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Estimation and prediction of a 2D lognormal diffusion random field

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Abstract This paper describes techniques for estimation and prediction of two-parameter lognormal diffusion random fields. The drift and diffusion coefficients, which characterize a two-parameter lognormal diffusion under certain conditions, are estimated by maximum likelihood. For data on a regular grid, an alternative method is proposed to estimate the diffusion coefficient. Both of these estimates are compared in several situations. The kriging predictors are formulated involving the drift and diffusion coefficients and the predictions are obtained using the estimates of these coefficients.

Keywords Diffusion random field · Kriging · Lognormal diffusion process

Introduction

Lognormal stochastic models play, at different technical levels, an important role in various scientific fields, in particular in Environmental Sciences. At the first level of complexity, two-parameter and three-parameter lognormal distributions have been used for statistical fitting of random variables describing environmental phenomena; see, for example, Crow (1988), Addiscott (1994), Small et al. (1998), in the univariate case; Buchanan and Leduc (1994), Indyk and Potocki (1994), in the multivariate case.

Dynamic models formulated in terms of lognormal stochastic processes have been also widely applied in Environmental Sciences and related fields (see, for

example, Smith and De Veaux 1992; Zielinski and Ponnambalam 1994; Tjeng and Chai 1999). In the recent years, significant analytical and statistical aspects related to univariate and multivariate lognormal processes have been addressed from both the forward-backward Kolmogorov equations and the Itô stochastic formulation points of view; for instance, parameter estimation and hypothesis testing, as well as first-passage time problems for certain time barriers, are solved in Gutiérrez et al. (1995), Gutiérrez et al. (1997b), and Gutiérrez et al. (1999). Furthermore, certain non-homogeneous versions of lognormal diffusions, with special incidence in this work, have been proposed and applied in different contexts (for example, to Economics, in relation to consumption of energetic products, etc.). Specifically, such models are constructed by formulating the drift term as dependent on certain deterministic functions in time (*exogenous factors*), and their applicability is based on establishing statistical inference results which allow model fitting to data obtained from discrete or continuous sampling (see Gutiérrez et al. 1991, 1997a, 2001).

Lognormal random fields represent the technically more complex stage of lognormal modelling. Usually introduced as a random field whose logarithm is a Gaussian random field (see, for example, Journel and Huijbregts 1978; Christakos 1992; Cressie 1993), the lognormal random field has been studied in the geostatistical context in relation to the associated lognormal kriging and to simulation aspects. Applications cover relevant problems in Geosciences, Radar Theory and Image Analysis, Astrophysics, Hydrology, etc. (see, for instance, Frankot and Chellappa 1987; Sheth 1995; Lee and Ellis 1997; Gómez-Hernández and Gorelick 1989; Noda and Hoshiya 1998; Corazza and Vatalaro 1994; Goldys et al. 2000). Problems as parameter estimation, lognormal simple kriging, estimation based on lognormal maximum entropy, among others, are generally undertaken by simply considering the lognormal random field as the exponential transformation of a Gaussian random field, without reference to any specific

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diffusion structure. This latter approach, however, constitutes an important alternative in relation to modeling, parameter estimation and inference, analysis of first passage through barriers, associated Itô equations and derivation of discrete simulation schemes, etc. Among the contribution to theoretical foundations for diffusion random fields, see Nualart (1983), and Ruiz-Medina and Valderrama (1998). In this context, Gutiérrez and Roldán (2001) develop a general study of homogeneous lognormal random fields from both the Kolmogorov and Itô equations.

It is expected that, in the next few years, important problems in Environmental Sciences, such as the definition and calculation of pollution indexes, which has been approached in some cases by consideration of homogeneous Gaussian random fields (see, for example, Christakos and Hristopulos 1997), will be modelled in terms of two-dimensional non-homogeneous lognormal random fields, taking into account the well-known lognormal distribution of pollutant elements. Subsequent development of space-time evolution equations involving lognormal random fields is also envisaged as an important direction for research, of particular interest for applications in Environmental Sciences.

In this paper, we study estimation and prediction of a 2D lognormal diffusion random field. The contents are organized as follows. First, the lognormal random field model is established and a related non-homogeneous version is introduced, involving exogenous factors affecting the drift term, following the same idea developed for the one-parameter case as mentioned above. Maximum-likelihood estimation of the model parameters based on discrete finite set of data is then explicitly solved. Finally, aspects related to kriging and simulation are addressed and illustrated.

