultaneously for all models $m \in \mathcal{M}_1$ with probability larger than $1 - \sum_{m\in\mathcal{M}_1\setminus\emptyset} e^{-K(d_m\vee 1)/24}$. If K is chosen large enough, the previous upper bound holds on an event of probability larger than $7/8$. Let us call K_2' such a value.

Let us now turn to the second part of the result. As previously, we decompose the difference of empirical contrasts

$$\gamma_{n,p,p}(\theta_{m,\rho}) - \gamma_{n,p,p}\left(\widehat{\theta}_{m,\rho}\right) = \overline{\gamma}_{n,p,p}(\theta_{m,\rho}) - \overline{\gamma}_{n,p,p}\left(\widehat{\theta}_{m,\rho}\right) - l\left(\widehat{\theta}_{m,\rho},\theta_{m,\rho}\right)$$

Arguing as in the proof of Theorem 3.1 in [Ver09], we obtain an upper bound analogous to Eq.(49) in [Ver09]

$$\overline{\gamma}_{n,p,p}(\theta_{m,\rho}) - \overline{\gamma}_{n,p,p}\left(\widehat{\theta}_{m,\rho}\right) \leq l(\widehat{\theta}_{m,\rho},\theta_{m,\rho}) + \rho^2\left\{\sup_{R\in\mathcal{B}^{\mathcal{H}'}_{m^2,m^2}}\frac{1}{p^2}tr\left[RD_\Sigma\left(\overline{\mathbf{Y}\mathbf{Y}^*} - I_{p^2}\right)\right]\right\}^2 .$$

The set $\mathcal{B}^{\mathcal{H}'}_{m^2,m^2}$ is defined in the proof of Lemma 8.2 in [Ver09]. Its precise definition is not really of interest in this proof. Coming back to the difference of $\gamma_{n,p,p}(.)$, we get

$$\gamma_{n,p,p}(\theta_{m,\rho}) - \gamma_{n,p,p}\left(\widehat{\theta}_{m,\rho}\right) \leq \rho^2\left\{\sup_{R\in\mathcal{B}^{\mathcal{H}'}_{m^2,m^2}}\frac{1}{p^2}tr\left[RD_\Sigma\left(\overline{\mathbf{Y}\mathbf{Y}^*} - I_{p^2}\right)\right]\right\}^2 .$$

We consecutively apply Lemma 8.3 and 8.4 in [Ver09] to bound the deviation of this supremum. Hence, for any positive number α,

$$\gamma_{n,p,p}(\theta_{m,\rho}) - \gamma_{n,p,p}\left(\widehat{\theta}_{m,\rho}\right) \leq L_1(1+\alpha/2)\rho^2\varphi_{\max}(\Sigma)\frac{d_m}{np^2} . \tag{20}$$

with probability larger than $1 - \exp[-L_2\sqrt{d_m}(\frac{\alpha}{\sqrt{1+\alpha/2}} \wedge \frac{\alpha^2}{1+\alpha/2})]$. Thus, there exists some numerical constant α_0 such that the upper bound (20) with $\alpha = \alpha_0$ holds simultaneously for all models $m \in \mathcal{M}_1 \setminus \emptyset$ with probability larger than $7/8$. Choosing K_2 to be the supremum of K_2' and $2L_1(1+\alpha_0/2)$ allows to conclude.

□

Proof of Lemma 8.3. Thanks to the definition (17) of $\gamma_{n,p,p}(.)$ we obtain

$$\gamma_{n,p,p}(\theta) - \gamma_{n,p,p}(\widehat{\theta}_{m',\rho}) = \frac{1}{p^2} \sup_{\theta' \in \Theta^+_{m',\rho}} tr\left[(C(\theta') - C(\theta)) \left(2I_{p^2} - C(\theta) - C(\theta') \right) \Sigma \overline{\mathbf{Z}\mathbf{Z}^*} \right] ,$$

