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Inference with a contrast-based posterior distribution and application in spatial statistics

S. Soubeyrand^{*†}, F. Carpentier^{*}, N. Desassis[‡] and J. Chadœuf^{*}

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Abstract. The likelihood function is often used for parameter estimation. Its use, however, may cause difficulties in specific situations. In order to circumvent these difficulties, we propose a parameter estimation method based on the replacement of the likelihood in the formula of the Bayesian posterior distribution by a function which depends on a contrast measuring the discrepancy between observed data and a parametric model. The properties of the contrast-based (CB) posterior distribution are studied to understand what the consequences of incorporating a contrast in the Bayes formula are. We show that the CB-posterior distribution can be used to make frequentist inference and to assess the asymptotic variance matrix of the estimator with limited analytical calculations compared to the classical contrast approach. Even if the primary focus of this paper is on frequentist estimation, it is shown that for specific contrasts the CB-posterior distribution can be used to make inference in the Bayesian way.

The method was used to estimate the parameters of a variogram (simulated data), a Markovian model (simulated data) and a cylinder-based autosimilar model describing soil roughness (real data). Even if the method is presented in the spatial statistics perspective, it can be applied to non-spatial data.

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Key words. Frequentist estimation; Quasi-Bayesian estimation; Spatial model.

1 Introduction

In both the frequentist and the Bayesian viewpoints, the likelihood function has become the major component of statistical inference under a parametric model. Its use, however, has drawbacks in specific situations. First, it may be impossible to write down the likelihood in a numerically tractable form; see the cases of Boolean models (Van Lieshout and Van Zwet, 2001), Markov point processes (Møller, 2003), Markov spatial processes (Guyon, 1985) and spatial generalized linear mixed models (spatial GLMM; Diggle et al., 1998) where multiple integrals cannot be reduced due to spatial dependences. Second, the likelihood may not be completely appropriate because of the associated assumptions. For instance, the likelihood is built under an assumption on the distribution of data, but such an assumption may be tricky to specify in the case of insufficient information as in classical geostatistics (Chilès and Delfiner, 1999); see also McCullagh and Nelder (1989, chap. 9). In the same vein, every data are assumed to have the same weights in the likelihood, but the influence of outliers may be too large according to the analyst (Markatou, 2000).

The difficulties encountered with the likelihood can be circumvented with the existing Bayesian and frequentist procedures.

- There are procedures which use conditional simulations to numerically approximate the likelihood. For instance, Markov chain Monte Carlo algorithms (MCMC; Robert and Casella, 1999) allow the approximation of the posterior distribution for Markov point processes (Møller, 2003) and spatial GLMMs (Diggle et al., 1998); Markov chain expectation maximization algorithms (MCEM; Wei and Tanner, 1990) allow the maximization of the likelihood for Boolean models (Van Lieshout and Van Zwet, 2001) and spatial GLMMs (Zhang, 2002).
- There are procedures where the likelihood function is simplified or replaced. For example, the likelihood can be replaced by a pseudo-likelihood which

only takes account of local dependence structures, like in Møller (2003) for Markov point processes and Besag (1975) and Guyon (1985) for Markov spatial processes. The generalized least squares estimation, which does not rely on assumptions on the distribution of data, is used in geostatistics for the estimation of variogram parameters; see Chilès and Delfiner (1999, chap. 2-3) and Stein (1999, chap. 1). Other examples of procedures where the likelihood function was replaced are: the weighted likelihood maximization (Markatou, 2000), the method of moments, the M-estimation (Serfling, 2002), the approximate Bayesian computation (ABC; Beaumont et al., 2002), the pseudo-posterior approach of Walker and Hjort (2001), the quasi-likelihood maximization (McCullagh and Nelder, 1989) and the quasi-Bayesian likelihood method (Lin, 2006).

In the pseudo-posterior approach of Walker and Hjort (2001), the likelihood is replaced by its square-root in the posterior distribution. This has the consequence of flattening the likelihood and leads to a robustifying posterior distribution. In the quasi-Bayesian likelihood approach (Lin, 2006), the likelihood appearing in the posterior distribution formula is replaced by a quasi-likelihood which does not rely on distribution assumptions. Then, the posterior distribution which is obtained is used to make inference as in classical Bayesian situations. In this communication we propose to generalize these approaches: the likelihood in the posterior distribution formula is replaced by a function of a contrast.

A contrast is a function of the model parameters and the observed data which is minimized to estimate the parameters (Dacunha-Castelle and Duflo, 1982). The minimum contrast approach is a generic estimation method which was developed in a frequentist perspective. The maximum likelihood estimation as well as the maximum pseudo, weighted or quasi likelihood estimation, the diverse least squares methods, the method of moments and the M-estimation can be formulated as minimum contrast estimation problems.

The procedure which is proposed —replacing the likelihood by a function of a contrast in the Bayesian formula— generalizes some of the existing approaches. It indeed includes the classical Bayesian approach (here and thereafter “classical” refers to “likelihood-based”), the pseudo-posterior approach of Walker and Hjort

(2001) and the quasi-Bayesian approach of Lin (2006). This procedure provides a contrast-based (CB) posterior distribution which does not coincide, in the general case, with the classical posterior distribution. In this paper, we investigate what are the posterior distribution and the MAP (maximum a posteriori) estimator based on a contrast.

Under mild conditions on the prior distribution, we show that the CB-MAP estimator inherits the asymptotic properties (consistency and asymptotic normality) of the minimum contrast estimator, as the classical MAP estimator inherits the asymptotic properties of the maximum likelihood estimator (Caillot and Martin, 1972). The limit variance matrix of the normalized estimator is $I_\theta^{-1}\Gamma_\theta I_\theta^{-1}$ where Γ_θ is the limit variance of the gradient of the contrast and I_θ is the limit Hessian matrix of the contrast.