Lognormal diffusion random fields

Lognormal diffusion processes are commonly used in the analysis of economic variables. When the parameter space is a subset of \mathbf{R}_+^2 , Nualart (1983) introduced a class of two-parameter random fields which are diffusions on each coordinate and satisfy a particular Markov property related to partial ordering in \mathbf{R}_+^2 . Using this theory, Gutiérrez and Roldán (2001) gave a characterization of a two parameter lognormal diffusion random field and proved that the transition density is determined by drift and diffusion coefficients, \tilde{a} and \tilde{B} . We next summarize the results related to this characterization.

Let $\{X(\mathbf{z}) : \mathbf{z} = (s, t) \in I = [0, S] \times [0, T] \subset \mathbf{R}_+^2\}$ be a positive-valued Markov random field, defined on a probability space (Ω, \mathcal{A}, P) , where $X(0, 0)$ is assumed to be constant or a lognormal random variable with $E[\ln X(0, 0)] = \phi_0$ and $\text{var}(\ln X(0, 0)) = \sigma_0^2$. The distribution of the random field is determined by the following transition probabilities:

$$\begin{aligned} P(B, (s + h, t + k)|(x_1, x, x_2), \mathbf{z}) \\ = P[X(s + h, t + k) \in B | X(s, t + k) = x_1, X(\mathbf{z}) \\ = x, X(s + h, k) = x_2 \end{aligned}$$

where $\mathbf{z} = (s, t) \in I, h, k > 0, (x_1, x, x_2) \in \mathbf{R}_+^3$ and B is a Borel subset. We suppose that the transition densities exist and are given by

$$\begin{aligned} g(y, (s + h, t + k)|(x_1, x, x_2), \mathbf{z}) \\ = \frac{1}{y\sqrt{2\pi\sigma_{\mathbf{z};h,k}^2}} \exp\left\{-\frac{1}{2}\left(\frac{\ln(yx/x_1x_2) - m_{\mathbf{z};h,k}}{\sigma_{\mathbf{z};h,k}}\right)^2\right\}, \end{aligned}$$

for $y \in \mathbf{R}_+$, with

$$\begin{aligned} m_{\mathbf{z};h,k} &= \int_s^{s+h} \int_t^{t+k} \tilde{a}(\sigma, \tau) \, d\sigma d\tau, \\ \sigma_{\mathbf{z};h,k}^2 &= \int_s^{s+h} \int_t^{t+k} \tilde{B}(\sigma, \tau) \, d\sigma d\tau, \end{aligned}$$

and \tilde{a}, \tilde{B} being continuous functions on I . Under these conditions we can assert that $\{X(\mathbf{z}) : \mathbf{z} \in I\}$ is a lognormal diffusion random field. The one-parameter drift and diffusion coefficients associated are given by

$$\begin{aligned} a_1(\mathbf{z})x &:= (\tilde{a}_1(\mathbf{z}) + \frac{1}{2}\tilde{B}_1(\mathbf{z}))x, & B_1(\mathbf{z})x^2 &:= \tilde{B}_1(\mathbf{z})x^2, \\ a_2(\mathbf{z})x &:= (\tilde{a}_2(\mathbf{z}) + \frac{1}{2}\tilde{B}_2(\mathbf{z}))x, & B_2(\mathbf{z})x^2 &:= \tilde{B}_2(\mathbf{z})x^2, \end{aligned}$$

where

$$\begin{aligned} \tilde{a}_1(s, t) &= \int_0^t \tilde{a}(s, \tau) \, d\tau, & \tilde{B}_1(s, t) &= \int_0^t \tilde{B}(s, \tau) \, d\tau, \\ \tilde{a}_2(s, t) &= \int_0^s \tilde{a}(\sigma, t) \, d\sigma, & \tilde{B}_2(s, t) &= \int_0^s \tilde{B}(\sigma, t) \, d\sigma, \end{aligned}$$

for all $\mathbf{z} = (s, t) \in I, x \in \mathbf{R}_+$.

The random field $\{Y(\mathbf{z}) : \mathbf{z} \in I\}$ defined as $Y(\mathbf{z}) = \ln X(\mathbf{z})$ is then a Gaussian diffusion random field, with \tilde{a} and \tilde{B} being, respectively, the drift and diffusion coefficients, and $\tilde{a}_1, \tilde{a}_2, \tilde{B}_1$ and \tilde{B}_2 being the corresponding one-parameter drift and diffusion coefficients. Furthermore, if $\mathbf{z}, \mathbf{z}' \in I, \mathbf{z} = (s, t), \mathbf{z}' = (s', t')$, then