where the $p^2 \times n$ matrix $\mathbf{Z}$ is defined by $\mathbf{Z} := \sqrt{\Sigma}^{-1} \mathbf{X}^{\mathbf{v}}$. We recall that the matrices Σ, $C(\theta)$ and $C(\theta')$ commute since they are jointly diagonalizable by Lemma 8.1. Let $(\Theta^+_{m',\rho} - \theta)$ be the set $\Theta^+_{m',\rho}$ translated by θ. Since $C(\theta) + C(\theta') = C(\theta + \theta')$, we lower bound the difference of $\gamma_{n,p,p}(.)$ as follows

$$\begin{aligned} \gamma_{n,p,p}(\theta) - \gamma_{n,p,p}(\widehat{\theta}_{m',\rho}) &= \frac{1}{p^2} \sup_{\theta' \in \left(\Theta^+_{m',\rho} - \theta \right)} 2\sigma^2 tr\left[C(\theta') \overline{\mathbf{Z}\mathbf{Z}^*} \right] - tr\left[C(\theta')^2 \Sigma \overline{\mathbf{Z}\mathbf{Z}^*} \right] \\ &\geq \frac{\sigma^2}{p^2} \sup_{\theta' \in \left(\Theta^+_{m',\rho} - \theta \right)} \left\{ 2tr\left[C(\theta') \overline{\mathbf{Z}\mathbf{Z}^*} \right] - \varphi_{\min}^{-1} \left[I_{p^2} - C(\theta) \right] tr\left[C(\theta')^2 \overline{\mathbf{Z}\mathbf{Z}^*} \right] \right\} . \end{aligned}$$

Let us consider $\Psi_{i_1,j_1}, \ldots, \Psi_{i_{d_{m'}},j_{d_{m'}}}$ a basis of the space $\Theta_{m'}$ defined in Eq.(14) of [Ver09]. Let α be a positive number that we shall define later. We then introduce θ' as

$$\theta' := \varphi_{\min} \left[I_{p^2} - C(\theta) \right] \frac{\alpha}{p^2} \sum_{k=1}^{d_{m'}} tr\left[C\left(\Psi_{i_k,j_k} \right) \overline{\mathbf{Z}\mathbf{Z}^*} \right] \Psi_{i_k,j_k} .$$

Since θ is assumed to belong to $\Theta^+_{m',\rho}$, the parameter θ' belongs to $(\Theta^+_{m',\rho} - \theta)$ if

$$\varphi_{\max}[C(\theta')] \leq \varphi_{\min}\left(I_{p^2} - C(\theta) \right) \quad \text{and} \quad \varphi_{\min}[C(\theta')] \geq -\rho + \varphi_{\max}\left(I_{p^2} - C(\theta) \right) .$$

. The largest eigenvalue of $C(\theta')$ is smaller than $\|\theta'\|_1$ whereas its smallest eigenvalue is larger than $-\|\theta'\|_1$. Let us upper bound the l_1 norm of θ':

$$\begin{aligned} \|\theta'\|_1 &= 2\varphi_{\min} \left[I_{p^2} - C(\theta) \right] \frac{\alpha}{p^2} \sum_{k=1}^{d_{m'}} \left| tr\left[C\left(\Psi_{i_k,j_k} \right) \overline{\mathbf{Z}\mathbf{Z}^*} \right] \right| \\ &\leq 2\sqrt{\frac{\alpha}{p^2} \varphi_{\min} \left[I_{p^2} - C(\theta) \right] d_{m'} tr\left[C(\theta') \overline{\mathbf{Z}\mathbf{Z}^*} \right]} . \end{aligned} \tag{21}$$

Hence, θ' belongs to $(\Theta^+_{m',\rho} - \theta)$ if

$$\|\theta'\|_1 \leq \varphi_{\min}\left(I_{p^2} - C(\theta) \right) \wedge \left[\rho - \varphi_{\max}\left(I_{p^2} - C(\theta) \right) \right] . \tag{22}$$

Thus, we get the lower bound

$$\gamma_{n,p,p}(\theta) - \gamma_{n,p,p}(\widehat{\theta}_{m',\rho}) \geq \frac{\sigma^2}{p^2} \left\{ 2tr\left[C(\theta') \overline{\mathbf{Z}\mathbf{Z}^*} \right] - \varphi_{\min}^{-1} \left[I_{p^2} - C(\theta) \right] tr\left[C(\theta')^2 \overline{\mathbf{Z}\mathbf{Z}^*} \right] \right\} , \tag{23}$$

as soon as Condition (22) is satisfied.