Moreover, we show that the CB-posterior distribution is asymptotically equivalent to a normal distribution whose variance matrix is I_θ^{-1} . Therefore, when building the contrast, particular attention must be paid to satisfy, if possible, $I_\theta^{-1}\Gamma_\theta I_\theta^{-1} = I_\theta^{-1}$. Indeed, with such a contrast, inference can be made without computing matrices Γ_θ and I_θ : the posterior distribution can either be used as a limit distribution in a frequentist viewpoint or be used to make inference in the Bayesian way. When building a contrast satisfying $I_\theta^{-1}\Gamma_\theta I_\theta^{-1} = I_\theta^{-1}$ is not possible, the CB-posterior distribution can nevertheless be used to estimate I_θ^{-1} . Thus, the computation of the limit Hessian matrix of the contrast is avoided.

The article is organized as follows. The method is presented in section 2, and its properties are derived. Then, it is applied in sections 3 and 4 to simulated and real cases in spatial statistics (estimation of the range parameter of a variogram; estimation of the parameters of a Markovian spatial process; and estimation of the parameters of a cylinder-based autosimilar model describing soil roughness). The three cases illustrate the application of the method when the parameter has one or several components and when $I_\theta^{-1}\Gamma_\theta I_\theta^{-1}$ is equal to or different from I_θ^{-1} .

2 Incorporating a contrast in the Bayesian formula

2.1 Minimum contrast estimation

Consider a family of parametric models $\{P_\alpha : \alpha \in \Theta\}$ and samples of increasing sizes $t \in T \subset \mathbb{N}$, drawn from the model P_θ with the true parameter θ . A contrast for θ is a random function $\alpha \mapsto U_t(\alpha)$ defined over Θ , depending on a sample of size t , and such that $\{U_t(\alpha) : t \in T\}$ converges in probability, as $t \rightarrow \infty$, to a function $\alpha \mapsto K(\alpha, \theta)$ which has a strict minimum at $\alpha = \theta$. The minimum contrast estimator is

$$\hat{\theta}_t = \operatorname{argmin}\{U_t(\alpha), \alpha \in \Theta\}.$$

The maximum likelihood estimation, the maximum pseudo, weighted or quasi likelihood estimation, the diverse least squares methods, the method of moments and the M-estimation can be formulated as minimum contrast estimation problems. A detailed presentation of minimum contrast estimation can be found in Dacunha-Castelle and Dufflo (1982). Molchanov (1997) illustrates the use of minimum contrast estimation in spatial statistics.

2.2 Posterior distribution and MAP estimator based on a contrast

Let $(X_i)_{i \leq t}$ be a sample of size t with distribution P_α . Then, the posterior distribution of α is

$$p(\alpha \mid X_i, i \leq t) = \frac{P_\alpha(X_i, i \leq t)c(\alpha)}{\int_{\Theta} P_\beta(X_i, i \leq t)c(\beta)d\beta},$$

where $P_\alpha(X_i, i \leq t)$ denotes the likelihood and $c(\cdot)$ is a prior distribution defined over Θ . The contrast corresponding to the likelihood being $U_t^{lik}(\alpha) = -\frac{1}{t} \log P_\alpha(X_i, i \leq t)$ (Dacunha-Castelle and Dufflo, 1982), the posterior distribution can be written by replacing $P_\alpha(X_i, i \leq t)$ by $\exp(-tU_t^{lik}(\alpha))$ in the previous equation.

Here, we propose to substitute the contrast associated with the likelihood in the Bayesian formula with any contrast $U_t(\alpha)$. This leads to a contrast-based (CB) posterior distribution denoted by $p_t(\alpha)$:

$$p_t(\alpha) = \frac{\exp(-tU_t(\alpha))c(\alpha)}{\int_{\Theta} \exp(-tU_t(\beta))c(\beta)d\beta}. \quad (1)$$

The CB-MAP estimator obtained by maximizing $p_t(\cdot)$ is denoted by

$$\tilde{\theta}_t = \operatorname{argmax}\{p_t(\alpha), \alpha \in \Theta\}.$$

$\tilde{\theta}_t$ is at the minimum of $\alpha \mapsto U_t(\alpha) - (1/t) \log c(\alpha)$ and, in general, does not coincide with the classical minimum contrast estimator $\hat{\theta}_t = \operatorname{argmin}\{U_t(\alpha), \alpha \in \Theta\}$.

Remark: The CB-posterior distribution proposed in equation (1) is one out of several possible alternatives to the classical posterior distribution. Indeed, other link functions, say g , could be used instead of the exponential function. The link g should be an increasing function and should satisfy regularity conditions in order to inherit the properties of the contrast. The use of the exponential link has two major advantages: (i) the classical Bayesian approach is included in the method which is proposed and (ii) the exponential link is particularly convenient for mathematical derivations allowing us to determine the properties of the CB-MAP estimator and the CB-posterior distribution. These properties are investigated below.

2.3 Consistency and asymptotic normality of the CB-MAP estimator

We noted above that the CB-MAP estimator $\tilde{\theta}_t$ is at the minimum of $\alpha \mapsto U_t(\alpha) - (1/t) \log c(\alpha)$. This function satisfies the definition of a contrast. Consequently, convergence properties of $\tilde{\theta}_t$ can be easily obtained by using the contrast theory (Dacunha-Castelle and Duflo, 1982). Assume that the hypotheses required for the convergence of the classical minimum contrast estimator (see Appendix A) are satisfied. Let us assume in addition that the prior distribution $c(\cdot)$ is proper, differentiable and strictly positive over Θ . It follows that, as $t \rightarrow \infty$,

- $\tilde{\theta}_t$ converges in probability to θ and
- $\sqrt{t}(\tilde{\theta}_t - \theta)$ converges in law to the Gaussian distribution $\mathcal{N}(0, I_\theta^{-1} \Gamma_\theta I_\theta^{-1})$,

where I_θ and Γ_θ are matrices satisfying:

$$\begin{aligned} \mathbf{H}U_t(\theta) &\rightarrow I_\theta \quad \text{in probability as } t \rightarrow \infty \\ \sqrt{t}\mathbf{grad}U_t(\theta) &\rightarrow \mathcal{N}(0, \Gamma_\theta) \quad \text{in law.} \end{aligned}$$