$$\begin{aligned} m_Y(\mathbf{z}) &:= E[Y(\mathbf{z})] = \phi_0 + \int_0^s \int_0^t \tilde{a}(\sigma, \tau) \, d\sigma d\tau, \\ \sigma_Y^2(\mathbf{z}) &:= \text{var}(Y(\mathbf{z})) = \sigma_0^2 + \int_0^s \int_0^t \tilde{B}(\sigma, \tau) \, d\sigma d\tau, \\ c_Y(\mathbf{z}, \mathbf{z}') &:= \text{cov}(Y(\mathbf{z}), Y(\mathbf{z}')) = \sigma_Y^2(\mathbf{z} \wedge \mathbf{z}'), \end{aligned}$$

where we write $\mathbf{z} \wedge \mathbf{z}'$ for $(s \wedge s', t \wedge t')$, with ‘ \wedge ’ denoting the minimum.

Henceforth we will assume that the condition usually considered for estimation of the drift and diffusion coefficients in the one-parameter case hold; that is, $P[\ln X(0, 0) = \phi_0] = 1$ (i.e. $\sigma_0^2 = 0$) and

$$\sigma_Y^2(\mathbf{z}) = \tilde{B}st, \quad \mathbf{z} = (s, t) \in I.$$

Estimation of the drift and diffusion coefficients

Let $\{X(\mathbf{z}) : \mathbf{z} \in I\}$ be a lognormal diffusion random field. Data $\mathbf{X} = (X(\mathbf{z}_1), \dots, X(\mathbf{z}_n))^t$ are assumed to be observed at known spatial locations $\mathbf{z}_1 = (s_1, t_1)$, $\mathbf{z}_2 = (s_2, t_2), \dots, \mathbf{z}_n = (s_n, t_n) \in I$. Let $\mathbf{x} = (x_1, x_2, \dots, x_n)^t$ be a sample. Let us consider the log-transformed n -dimensional random vector, $\mathbf{Y} = (Y(\mathbf{z}_1), Y(\mathbf{z}_2), \dots, Y(\mathbf{z}_n))^t = (\ln X(\mathbf{z}_1), \ln X(\mathbf{z}_2), \dots, \ln X(\mathbf{z}_n))^t = \ln \mathbf{X}$, and the log-transformed sample, $\mathbf{y} = (y_1, y_2, \dots, y_n)^t = \ln \mathbf{x}$. We denote

$$\mathbf{m}_Y = (m_Y(\mathbf{z}_1), \dots, m_Y(\mathbf{z}_n))^t,$$

$$\Sigma_Y = (\sigma_Y^2(\mathbf{z}_i \wedge \mathbf{z}_j))_{i,j=1,\dots,n}.$$

MLE for the drift and diffusion coefficients using exogenous factors

Suppose that the drift coefficient \tilde{a} of Y is a linear combination of several known functions, set $\{h_1(\mathbf{z}), \dots, h_p(\mathbf{z}) : \mathbf{z} \in I\}$, with real coefficients ϕ_1, \dots, ϕ_p :

$$\tilde{a}(\mathbf{z}) = \sum_{\alpha=1}^p \phi_\alpha h_\alpha(\mathbf{z}), \quad \mathbf{z} \in I.$$

Defining, for $\mathbf{z} = (s, t) \in I$,

$$f_0(z) = 1,$$

$$f_\alpha(z) = \int_0^s \int_0^t h_\alpha(\sigma, \tau) d\sigma d\tau, \quad \alpha = 1, \dots, p,$$

the mean of Y is given by

$$m_Y(s, t) = \phi_0 + \sum_{\alpha=1}^p \phi_\alpha \int_0^s \int_0^t h_\alpha(\sigma, \tau) d\sigma d\tau$$

$$= \sum_{\alpha=0}^p \phi_\alpha f_\alpha(\mathbf{z}).$$

Thus, denoting $\mathbf{F} = (\mathbf{f}_0, \mathbf{f}_1, \dots, \mathbf{f}_p)$, with $\mathbf{f}_\alpha = (f_\alpha(\mathbf{z}_1), f_\alpha(\mathbf{z}_2), \dots, f_\alpha(\mathbf{z}_n))^t$, for $\alpha=0, 1, \dots, p$, and $\phi = (\phi_0, \phi_1, \dots, \phi_p)^t$, we have

$$\phi_Y = (\phi_0 \mathbf{f}_0 + \phi_1 \mathbf{f}_1 + \dots + \phi_p \mathbf{f}_p) = \mathbf{F}\phi.$$