Let us now bound the deviations of the two random variables involved in (21) and (23) by applying Markov's and Tchebychev's inequality. For the sake of simplicity, we assume that $d_{m'}$ is

smaller than $(p^2-2p)/2$. In such a case, all the nodes in m' are different from their symmetric in Λ. We omit the proof for $d_{m'}$ larger than $(p^2-2p)/2$ because the approach is analogous but the computations are slightly more involved. Straightforwardly, we get

$$\mathbb{E}\left[tr\left(C(\theta')\overline{\mathbf{Z}\mathbf{Z}^*}\right)\right] = 4\alpha\varphi_{\min}\left[I_{p^2}-C(\theta)\right]\frac{d_{m'}}{n}\ ,$$

since the neighborhood m' only contains points (i,j) whose symmetric $(-i,-j)$ is different. A cumbersome but pedestrian computation leads to the upper bound

$$\mathrm{var}\left[tr\left(C(\theta')\overline{\mathbf{Z}\mathbf{Z}^*}\right)\right] \leq L_1\alpha^2\varphi^2_{\min}\left[I_{p^2}-C(\theta)\right]\frac{d_{m'}}{n^2}\ ,$$

where L_1 is a numerical constant. Similarly, we upper bound the expectation of $tr\left[C(\theta')^2\overline{\mathbf{Z}\mathbf{Z}^*}\right]$

$$\mathbb{E}\left[tr\left(C(\theta')^2\overline{\mathbf{Z}\mathbf{Z}^*}\right)\right] \leq L_2\alpha^2\varphi^2_{\min}\left[I_{p^2}-C(\theta)\right]\frac{d_{m'}}{n}\ .$$

Let us respectively apply Tchebychev's inequality and Markov's inequality to the variables $tr\left[C(\theta')\overline{\mathbf{Z}\mathbf{Z}^*}\right]$ and $tr\left[C(\theta')^2\overline{\mathbf{Z}\mathbf{Z}^*}\right]$. Hence, there exists an event Ω of probability larger than $3/4$ such that

$$2tr\left[C(\theta')\overline{\mathbf{Z}\mathbf{Z}^*}\right] - \varphi^{-1}_{\min}\left[I_{p^2}-C(\theta)\right]tr\left[C(\theta')^2\overline{\mathbf{Z}\mathbf{Z}^*}\right] \geq \varphi_{\min}\left[I_{p^2}-C(\theta)\right]\frac{d_{m'}}{n}\left\{8\alpha\left(1-\sqrt{\frac{L_1'}{d_{m'}}}\right)-\alpha^2L_2'\right\}$$

and

$$tr\left[C(\theta')\overline{\mathbf{Z}\mathbf{Z}^*}\right] \leq 4\alpha\varphi_{\min}\left[I_{p^2}-C(\theta)\right]\frac{d_{m'}}{n}\left(1+\sqrt{\frac{L_1'}{d_{m'}}}\right)\ .$$

In the sequel, we assume that p is larger than some universal constant p_0, which ensures the dimension $d_{m'}$ to be larger than $4L_1'$. Gathering (21) with the upper bound on $tr\left[C(\theta')\overline{\mathbf{Z}\mathbf{Z}^*}\right]$ yields

$$\|\theta'\|_1 \leq 2\sqrt{2}\alpha\varphi_{\min}\left[I_{p^2}-C(\theta)\right]\frac{d_{m'}}{\sqrt{np^2}} \leq 2\sqrt{2}\alpha\varphi_{\min}\left[I_{p^2}-C(\theta)\right]\ ,$$