Remark 1: The convergence results given above can also be obtained by noting that the asymptotic deviation between the classical minimum contrast estimator $\hat{\theta}_t$ and the CB-MAP estimator $\tilde{\theta}_t$ is of order $1/t$. More exactly, it is shown in Appendix B that

$$\tilde{\theta}_t - \hat{\theta}_t = \frac{1 + o_{\text{proba}}(1)}{tc(\theta)} I_\theta^{-1} \mathbf{grad}c(\theta). \quad (2)$$

Remark 2: It would be interesting to study not only the asymptotics of the CB-posterior maximum but also the asymptotics of the CB-posterior mean and median which are commonly used in classical Bayesian estimation.

2.4 Convergence of the CB-posterior distribution

The CB-posterior distribution $p_t(\cdot)$ is asymptotically equivalent to the density function of the Gaussian distribution $\mathcal{N}(\tilde{\theta}_t, (tI_\theta)^{-1})$ (see Appendix C):

$$p_t(\alpha) \underset{t \rightarrow \infty}{\sim} \frac{1}{(2\pi)^{p/2} |(tI_\theta)^{-1}|^{1/2}} \exp\left(-\frac{1}{2}(\alpha - \tilde{\theta}_t)'(tI_\theta)(\alpha - \tilde{\theta}_t)\right). \quad (3)$$

This result allows us to figure out what the CB-posterior distribution is and how it can be used to make inference in the frequentist and Bayesian ways.

In the contrast theory, the distribution $\mathcal{N}(\tilde{\theta}_t, (tI_\theta)^{-1} \Gamma_\theta I_\theta^{-1})$ is used to make frequentist inference about θ : the point estimator is $\tilde{\theta}_t$, and confidence zones are provided based on the this normal distribution. Consequently, if the contrast is such that $I_\theta^{-1} \Gamma_\theta I_\theta^{-1} = I_\theta^{-1}$, then the CB-posterior distribution $p_t(\cdot)$ which approximates the density of $\mathcal{N}(\tilde{\theta}_t, (tI_\theta)^{-1})$ can be directly used to make frequentist inference about θ : the mode of $p_t(\cdot)$ is the point estimator, and confidence zones can be directly determined from $p_t(\cdot)$. This case is particularly

interesting since the calculation of the limit matrices $I_\theta = \lim_{t \rightarrow \infty} \mathbf{H}U_t(\theta)$ and $\Gamma_\theta = \lim_{t \rightarrow \infty} V_\theta(\sqrt{t} \mathbf{grad} U_t(\theta))$ is no more required.

Moreover, when the contrast which is considered satisfies $I_\theta^{-1} \Gamma_\theta I_\theta^{-1} = I_\theta^{-1}$, we propose to use the CB-posterior distribution $p_t(\cdot)$ to make inference in the Bayesian way, i.e. to use $p_t(\cdot)$ as a real posterior density. The motivation is based on the following analogy: when the contrast corresponding to the likelihood is employed (in this case, $I_\theta^{-1} \Gamma_\theta I_\theta^{-1} = I_\theta^{-1}$), then $p_t(\cdot)$ can be used (i) to make frequentist inference since it is an approximation of the limit distribution of the estimator (see above) and (ii) to make Bayesian inference since it is the classical posterior density. It has to be noted that, in general, the CB-posterior density $p_t(\cdot)$ does not coincide with the classical posterior density. It is a posterior density based on the information brought by the contrast under consideration.

If the contrast does not satisfy $I_\theta^{-1} \Gamma_\theta I_\theta^{-1} = I_\theta^{-1}$, then the CB-posterior distribution $p_t(\cdot)$ cannot be used to approximate the limit distribution of $\tilde{\theta}_t$ or to make Bayesian inference. However, $p_t(\cdot)$ can be used to estimate the matrix I_θ , so avoiding the calculation of the second derivatives of the contrast. Indeed, one can see from (3) that an estimate of I_θ is the matrix Ω^{-1}/t where Ω is the variance matrix of the normal density function centered around $\tilde{\theta}_t$ and fitted to $p_t(\cdot)$ (using a least square technique for example). If θ is real, I_θ can be more simply estimated by $2\pi p_t(\tilde{\theta}_t)^2/t$ since equation (3) yields $p_t(\tilde{\theta}_t) \underset{t \rightarrow \infty}{\sim} (tI_\theta/2\pi)^{1/2}$. We have not found an equivalent way to easily estimate Γ_θ without analytical calculation of the second derivatives and without simulations.

3 Application in spatial statistics: simulated data

This section illustrates the properties of the CB-posterior distribution and shows the possible discrepancy between this posterior and the limit distribution of the CB-MAP.

3.1 Least-square estimation of a variogram range

This simulated case illustrates the application of the method for a real parameter. Here, the CB-posterior distribution cannot be directly used to make

inference but can be used to estimate I_θ .

We built a data set by simulating a centered Gaussian random field whose variogram at distance h is $\gamma_\theta(h) = 1 - \exp(-\theta h)$ with $\theta = 1$; θ is the inverse of the range parameter. The field was simulated over a square grid $\{i = (i_1, i_2) : 0 \leq i_1, i_2 \leq n\}$ with size $t = n^2 = 20^2$ and inter-node distance one. Figure 1 (left) shows the simulated random field. The sample variogram $\hat{\gamma}(h)$ (Chilès and Delfiner, 1999) was estimated for every possible inter-points distance h less than the half diagonal of the grid; let \mathcal{H} denote the set of these distances.