Let us write

$$\Sigma_Y = \tilde{B}\mathbf{M}:$$

$$= \tilde{B} \begin{pmatrix} s_1 t_1 & (s_1 \wedge s_2)(t_1 \wedge t_2) & \dots & (s_1 \wedge s_n)(t_1 \wedge t_n) \\ (s_1 \wedge s_2)(t_1 \wedge t_2) & s_2 t_2 & \dots & (s_2 \wedge s_n)(t_2 \wedge t_n) \\ \vdots & \vdots & \ddots & \vdots \\ (s_1 \wedge s_n)(t_1 \wedge t_n) & (s_2 \wedge s_n)(t_2 \wedge t_n) & \dots & s_n t_n \end{pmatrix}.$$

With this notation, the joint density function of the random vector \mathbf{Y} is

$$f(\mathbf{y}) = \frac{1}{(2\pi)^{n/2} |\tilde{B}\mathbf{M}|^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{y} - \mathbf{F}\phi)^t (\tilde{B}\mathbf{M})^{-1} (\mathbf{y} - \mathbf{F}\phi) \right\},$$

and then, the joint density function of \mathbf{X} is given by

$$g(\mathbf{x}) = \frac{1}{(2\pi)^{n/2} |\tilde{B}\mathbf{M}|^{1/2} \prod_{i=1}^n x_i} \times \exp \left\{ -\frac{1}{2} (\ln \mathbf{x} - \mathbf{F}\phi)^t (\tilde{B}\mathbf{M})^{-1} (\ln \mathbf{x} - \mathbf{F}\phi) \right\}.$$

Therefore, the associated log-likelihood function is

$$\ln L(\mathbf{x}; \phi, \tilde{B}) = -\frac{n}{2} \ln(2\pi) - \frac{1}{2} \ln |\tilde{B}\mathbf{M}| - \ln \left(\prod_{i=1}^n x_i \right)$$

$$- \frac{1}{2} (\ln \mathbf{x} - \mathbf{F}\phi)^t (\tilde{B}\mathbf{M})^{-1} (\ln \mathbf{x} - \mathbf{F}\phi)$$

$$= -\frac{n}{2} \ln(2\pi) - \frac{n}{2} \ln \tilde{B} - \frac{1}{2} \ln |\mathbf{M}| - \ln \left(\prod_{i=1}^n x_i \right)$$

$$- \frac{1}{2\tilde{B}} (\ln \mathbf{x} - \mathbf{F}\phi)^t \mathbf{M}^{-1} (\ln \mathbf{x} - \mathbf{F}\phi).$$

Differentiating with respect to ϕ and \tilde{B} , and equating to 0, we have

$$(\ln \mathbf{x} - \mathbf{F}\phi)^t \mathbf{M}^{-1} \mathbf{F} = \mathbf{0},$$

$$-\frac{n}{2\tilde{B}} + \frac{n}{2\tilde{B}^2} (\ln \mathbf{x} - \mathbf{F}\phi)^t \mathbf{M}^{-1} (\ln \mathbf{x} - \mathbf{F}\phi) = 0,$$

with $\mathbf{0} = (0, \dots, 0)$. Solving for ϕ and \tilde{B} , we obtain

$$\phi^* = (\phi_0^*, \phi_1^*, \dots, \phi_p^*)^t = (\mathbf{F}' \mathbf{M}^{-1} \mathbf{F})^{-1} \mathbf{F}' \mathbf{M}^{-1} \ln \mathbf{x} \quad (1)$$

and

$$\tilde{B}^* = \frac{1}{n} (\ln \mathbf{x} - \mathbf{m}_Y^*)^t \mathbf{M}^{-1} (\ln \mathbf{x} - \mathbf{m}_Y^*), \quad (2)$$

where $\mathbf{m}_Y^* = \mathbf{F}\phi^*$.

Remark.

In many practical applications, a polynomial trend provides a suitable representation for the drift surface,

$$m(\mathbf{z}) = \sum_{0 \leq k+l \leq r} \phi_{kl} s^k t^l, \quad \mathbf{z} = (s, t),$$

for some appropriate choice of r .

Estimation of the drift and diffusion coefficients from data on a regular grid

Suppose now that the data are obtained on a regular grid in \mathbf{R}_+^2 . Let $\mathbf{z} = (s, t)$ be a point on a set S of locations included in the regular grid and let us denote the 2D four-point increment of Y by

$$Y(\Delta_{hk}(\mathbf{z})) = Y(s+h, t+k) - Y(s, t+k) - Y(s+h, t) + Y(s, t),$$

for $h, k > 0$. Taking into account that the variance of this increment,

$$\text{var}(Y(\Delta_{hk}(\mathbf{z}))) = \sigma_{\mathbf{z};h,k}^2 = \int_s^{s+h} \int_t^{t+k} \tilde{B}(\sigma, \tau) d\sigma d\tau = \tilde{B}hk,$$

does not depend on the location \mathbf{z} , but only on the area hk , the diffusion coefficient \tilde{B} can be estimated using a similar approach to Matheron's (1962) estimator for the variogram (see also Cressie 1993), considering here 2D four-point increments, as follows.