since $d_{m'} \leq p\sqrt{n}$. If $2\sqrt{2}\alpha$ is smaller than $1 \wedge \left\{\left[\rho-\varphi_{\max}\left(I_{p^2}-C(\theta)\right)\right]\varphi^{-1}_{\min}\left[I_{p^2}-C(\theta)\right]\right]$, then Condition (22) is fulfilled on the event Ω and it follows from (23) that

$$\mathbb{P}\left\{\gamma_{n,p,p}(\theta)-\gamma_{n,p,p}(\widehat{\theta}_{m',\rho}) \geq 4\sigma^2\varphi_{\min}\left[I_{p^2}-C(\theta)\right]\frac{d_{m'}}{np^2}\left[\alpha-\alpha^2L_2'/4\right]\right\} \geq \frac{3}{4}\ .$$

Choosing $\alpha = \frac{2}{L_2'} \wedge \frac{\sqrt{2}}{4} \wedge \sqrt{2}\frac{\rho-\varphi_{\max}\left(I_{p^2}-C(\theta)\right)}{4\varphi_{\min}\left(I_{p^2}-C(\theta)\right)}$, we get

$$\mathbb{P}\left\{\gamma_{n,p,p}(\theta)-\gamma_{n,p,p}(\widehat{\theta}_{m',\rho}) \geq K_3\sigma^2\left\{\varphi_{\min}\left[I_{p^2}-C(\theta)\right] \wedge \left[\rho-\varphi_{\max}\left(I_{p^2}-C(\theta)\right)\right]\right\}\frac{d_{m'}}{np^2}\right\} \geq \frac{3}{4}\ ,$$

where K_3 is an universal constant. □

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References

[Aka73] H. Akaike. Information theory and an extension of the maximum likelihood principle. In *Second International Symposium on Information Theory (Tsahkadsor, 1971)*, pages 267–281. Akadémiai Kiadó, Budapest, 1973.

[AM09] S. Arlot and P. Massart. Data-driven calibration of penalties for least-squares regression. *J. Mach. Learn. Res. (to appear)*, 2009.

[Ayk98] R.G. Aykroyd. Bayesian estimation for homogeneous and inhomogeneous gaussian random fields. *IEEE Trans. Pattern Anal. Machine Intell.*, 20(5):533–539, 1998.

[BCM08] J.P. Baudry, G. Celeux, and J.M. Marin. Selecting models focussing the modeller's purpose. In *Compstat 2008: Proceedings in Computational Statistics*. Springer-Verlag, 2008.

[Bes75] J. E. Besag. Statistical Analysis of Non-Lattice Data. *The Statistician*, 24(3):179–195, 1975.

[BK95] J. E. Besag and C. Kooperberg. On conditional and intrinsic autoregressions. *Biometrika*, 82(4):733–746, 1995.

[BM07] L. Birgé and P. Massart. Minimal penalties for Gaussian model selection. *Probab. Theory Related Fields*, 138(1-2):33–73, 2007.

[CNB98] M. Crouse, R. Nowak, and R. Baraniuk. Wavelet-based statistical signal processing using hidden Markov models. *IEEE Trans. Signal Process.*, 46(4):886–902, 1998.

[Cre85] N. Cressie. Fitting variogram models by weighted least squares. *Mathematical Geology*, 17:563–586, 1985.

[Cre93] N. A. C. Cressie. *Statistics for spatial data*. Wiley Series in Probability and Mathematical Statistics: Applied Probability and Statistics. John Wiley & Sons Inc., New York, 1993.

[CV08] N. A. C. Cressie and N. Verzelen. Conditional-mean least-squares of Gaussian Markov random fields to Gaussian fields. *Comput. Statist. Data Analysis*, 52(5):2794–2807, 2008.

[DN03] S. C. Dass and V. N. Nair. Edge detection, spatial smoothing, and image reconstruction with partially observed multivariate data. *J. Amer. Statist. Assoc.*, 98(461):77–89, 2003.