For the estimation of θ , we chose a uniform prior density over $[0, 4]$ (horizontal dotted line in Fig. 1, right) and we used the least-square contrast between the sample variogram and the theoretical variogram

$$U_{n^2}(\alpha) = \frac{1}{2} \sum_{h \in \mathcal{H}} \{\hat{\gamma}(h) - \gamma_\alpha(h)\}^2. \quad (4)$$

The CB-posterior density is shown in Figure 1 (right, dotted curve). The MAP estimate is $\tilde{\theta}_t = 1.34$ (vertical line).

Estimation uncertainty was assessed by estimating the limit variance $\Gamma_\theta/(nI_\theta)^2$ of $\tilde{\theta}_t$. The term $\Gamma_\theta = \lim_{t \rightarrow \infty} V_\theta(\sqrt{t} \mathbf{grad} U_t(\theta))$ (here, $t = n^2$) was estimated based on Monte-Carlo simulations: 1000 Gaussian random fields were simulated under $\tilde{\theta}_t$; for each simulation the sample variogram $\{\hat{\gamma}(h) : h \in \mathcal{H}\}$ was computed, and the first derivative of the contrast in $\tilde{\theta}_t$, i.e. $-\sum_{h \in \mathcal{H}} h e^{-\tilde{\theta}_t h} \{\hat{\gamma}(h) - (1 - e^{-\tilde{\theta}_t h})\}$, was calculated; the sample variance of the derivatives multiplied by n^2 gave the estimate 1.97 for Γ_θ .

The term $I_\theta = \lim_{t \rightarrow \infty} \mathbf{H} U_t(\theta)$ was estimated in two ways: with the estimator $2\pi p_t(\tilde{\theta}_t)^2/t$ as suggested in section 2.4 and with Monte-Carlo simulations. In the former way, the estimate of I_θ is 0.20. The second way was carried out as follows: for each of the 1000 simulated Gaussian fields mentioned above, the second derivative of the contrast in $\tilde{\theta}_t$, i.e. $\sum_{h \in \mathcal{H}} h^2 e^{-\tilde{\theta}_t h} [e^{-\tilde{\theta}_t h} - \{\hat{\gamma}(h) - (1 - e^{-\tilde{\theta}_t h})\}]$, was computed; then, the sample mean of these derivatives gave the estimate 0.27 for I_θ .

Thus, the estimate of the limit variance $\Gamma_\theta/(nI_\theta)^2$ of $\tilde{\theta}_t$ is 0.07 when I_θ is assessed by simulations and 0.12 when I_θ is computed from the CB-posterior distribution. The density function of the limit distribution $\mathcal{N}(\tilde{\theta}_t, \Gamma_\theta/(nI_\theta)^2)$ is

drawn in Figure 1 (right). The continuous and dashed lines show this density when the estimate of the limit variance is 0.07 and 0.12, respectively. The true value $\theta = 1$ belongs to the 95%-confidence interval whatever the estimate of the limit variance is. We see how the two versions of the limit density are different from the CB-posterior density.

To assess the efficiency of the method, the coverage rate of the 95%-confidence interval was measured by applying the estimation procedure to 1000 simulated fields. The coverage rate was 94.6% when the estimate of I_θ is based on Monte-Carlo simulations and 94.7% when the estimate of I_θ comes from the contrast-based posterior density.

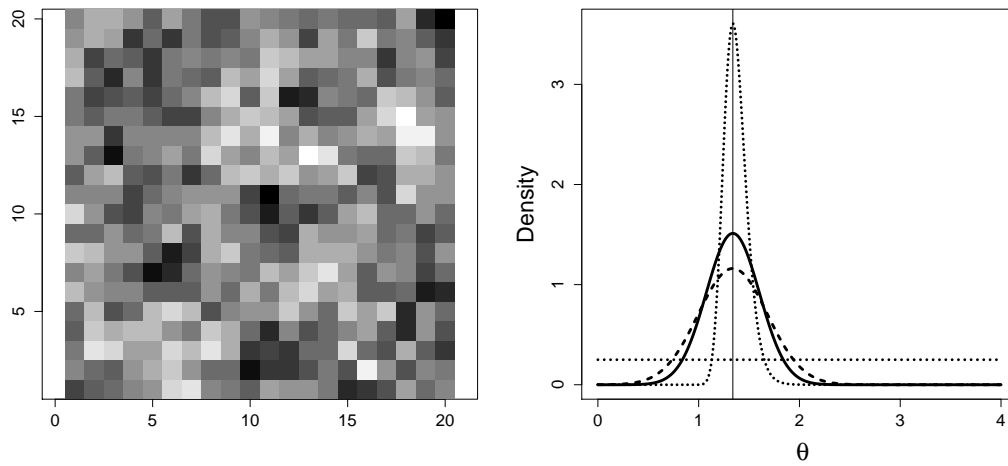


Figure 1: Left: realization of a centered Gaussian random field with exponential variogram parameterized with $\theta = 1$, over a 20×20 square-grid. Right: prior density (horizontal dotted line), contrast-based posterior density (dotted curve), density function of the limit distribution $\mathcal{N}(\tilde{\theta}_t, \Gamma_\theta / (nI_\theta)^2)$ (continuous and dashed lines when the estimate of the limit variance is based on simulations and when it is based on the posterior distribution), and MAP estimator (vertical line).

3.2 Pseudo-likelihood estimation of a Markovian spatial model

This simulated case illustrates the application of the method for a bivariate parameter. Here, the CB-posterior distribution is different from the limit distribution of the estimator; it cannot be directly used to make inference but can be used for estimating I_θ .

We built a data set by simulating a spatial Markov field X with two states, 0 and 1. The model is defined by the conditional probability of X_i given X_j , $j \in V(i)$ ($V(i)$ is the set of the four nearest neighbors of i) satisfying (Guyon, 1985)

$$\begin{aligned} P_\theta(X_i | X_j, j \neq i) &= P_\theta(X_i | X_j, j \in V(i)) \\ &= \frac{\exp\left(\theta_1 X_i + \theta_2 \sum_{j \in V(i)} X_i X_j\right)}{\left\{1 + \exp\left(\theta_1 + \theta_2 \sum_{j \in V(i)} X_j\right)\right\}}. \end{aligned}$$

The field was simulated on a $n \times n$ square grid \mathcal{I} (here, $t = n^2 = 20^2$); see Figure 2 (left).