Under the implicit condition that $\mathbf{z}_i = (s_i, t_i) < \mathbf{z}_j = (s_j, t_j)$, we denote

$$[\mathbf{z}_i, \mathbf{z}_j] = \{(s_i, t_i), (s_i, t_j), (s_j, s_i), (s_j, t_j)\}.$$

Assuming first that the mean is constant, we propose the estimator

$$\text{var}(Y(\Delta_{hk}(\mathbf{z}))) = \frac{1}{|N(hk)|} \sum_{N(hk)} [Y(s+h, t+k) - Y(s, t+k) - Y(s+h, t) + Y(s, t)]^2, \quad (3)$$

where

$$N(hk) \equiv \{(\mathbf{z}_i, \mathbf{z}_j) : [\mathbf{z}_i, \mathbf{z}_j] \in S,$$

$$v(s_j - s_i)(t_j - t_i) = hk, i, j = 1, \dots, n\}$$

and $|N(hk)|$ is the number of distinct elements of $N(hk)$. Note that, in this case, the mean does not need to be estimated. From Eq. 3, we can estimate variances for the different areas hk associated with the grid subset S considered. Then, an estimate for \tilde{B} can be obtained from the slope of the 'best' straight line starting at the origin and approximating the set of points $(hk, \widehat{\text{var}}(Y(\Delta_{hk}(\mathbf{z}))))$ calculated. Here we adopt the usual least-squares criterion for optimality, and denote \tilde{B}^{**} the corresponding estimator for \tilde{B} .

If the mean is not constant, we can also estimate the increment variances as follows:

$$\text{var}(Y(\Delta_{hk}(\mathbf{z}))) = \frac{1}{|N(hk)|} \sum_{N(hk)} (Y(s+h, t+k) - Y(s, t+k) - Y(s+h, t) + Y(s, t) - m_Y(s+h, t+k) + m_Y(s, t+k) + m_Y(s+h, t) - m_Y(s, t))^2, \quad (4)$$

for $\mathbf{z} = (s, t)$. If the mean is unknown, it can be estimated using Eq. 1 by $m_Y^*(\mathbf{z}) = \sum_{x=0}^p \phi_x^* f_x(\mathbf{z})$.

Lognormal kriging

Let \mathbf{z}_0 be a known spatial location where we are interested to estimate X from observations at locations $\mathbf{z}_1, \dots, \mathbf{z}_n \in I$. Here we follow the usual approach which con-

sists of transforming the data from the X scale to the Y scale,

$$\begin{aligned} \mathbf{Y} &= (Y(\mathbf{z}_1), \dots, Y(\mathbf{z}_n))^t \\ &= (\ln(\mathbf{z}_1), \dots, \ln(\mathbf{z}_n))^t. \end{aligned}$$

Using this data we obtain the kriging predictor for $Y(\mathbf{z}_0)$,

$$\hat{Y}(\mathbf{z}_0) = \sum_{i=1}^n \lambda_i Y(\mathbf{z}_i) = \lambda^t \mathbf{Y}.$$

Then, the predictor for $X(\mathbf{z}_0)$, $\hat{X}(\mathbf{z}_0)$, is obtained using an appropriate unbiased back transformation of $\hat{Y}(\mathbf{z}_0)$, (Cressie 1993). We next summarize the results obtained under the different hypotheses that are usually considered.

We denote

$$\mathbf{c}_Y = (\sigma_Y^2(\mathbf{z}_0 \wedge \mathbf{z}_1), \dots, \sigma_Y^2(\mathbf{z}_0 \wedge \mathbf{z}_n))^t,$$

where $\mathbf{z}_0, \mathbf{z}_1, \dots, \mathbf{z}_n \in I$.