[FARMA08] M.P. Frías, F.J. Alonso, M.D. Ruiz-Medina, and J.M. Angulo. Semiparametric estimation of spatial long-range dependence. *J. Statist. Plann. Inference*, 138(5):1479–1495, 2008.

[Gra06] R.M. Gray. *Toeplitz and Circulant Matrices: A Review*. Now Publishers, Norwell, Massachusetts, rev. edition, 2006.

[Guy87] X. Guyon. Estimation d'un champ par pseudo-vraisemblance conditionnelle: étude asymptotique et application au cas markovien. In *Spatial processes and spatial time series analysis (Brussels, 1985)*, volume 11 of *Travaux Rech.*, pages 15–62. Publ. Fac. Univ. Saint-Louis, Brussels, 1987.

[Guy95] X. Guyon. *Random fields on a network*. Probability and its Applications (New York). Springer-Verlag, New York, 1995.

[GY99] X. Guyon and J.F. Yao. On the underfitting and overfitting sets of models chosen by order selection criteria. *J. Multivariate Anal.*, 70(2):221–249, 1999.

[HFH94] P. Hall, N. Fisher, and B. Hoffmann. On the nonparametric estimation of covariance functions. *Ann. Statist.*, 22(4):2115–2134, 1994.

[ISZ07] H.K. Im, M.L. Stein, and Z. Zhu. Semiparametric estimation of spectral density with irregular observations. *J. Amer. Statist. Assoc.*, 102(478):726–735, 2007.

[Lau96] S. L. Lauritzen. *Graphical models*, volume 17 of *Oxford Statistical Science Series*. The Clarendon Press Oxford University Press, New York, 1996. Oxford Science Publications.

[LD93] S. Lakshmanan and H. Derin. Valid parameter space for 2-D Gaussian Markov random fields. *IEEE Trans. Inform. Theory*, 39(2):703–709, 1993.

[Leb05] E. Lebarbier. Detecting multiple change-points in the mean of a gaussian process by model selection. *Signal processing*, 85(4):717–736, 2005.

[Lep02] V. Lepez. *Some estimation problems related to oil reserves*. PhD thesis, University Paris XI, 2002.

[LM00] B. Laurent and P. Massart. Adaptive estimation of a quadratic functional by model selection. *Ann. Statist.*, 28(5):1302–1338, 2000.

[Mas07] P. Massart. *Concentration inequalities and model selection*, volume 1896 of *Lecture Notes in Mathematics*. Springer, Berlin, 2007.

[Mat86] B. Matérn. *Spatial variation*, volume 36 of *Lecture Notes in Statistics*. Springer-Verlag, Berlin, second edition, 1986. With a Swedish summary.

[MM08] C. Maugis and B. Michel. Slope heuristics for variable selection and clustering via gaussian mixtures. Technical Report RR-6550, INRIA, 2008.

[MT98] A. D. R. McQuarrie and C.-L. Tsai. *Regression and time series model selection*. World Scientific Publishing Co. Inc., River Edge, NJ, 1998.

[PSWS03] J. Portilla, V. Strela, M. J. Wainwright, and E. P. Simoncelli. Image denoising using scale mixtures of Gaussians in the wavelet domain. *IEEE Trans. Image Process.*, 12(11):1338–1351, 2003.

[R D08] R Development Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2008. ISBN 3-900051-07-0.

[RH05] H. Rue and L. Held. *Gaussian Markov Random Fields: Theory and Applications*, volume 104 of *Monographs on Statistics and Applied Probability*. Chapman & Hall/CRC, London, 2005.

[RJD01] P. J. Ribeiro Jr and P. J. Diggle. geoR: a package for geostatistical analysis. *R-NEWS*, 1(2):14–18, June 2001. ISSN 1609-3631.

[RMC09] H. Rue, S. Martino, and N. Chopin. Approximate bayesian inference for latent gaussian models by using integrated nested laplace approximations. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, 71(2):319–392, 2009.

[RT02] H. Rue and H. Tjelmeland. Fitting Gaussian Markov random fields to Gaussian fields. *Scand. J. Statist.*, 29(1):31–49, 2002.