The classical likelihood cannot be analytically calculated for this model. Therefore, a pseudo-likelihood was proposed to make inference (Guyon, 1985). The pseudo-likelihood is the product of the conditional probabilities $\prod_{i \in \mathcal{I}} P_\theta(X_i | X_j, j \neq i)$. To estimate θ_1 and θ_2 , we applied the estimation method proposed in this article by using a uniform prior density over $[-1.5, 1.5]^2$ and the contrast corresponding to the pseudo-likelihood:

$$U_{n^2}(\alpha) = -\frac{1}{n^2} \sum_{i \in \mathcal{I}} \log P_\alpha(X_i | X_j, j \in V(i)). \quad (5)$$

The CB-posterior density is shown in Figure 2 (center). The MAP estimate is $\tilde{\theta}_t = (-0.21, 0.38)$.

To give the limit distribution $\mathcal{N}(\tilde{\theta}_t, I_\theta^{-1} \Gamma_\theta I_\theta^{-1} / n^2)$ of the estimator, matrices Γ_θ and I_θ must be estimated. We computed the gradient and the Hessian of the contrast for $N = 1000$ Markov fields simulated under $\tilde{\theta}_t$, and we used the sample variance of the gradients for estimating Γ_θ and the sample mean of the Hessians

for estimating I_θ ; see Appendix D. The estimate of the limit variance matrix $I_\theta^{-1}\Gamma_\theta I_\theta^{-1}/n^2$ was finally

$$\begin{pmatrix} 0.14 & -0.055 \\ -0.055 & 0.022 \end{pmatrix}.$$

Almost the same limit variance matrix was obtained when I_θ was estimated by fitting a normal density to the CB-posterior density as suggested in section 2.4. Figure 2 (right) shows the limit density function of the estimator together with the 95%-confidence zone. We can see that the true parameter belongs to this zone. Moreover, Figure 2 shows the limit density is quite close from the posterior density. The pseudo-likelihood which takes account of short-distance interactions certainly brings almost the same information than the likelihood brings. It has however to be noted that this would not be the case if long-distance interactions had been introduced in the spatial Markov model.

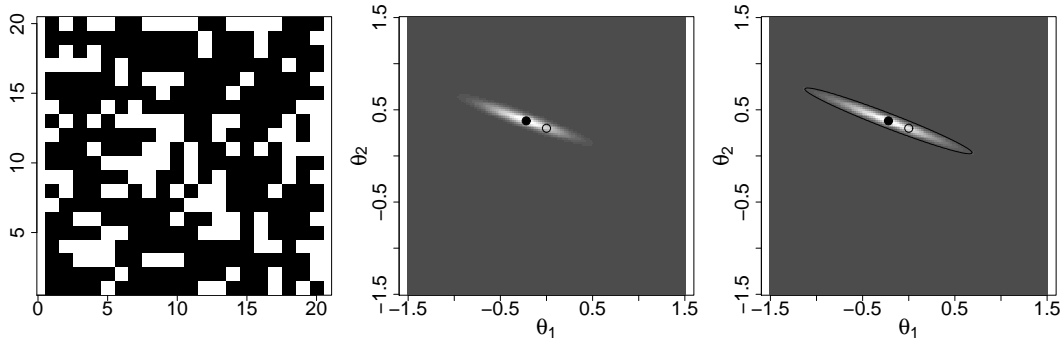


Figure 2: Left: realization of a Markovian spatial process with two states over a 20×20 grid. Center: contrast-based posterior density. Right: limit density $\mathcal{N}(\tilde{\theta}_t, I_\theta^{-1}\Gamma_\theta I_\theta^{-1}/n^2)$. On the center and right panels, the MAP estimate and the true parameter are drawn with a black dot and a circle, respectively. On the right panel, the continuous line circumscribes the 95%-confidence zone.

4 Application in spatial statistics: real data

This section presents a case where the CB-posterior distribution can be directly used to make inference in the frequentist and Bayesian ways (the estimation

of the limit matrices I_θ and Γ_θ being not required). The method is applied to a real data set dealing with soil roughness.

4.1 Cylinder-based autosimilar model

Soil roughness plays an important role in rain water absorption, pond and streaming. It also modifies reflectance properties of soils used to estimate soil moisture with remote detection for example. An experiment was carried out to measure soil roughness at a small scale. Soil heights were measured every 2mm along 1.18m-transects in a cultivated field (Bertuzzi et al., 1995). Figure 3 (top) shows the distributions of heights for two among twelve sampled transects. The mean height computed from the 12 transects is 7.6mm, the maximum is 22.9mm.

Object based models (Lantuéjoul, 2002, chap. 14) have been used to describe soil surface (Bertuzzi et al., 1995; Goulard and Chadœuf, 1994). Here, we use a cylinder-based autosimilar models defined as follows. For any $x \in \mathbb{R}^2$ and $r > 0$, let $f(x, r) = r 1_{\{\|x\| < r\}}$ be the function describing the cylinder which is centered in x and whose radius and height are equal to r ($1_{\{\cdot\}}$ is the indicator function). In addition, let (X, R) be a marked Poisson point process defined over $\mathbb{R}^2 \times \mathbb{R}_+^*$ with intensity function $\mu(x, r) = \alpha \exp \{-\beta r\}$. The random surface Y representing the soil surface is defined by

$$Y_M = \sum_{(x,r) \in (X,R)} f(x - M, r).$$

4.2 Parameter estimation using moments

For such a process, it is difficult to calculate the joint distribution of the heights whereas the moments can easily be written. We propose to estimate the bivariate parameter vector $\theta = (\alpha, \beta)$ using the first two moments: $\hat{\mu}_A = (\frac{1}{\nu(A)} \int_A Y_M dM, \frac{1}{\nu(A)} \int_A Y_M^2 dM)$, where A is the set of the sampled transects and $\nu(A)$ is its measure.