Simple lognormal kriging

Assuming that ϕ_0 and \tilde{B} are known constants and \tilde{a} is a known continuous function on I , an unbiased predictor of $X(\mathbf{z}_0)$ is given by

$$\begin{aligned} \hat{X}(\mathbf{z}_0) &= \exp \left\{ \mathbf{c}_Y^t \Sigma_Y^{-1} (\mathbf{Y} - \mathbf{m}_Y) + m_Y(\mathbf{z}_0) \right. \\ &\quad \left. + \frac{\sigma_Y^2(\mathbf{z}_0) - \mathbf{c}_Y^t \Sigma_Y^{-1} \mathbf{c}_Y}{2} \right\} \\ &= \exp \left\{ \hat{Y}(\mathbf{z}_0) + \frac{\sigma_{Ysk}^2(\mathbf{z}_0)}{2} \right\}, \end{aligned} \quad (5)$$

where

$$\hat{Y}(\mathbf{z}_0) = \mathbf{c}_Y^t \Sigma_Y^{-1} (\mathbf{Y} - \mathbf{m}_Y) + m_Y(\mathbf{z}_0).$$

The corresponding minimum mean-squared prediction error is

$$\begin{aligned} E \left[(X(\mathbf{z}_0) - \hat{X}(\mathbf{z}_0))^2 \right] &= \exp \{ 2m_Y(\mathbf{z}_0) + \sigma_Y^2(\mathbf{z}_0) \} \\ &\quad \times [\exp \{ \sigma_Y^2(\mathbf{z}_0) \} - \exp \{ \text{var}(\hat{Y}(\mathbf{z}_0)) \}], \end{aligned}$$

where

$$\text{var}(\hat{Y}(\mathbf{z}_0)) = \lambda^t \Sigma_Y \lambda, \text{ with } \lambda^t = \mathbf{c}_Y^t \Sigma_Y^{-1}.$$

Ordinary lognormal kriging

We now consider ϕ_0 to be an unknown constant, $\tilde{a}(\mathbf{z}) = 0$, for all $\mathbf{z} \in I$, and \tilde{B} a known constant. In this case, an unbiased predictor of $X(\mathbf{z}_0)$ is given by

$$\begin{aligned}\hat{X}(\mathbf{z}_0) &= \exp \left\{ \mathbf{c}_Y^t \Sigma_Y^{-1} \mathbf{Y} + (1 - \mathbf{1}' \Sigma_Y^{-1} \mathbf{c}_Y) \hat{\phi}_0 \right. \\ &\quad \left. + \frac{1}{2} \left(\sigma_Y^2(\mathbf{z}_0) - \mathbf{c}_Y^t \Sigma_Y^{-1} \mathbf{c}_Y + \frac{(1 - \mathbf{1}' \Sigma_Y^{-1} \mathbf{c}_Y)^2}{\mathbf{1}' \Sigma_Y^{-1} \mathbf{1}} \right) \right. \\ &\quad \left. - \frac{1 - \mathbf{1}' \Sigma_Y^{-1} \mathbf{c}_Y}{\mathbf{1}' \Sigma_Y^{-1} \mathbf{1}} \right\} \\ &= \exp \left\{ \hat{Y}(\mathbf{z}_0) + \frac{\sigma_{Yok}^2(\mathbf{z}_0)}{2} - M \right\},\end{aligned}$$

where

$$\hat{\phi}_0 = \frac{\mathbf{1}' \Sigma_Y^{-1} \mathbf{Y}}{\mathbf{1}' \Sigma_Y^{-1} \mathbf{1}},$$

$$\hat{Y}(\mathbf{z}_0) = \mathbf{c}_Y^t \Sigma_Y^{-1} \mathbf{Y} + (1 - \mathbf{1}' \Sigma_Y^{-1} \mathbf{c}_Y) \hat{\phi}_0, \quad \text{and}$$

$$M = (1 - \mathbf{1}' \Sigma_Y^{-1} \mathbf{c}_Y) (\mathbf{1}' \Sigma_Y^{-1} \mathbf{1})^{-1} \quad (\text{Lagrange multiplier}).$$

The minimized mean-squared prediction error is

$$\begin{aligned}\hat{E} \left[(X(\mathbf{z}_0) - \hat{X}(\mathbf{z}_0))^2 \right] &= \exp \left\{ 2\hat{\phi}_0 + \sigma_Y^2(\mathbf{z}_0) \right\} \\ &\quad \times \left[\exp \left\{ \sigma_Y^2(\mathbf{z}_0) \right\} \right. \\ &\quad \left. + \exp \left\{ \text{var}(\hat{Y}(\mathbf{z}_0)) \right\} (1 - 2e^{-M}) \right],\end{aligned}$$

where

$$\begin{aligned}\text{var}(\hat{Y}(\mathbf{z}_0)) &= \lambda^t \Sigma_Y \lambda, \quad \text{with } \lambda^t \\ &= \mathbf{c}_Y^t \Sigma_Y^{-1} + (1 - \mathbf{1}' \Sigma_Y^{-1} \mathbf{c}_Y) (\mathbf{1}' \Sigma_Y^{-1} \mathbf{1})^{-1} \mathbf{1}' \Sigma_Y^{-1}.\end{aligned}$$