[Sch78] G. Schwarz. Estimating the dimension of a model. *Ann. Statist.*, 6(2):461–464, 1978.

[Sch09] M. Schlather. *RandomFields: Simulation and Analysis of Random Fields*, 2009. R package version 1.3.40.

[SFG08] H.-R. Song, M. Fuentes, and S. Ghosh. A comparative study of gaussian geostatistical models and gaussian markov random field models. *Journal of Multivariate Analysis*, 99:1681–1697, 2008.

[Ste99] M. L. Stein. *Interpolation of spatial data*. Springer Series in Statistics. Springer-Verlag, New York, 1999. Some theory for Kriging.

[Ver09] N Verzelen. Adaptive estimation of regular Gaussian Markov random fields. Technical Report RR-6797, INRIA, 2009. Arxiv:math.ST/0901.2212v2.

[Vil07] F. Villers. *Tests et sélection de modèles pour l'analyse de données protéomiques et transcriptomiques*. PhD thesis, University Paris XI, December 2007.

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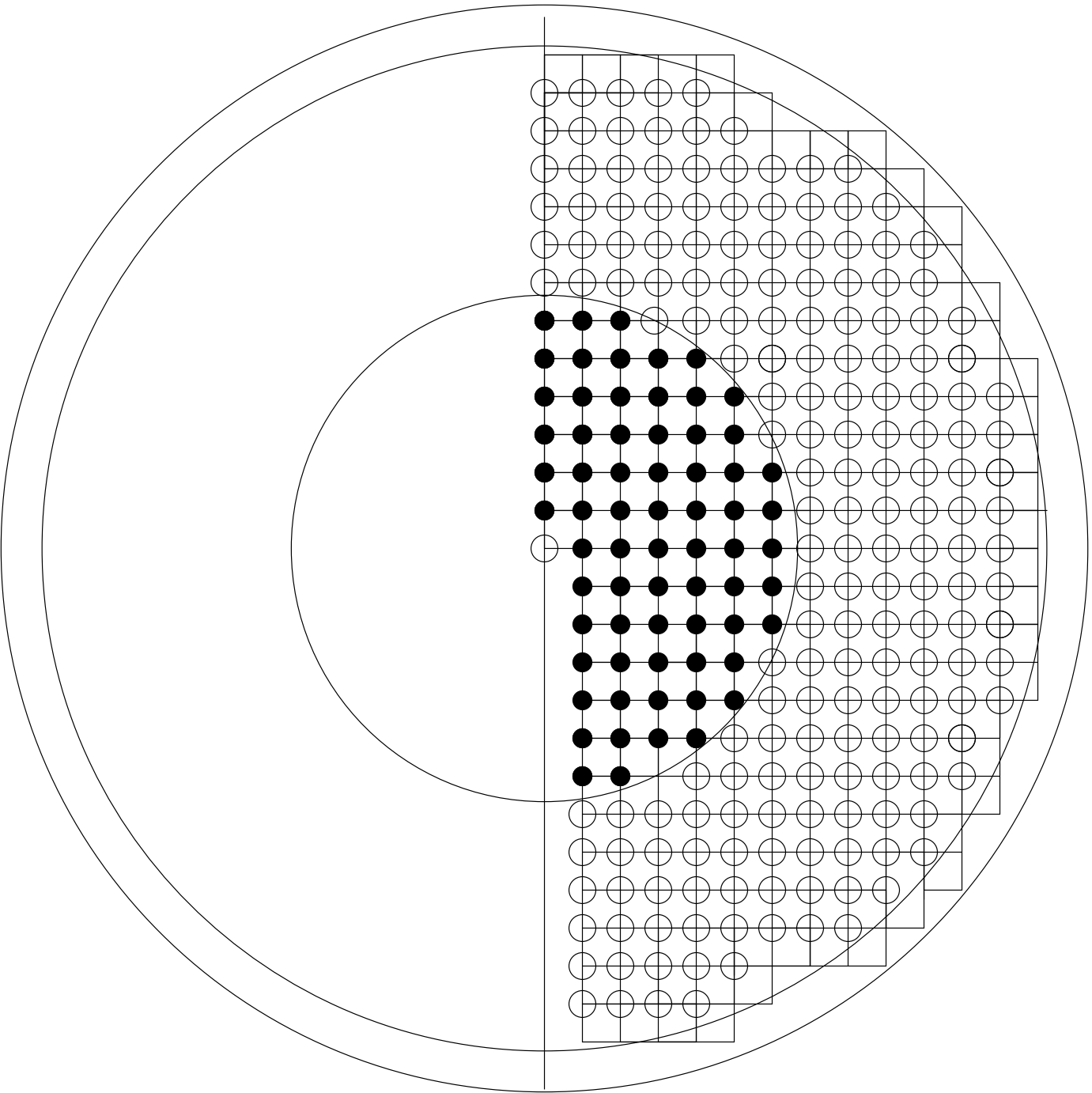