If border effects are neglected, the expected value of $\hat{\mu}_A$ is

$$E(\hat{\mu}_A) = \left(6\pi \frac{\alpha}{\beta^4}, 36\pi^2 \frac{\alpha^2}{\beta^8} + 24\pi \frac{\alpha}{\beta^5} \right).$$

Moreover, the variance matrix of $\hat{\mu}_A$ satisfies

$$\nu(A)\text{var}(\hat{\mu}_A) \rightarrow V,$$

where the components of V are

$$\begin{aligned} V_{11} &= 5! \frac{16}{3} \frac{\alpha}{\beta^6} \\ V_{12} &= 6! \frac{16}{3} \frac{\alpha}{\beta^7} + (5!)64\pi \frac{\alpha^2}{\beta^{10}} \\ V_{22} &= 7! \frac{16}{3} \frac{\alpha}{\beta^8} + \{(6!)128\pi + (10!)32\kappa\} \frac{\alpha^2}{\beta^{11}} + (3!)(5!)128\pi^2 \frac{\alpha^3}{\beta^{14}}, \end{aligned}$$

with $\kappa = \int_0^1 \int_0^1 (\arccos(u) - u\sqrt{1-u^2})(\arccos(v) - v\sqrt{1-v^2}) \frac{(uv)^5}{(u+v)^{11}} dudv$.

The estimation method is applied by using a uniform prior over $[1,100] \times [1,5]$ and a contrast based on the weighted least squares of the first two moments:

$$U_A(\theta) = (\hat{\mu}_A - E(\hat{\mu}_A))' V^{-1} (\hat{\mu}_A - E(\hat{\mu}_A)) / 2.$$

For this contrast, the matrices I_θ and Γ_θ are equal and their component (i, j) is

$$\frac{\partial E(\hat{\mu}_A)'}{\partial \theta_i} V^{-1} \frac{\partial E(\hat{\mu}_A)}{\partial \theta_j}.$$

Consequently, $I_\theta^{-1} \Gamma_\theta I_\theta^{-1} = I_\theta^{-1}$ and the CB-posterior density can be used as an approximation of the limit density of the MAP estimator $\tilde{\theta}_A$ or as a posterior distribution of the parameter θ (see section 2.4). Figure 3 (bottom) shows the joint CB-posterior distribution and the marginals. The MAP estimate of θ is $\tilde{\theta}_A = (46.6, 3.28)$. Marginal 95%-confidence intervals of α and β are $[36.1, 58.5]$ and $[3.07, 3.48]$, respectively.

5 Discussion

5.1 Summary

We have proposed an estimation method exploiting a contrast-based posterior distribution (CBPD). This method includes the classical likelihood-based procedures (MLE and Bayesian estimation), but has been mainly developed to circumvent difficulties encountered with the likelihood by generalizing the Bayesian

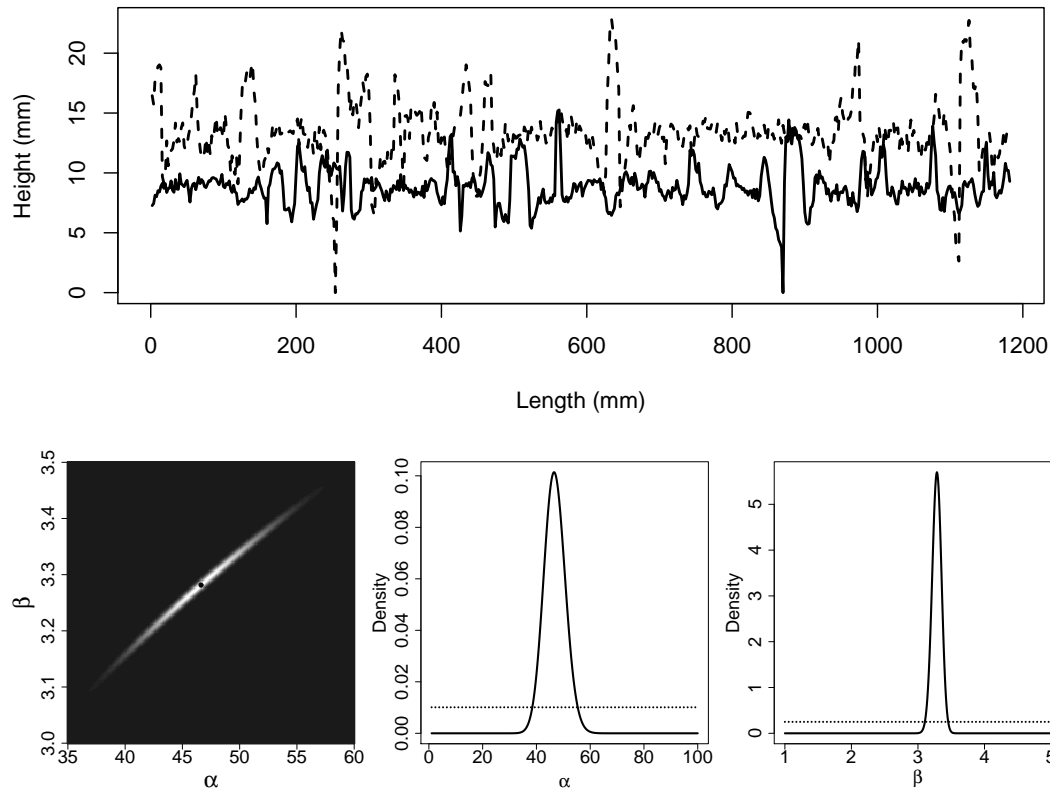


Figure 3: Top: distribution of heights for two transects. Bottom left: contrast-based posterior density for (α, β) ; the MAP estimate is at the black dot. Bottom center and right: contrast-based posterior marginal densities for α et β (continuous lines) and prior marginal densities (dashed lines).

formula of the posterior distribution, so extending the proposal of Lin (2006). The CBPD can be used to make frequentist inference and, in specific situations, Bayesian inference. In case of frequentist inference, the use of the CBPD allows the reduction of analytical calculations usually required to compute the limit variance matrix of the estimator. In this article, the method has been applied to spatial data sets, but can be applied to other cases where likelihood-based procedures are not appropriate.