Numerical examples

In this section we describe some numerical examples illustrating estimation and prediction for a lognormal diffusion random field under the approaches considered. First, using simulated data on a regular grid, the two estimation methods for the diffusion coefficient respectively described in Sects. 3.1 and 3.2 are compared. Both cases of known mean and unknown constant mean (for the associated Gaussian random field; see Sect. 4) are studied. For the latter case, we obtain (lognormal) kriging predictions of the field.

The parameter space considered is $I = [0, 1.67] \times [0, 1.07]$. Realizations are generated on a regular 19×19 grid with SW corner at point (0.05, 0.05) and NE corner at point (1.67, 1.07) using the method of unconstrained simulation (see Christakos 1992). Parameter estimates and predictions are obtained on this grid based on the data \mathbf{X} , consisting of the values corresponding to the 7×7 grid subset determined by the same corner points. Both sets are displayed in Fig. 1.

We first consider a lognormal diffusion random field with non constant mean, and with $\phi_0 = 0.25$, $\tilde{a}(\mathbf{z}) = -2$, for all $\mathbf{z} \in I$, and $\tilde{B} = 1$. Table 1 gives the

estimates of \tilde{B}^* and \tilde{B}^{**} obtained for 16 independent unconstrained simulations for this random field, assuming that the mean of the associated Gaussian random field is known.

In particular, the values obtained for $\widehat{\text{var}}(Y(\Delta_{hk}(\mathbf{z})))$ (see Eq. 4) from simulation 1, for the possible values of hk and $|N(hk)|$ determined by the 7×7 grid considered, are given in Table 2. The corresponding regression line from which \tilde{B}^{**} was obtained is represented in Fig. 2. For these data, the slope is $\tilde{B}^{**} = 1.2778$.

Assuming now that the mean is constant, $\tilde{a}(\mathbf{z}) = 0$, for all $\mathbf{z} \in I$, for all $\mathbf{z} \in I$, we have generated 16 unconstrained simulations for a lognormal diffusion random field with $\phi_0 = 0.25$, and $\tilde{B} = 1$, as before. Estimates ϕ_0^* , \tilde{B}^* and \tilde{B}^{**} are given in Table 3. (In this case, the values of $\widehat{\text{var}}(Y(\Delta_{hk}(\mathbf{z})))$ are obtained using the Eq. 3.)

As for kriging, we have considered the latter case, that is, the lognormal diffusion random field with $\phi_0 = 0.25$, $\tilde{a} = 0$ and $\tilde{B} = 1$. Using the 49 values obtained from simulation 1 (see Fig. 3) and $\tilde{B}^* = 1.1328$ we have obtained 361 predictions by ordinary lognormal kriging (see Eq. 6). The results are plotted in Fig. 4.

Figure 5 displays a contour-level plot for the 19×19 realization obtained from simulation 1.

From the results obtained in both cases studied, we can observe that the maximum-likelihood estimation method overall provides more accurate estimates for the diffusion coefficient than the alternative method based on evaluation of 2D four-point increments. A similar behavior has been observed in several other cases studied by the authors. Lack of stability in the estimate \tilde{B}^* can be possibly overcome by robust estimation of the slope of $\widehat{\text{var}}(Y(\Delta_{hk}(\mathbf{z})))$ versus hk instead of using the least-squares approach.

Conclusions

In this paper we study estimation of the drift and diffusion coefficients and prediction for a 2D lognormal

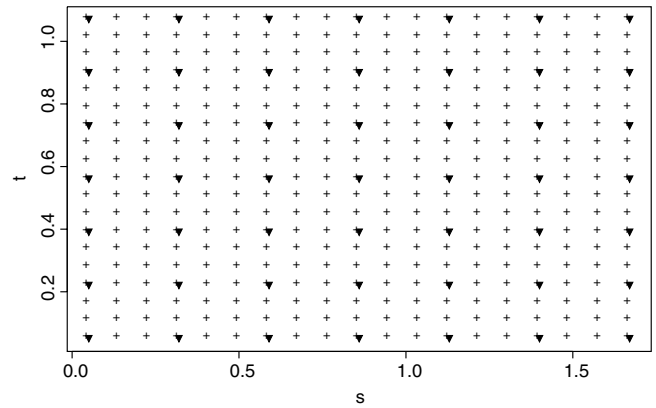


Fig. 1 Grids with the 49 observation locations and the 361 locations for prediction