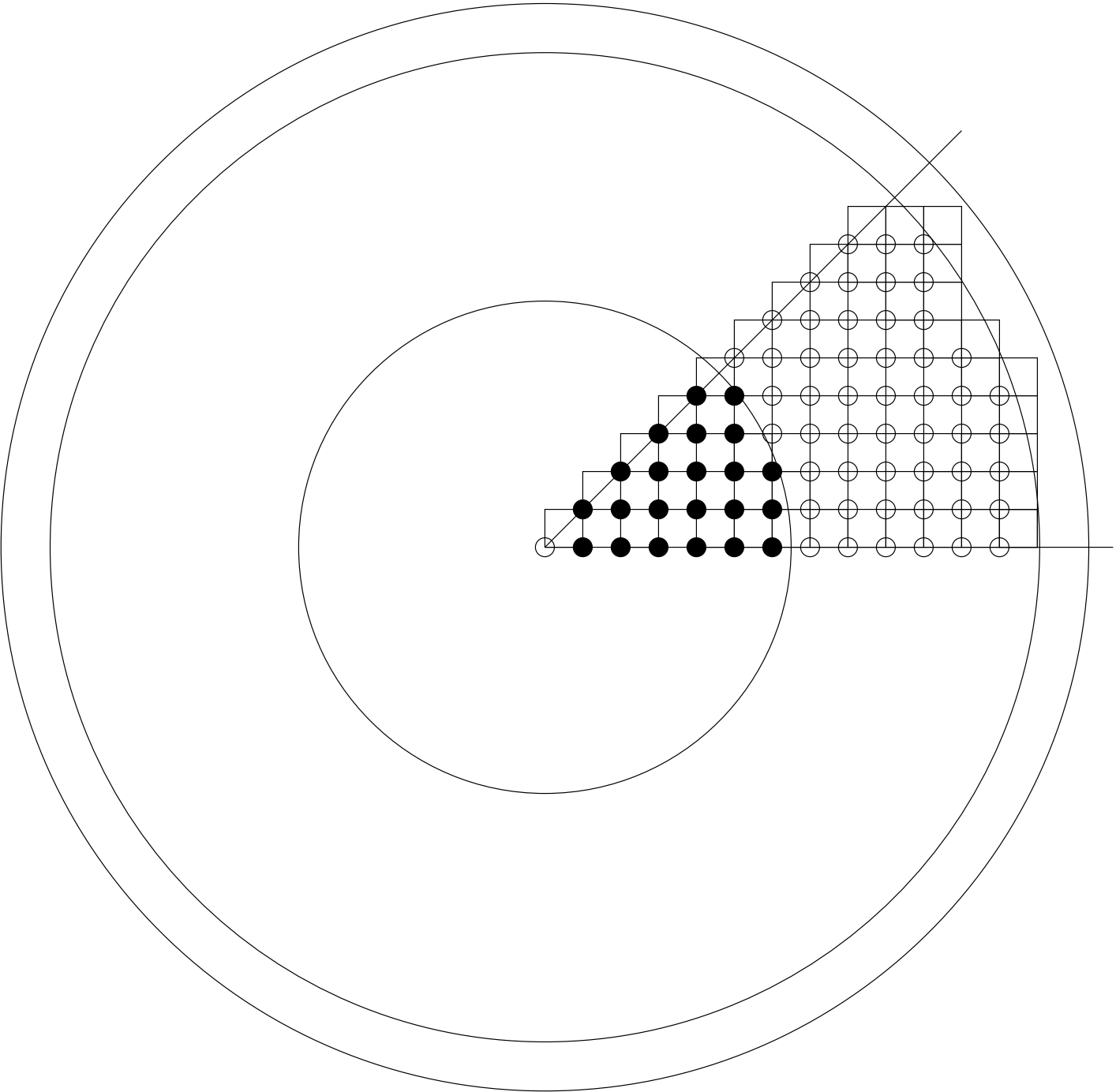

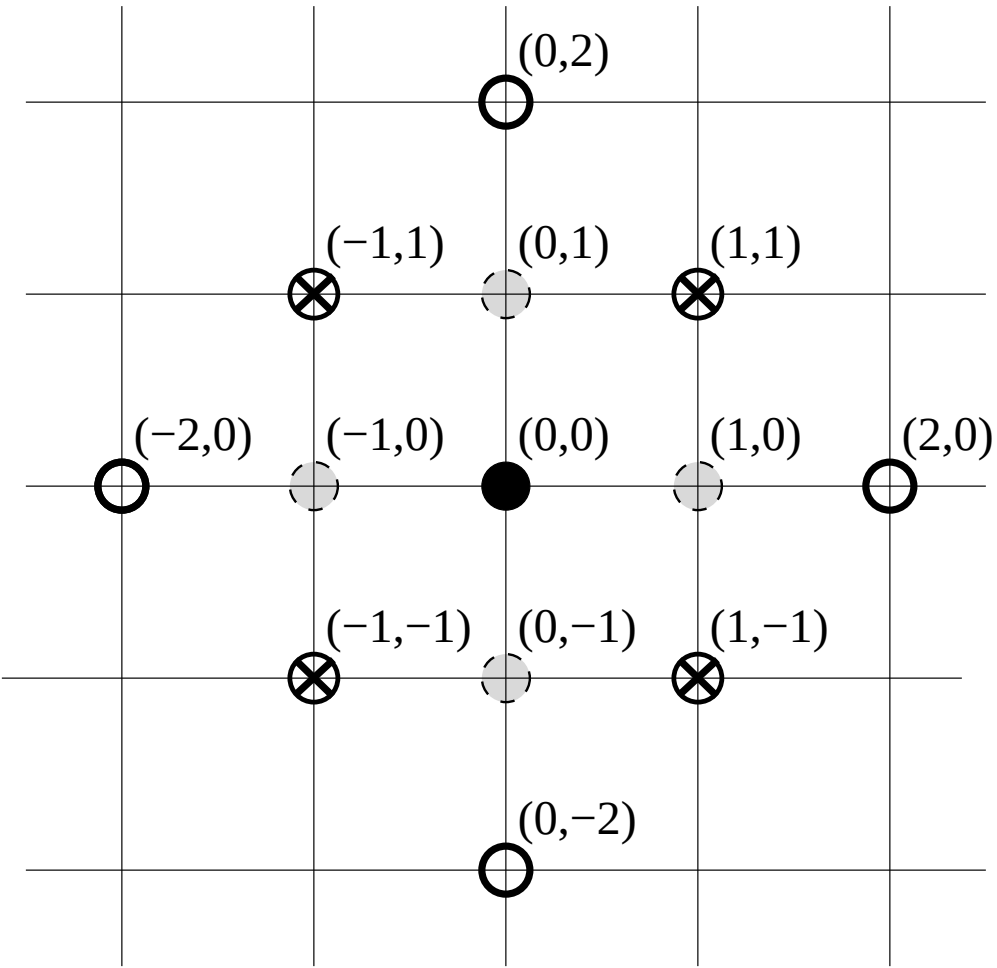
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