5.2 Frequentist and Bayesian inference

In the frequentist viewpoint, the CBPD can be used to provide a point estimator (the posterior mode) and the limit distribution of this estimator. The limit distribution is directly approximated by the CBPD if the variance of the gradient vector of the contrast is equal to the inverse of the limit Hessian matrix of the contrast (i.e. $I_\theta^{-1}\Gamma_\theta I_\theta^{-1} = I_\theta^{-1}$; see the third application). In this case, it is not required to calculate and estimate the variance matrix of the estimator. In other cases, the limit distribution is not directly available, but the Hessian matrix of the contrast can be easily estimated from the CBPD and, consequently, the calculation of the second derivatives of the contrast is avoided (see the first two applications). It has to be noted that using Bayesian calculation to make frequentist estimation has been proposed in the literature (Robert and Hwang, 1996; Robert and Titterton, 1998; Jacquier et al., 2007), but the proposals were restricted to maximum likelihood estimation.

In the Bayesian viewpoint, the CBPD can be used as a classical posterior distribution when $I_\theta^{-1}\Gamma_\theta I_\theta^{-1} = I_\theta^{-1}$, as in the third application. However, the CBPD does not coincide with the classical posterior distribution: It has to be viewed as a posterior distribution based on the information brought by the contrast which is used.

Regarding the reconciliation of the frequentist and the Bayesian approaches, it has to be noted that the Bernstein–Von Mises (BVM) theorem, translated to our context, does not hold in general. The classical BVM theorem asserts that, under specific conditions, the posterior distribution converges to a Gaussian distribution with variance matrix equal to the asymptotic variance of the maximum likelihood estimator (Freedman, 1999). In this paper we saw that the CBPD is asymptotically equivalent to a Gaussian distribution with variance matrix I_θ^{-1} whereas the asymptotic variance matrix of the minimum contrast estimator is $I_\theta^{-1}\Gamma_\theta I_\theta^{-1}$.

5.3 Limits of the approach and perspectives

Even if the proposed procedure has advantages, it also faces two classical limits: the choice of the prior distribution (or the penalization function in the frequentist viewpoint) which can influence the posterior inference, and the choice of the contrast. Regarding the former limit, we refer to Clarke and Gustafson (1998) and Rootzén and Olsson (2006) for example. Regarding the choice of the contrast, two comments arise.

The first comment concerns the possibility to build a contrast such that $I_{\theta}^{-1}\Gamma_{\theta}I_{\theta}^{-1} = I_{\theta}^{-1}$ (case where our method has favorable properties). Necessary and sufficient conditions for obtaining this equation are not known to us. However, sufficient conditions can be given. For example, using a coding technique (Besag, 1975) based on conditional independence between sets of data is a sufficient condition. We could have applied such a technique instead of the pseudo-likelihood method for the estimation of the parameters of the Markovian spatial model (second simulated case-study). But, the use of the coding method would have induced a loss of information (Guyon, 1985). It is also possible to obtain $I_{\theta}^{-1}\Gamma_{\theta}I_{\theta}^{-1} = I_{\theta}^{-1}$ for specific models by rescaling the contrast with a variance matrix. We applied this approach in the real case-study because we could provide the analytical form for the variance matrix of the sample moments. To apply the same approach for the estimation of the range parameter of a variogram (first case-study), we should have modeled the variance of the sample variogram. However, such a practice is not common in geostatistics when the field is not assumed to be Gaussian (and it may be cumbersome). It has to be noted that if an approximate likelihood is used and its discrepancy from the true likelihood can be analytically quantified, it may be possible to assess the discrepancy between $I_{\theta}^{-1}\Gamma_{\theta}I_{\theta}^{-1}$ and I_{θ}^{-1} , and to correct the CBPD accordingly.

Our second comment concerns the information brought by contrasts. We see that in the real case-study the two estimators are strongly correlated. We could have tried to use another contrast to avoid correlation. For example, together with the sample mean, we could have used the covariance at a given distance instead of the variance to get two moments which are less correlated. However, the calculation of the expected value and the variance-covariance of these moments

is much more tricky. Thus, to be able to derive analytical expressions and apply the method as it is presented, the choice of the contrast is limited. Nevertheless, simulations could be used to circumvent this difficulty. This could be an interesting extension of the estimation method proposed in this paper.

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A Hypotheses for minimum contrast estimation

- H_1 : $\Theta \subset \mathbb{R}^p$, $p < \infty$, is compact and θ is in the interior of Θ ,
- H_2 : $\alpha \mapsto K(\alpha, \theta)$ has a strict minimum at θ ,
- H_3 : $\alpha \mapsto U_t(\alpha)$ is C^2 (it has two continuous derivatives) over Θ ,
- H_4 : the normalized gradient vector $\sqrt{t}\mathbf{grad}U_t(\theta)$ (first derivatives of $U_t(\theta)$ with respect to θ) converges in law to the normal distribution $\mathcal{N}(0, \Gamma_\theta)$:

$$\sqrt{t}\mathbf{grad}U_t(\theta) \rightarrow \mathcal{N}(0, \Gamma_\theta) \quad \text{in law as } t \rightarrow \infty,$$

H_5 : the Hessian matrix $\mathbf{H}U_t(\theta)$ (second derivatives of $U_t(\theta)$ with respect to θ) converges in probability to an invertible matrix I_θ :

$$\mathbf{H}U_t(\theta) \rightarrow I_\theta \quad \text{in probability as } t \rightarrow \infty,$$

H_6 : $\sup_{\|\beta\| < \epsilon} |\mathbf{H}_{kl}U_t(\theta + \beta) - \mathbf{H}_{kl}U_t(\theta)| \rightarrow 0$ in probability, where $\epsilon > 0$ and \mathbf{H}_{kl} is the component (k, l) , $1 \leq k, l \leq p$, of the Hessian operator.

Under these assumptions, the minimum contrast estimator is consistent and asymptotically normal (Dacunha-Castelle and Duflo, 1982): as $t \rightarrow \infty$,

- $\hat{\theta}_t$ converges in probability to θ and
- $\sqrt{t}(\hat{\theta}_t - \theta)$ converges in law to the Gaussian distribution $\mathcal{N}(0, I_\theta^{-1} \Gamma_\theta I_\theta^{-1})$.

B Proof of equation (2)

Since $\tilde{\theta}_t$ satisfies $\mathbf{grad}p_t(\tilde{\theta}_t) = 0$,

$$0 = -tc(\tilde{\theta}_t)\mathbf{grad}U_t(\tilde{\theta}_t) + \mathbf{grad}c(\tilde{\theta}_t).$$

Then, applying a first order Taylor's expansion for $\mathbf{grad}U_t(\tilde{\theta}_t)$ around $\hat{\theta}_t$ yields

$$0 = -tc(\tilde{\theta}_t)\{\mathbf{grad}U_t(\hat{\theta}_t) + (\mathbf{H}U_t(\hat{\theta}_t))(\tilde{\theta}_t - \hat{\theta}_t)\}(1 + o_{\text{proba}}(1)) + \mathbf{grad}c(\tilde{\theta}_t).$$

In this equation, $\mathbf{grad}U_t(\hat{\theta}_t) = 0$ because $\hat{\theta}_t$ is the maximizer of $U_t(\cdot)$. Moreover, applying zero order Taylor's expansions for $c(\tilde{\theta}_t)$, $\mathbf{H}U_t(\hat{\theta}_t)$ and $\mathbf{grad}c(\tilde{\theta}_t)$ around θ yields

$$\begin{aligned} 0 &= -tc(\theta)(\mathbf{H}U_t(\theta))(\tilde{\theta}_t - \hat{\theta}_t)(1 + o_{\text{proba}}(1)) + \mathbf{grad}c(\theta) \\ &= -tc(\theta)I_\theta(\tilde{\theta}_t - \hat{\theta}_t)(1 + o_{\text{proba}}(1)) + \mathbf{grad}c(\theta), \end{aligned}$$

since $\lim_{t \rightarrow \infty} \mathbf{H}U_t(\theta) = I_\theta$ in probability. Then equation (2) follows.

C Proof of equation (3)

Let $\delta > 0$. For any a such that $\sup_{1 \leq i \leq p} |a_i| < t^\delta$, a third order Taylor's expansion yields

$$\log p_t(\tilde{\theta}_t + a/\sqrt{t}) - \log p_t(\tilde{\theta}_t) = -\sqrt{t}a' \mathbf{grad} U_t(\tilde{\theta}_t) - \frac{1}{2}a' I_\theta a + o_{\text{proba}}(t^{2\delta} + t^{3\delta-1/2}).$$

Given that $\mathbf{grad} U_t(\hat{\theta}_t) = 0$ (definition of the classical minimum contrast estimator $\hat{\theta}_t$) and that $\tilde{\theta}_t - \hat{\theta}_t = o_{\text{proba}}(t^{-1+\delta})\mathbf{1}_p$ where $\mathbf{1}_p$ is the unit vector of size p , the dimension of Θ (see eq. (2)), the previous equation becomes

$$\log p_t(\tilde{\theta}_t + a/\sqrt{t}) - \log p_t(\tilde{\theta}_t) = -\frac{1}{2}a' I_\theta a + o_{\text{proba}}(t^{2\delta} + t^{3\delta-1/2}).$$

Ensuring that $\delta < 1/2$ (and not only $\delta > 0$), then

$$\begin{aligned} \log p_t(\tilde{\theta}_t + a/\sqrt{t}) - \log p_t(\tilde{\theta}_t) &= -\frac{1}{2}a' I_\theta a + o_{\text{proba}}(t^{2\delta}) \\ &= -\frac{1}{2}a' I_\theta a \{1 + o_{\text{proba}}(1)\}. \end{aligned}$$

Let us introduce $g_t : a \mapsto t^{-p/2}p_t(\tilde{\theta}_t + a/\sqrt{t})$ defined over \mathbb{R}^p . This density function satisfies, from the previous result,

$$g_t(a) \underset{t \rightarrow \infty}{\sim} t^{-p/2}p_t(\tilde{\theta}_t) \exp\left(-\frac{1}{2}a' I_\theta a\right).$$

Since $g_t(\cdot)$ is a density function and given the form of the right-hand-side term of this equation, $g_t(\cdot)$ is equivalent to the density function of the normal law with variance matrix I_θ^{-1} . Equation (3) is then obtained with the change of variable $\alpha = \tilde{\theta}_t + a/\sqrt{t}$.

D Spatial Markovian model: Limit matrices

I_θ and Γ_θ satisfy $I_\theta = \text{var}(Z_0)$ and $\Gamma_\theta = M_0 + 4 \sum_{0 \leq i_1, i_2 \leq 2} M_i$ where $M_i = \text{cov}(Z_0, Z_i)$, $i \in \mathcal{I}$, and

$$Z_i = \left(X_i - \frac{\exp\left(\theta_1 + \theta_2 \sum_{j \in V(i)} X_j\right)}{1 + \exp\left(\theta_1 + \theta_2 \sum_{j \in V(i)} X_j\right)} \right) \begin{pmatrix} 1 \\ \sum_{j \in V(i)} X_j \end{pmatrix}.$$