Table 1 Estimates of \tilde{B} by the two methods considered, for 16 simulations of the lognormal diffusion random field (known non constant mean case)

| Simulation number | \tilde{B}^* | \tilde{B}^{**} |
|-------------------|---------------|------------------|
| 1 | 1.0045 | 1.2778 |
| 2 | 0.9528 | 0.7436 |
| 3 | 1.1243 | 0.8203 |
| 4 | 0.9492 | 1.7679 |
| 5 | 0.7116 | 0.2694 |
| 6 | 0.7615 | 0.4587 |
| 7 | 1.0214 | 0.3270 |
| 8 | 1.0359 | 3.9383 |
| 9 | 0.7809 | 0.3710 |
| 10 | 0.7884 | 0.5202 |
| 11 | 0.8757 | 0.5730 |
| 12 | 0.9804 | 0.9938 |
| 13 | 1.2311 | 0.3689 |
| 14 | 0.5693 | 1.1436 |
| 15 | 1.0823 | 0.4155 |
| 16 | 0.8557 | 0.8566 |

diffusion random field, including exogenous factors in its formulation. This is an important case of random fields which are not intrinsically stationary, then well-known related techniques cannot be applied. Such models are useful to represent diffusion-type positive valued characteristics associated to phenomena of interest in different fields, in particular pollutant indicators in environmental studies.

Two approaches are considered for parameter estimation from discrete observations: one is based on MLE, which can be applied to irregularly spaced observations; the other one exploits the Gaussian distribution of the log-transformation of the random field and stationarity of the 2D four-point increments, which can be applied to the case of observations lying on a regular grid. Unbiased kriging predictors are obtained for the cases of known and constant unknown mean for

Table 2 Values of $|N(hk)|$ and $\widehat{\text{var}}(Y(\Delta_{hk}(\mathbf{z})))$ for the possible values of the areas hk

| hk | $ N(hk) $ | $\widehat{\text{var}}(Y(\Delta_{hk}(\mathbf{z})))$ |
|--------|-----------|--|
| 0.0459 | 36 | 0.0441 |
| 0.0918 | 60 | 0.0725 |
| 0.1377 | 48 | 0.0996 |
| 0.1836 | 61 | 0.1511 |
| 0.2295 | 24 | 0.2242 |
| 0.2754 | 52 | 0.2531 |
| 0.3672 | 30 | 0.3423 |
| 0.4131 | 16 | 0.3560 |
| 0.4590 | 20 | 0.4099 |
| 0.5508 | 34 | 0.6100 |
| 0.6885 | 16 | 0.7041 |
| 0.7344 | 9 | 0.9754 |
| 0.8262 | 8 | 0.9570 |
| 0.9180 | 12 | 1.1385 |
| 1.1016 | 6 | 1.6370 |
| 1.1475 | 4 | 1.1602 |
| 1.3770 | 4 | 1.7207 |
| 1.6524 | 1 | 2.5249 |

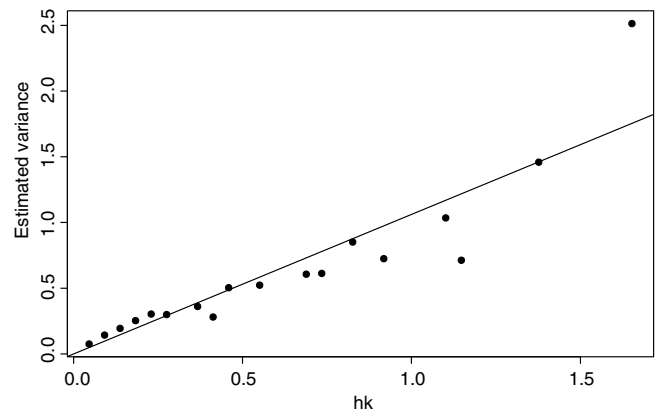


Fig. 2 Straight line fitted by least squares

the associated Gaussian field. Numerical examples illustrating the methods considered, are provided.

The approach considered allows us to use well-known techniques for estimation and prediction, such as simple kriging. The numerical examples show that both methods of estimation considered provide reasonable results. However, as commented in Sect. 5, our experience with these and other cases studied suggests that the implementation of the 2D four-point increment approach might be improved, e.g. by using robust regression for estimating the diffusion coefficient, for increasing the stability of estimates. A rigorous formal comparative study on the statistical performance of both methods is not available at this stage.

Possible extensions under investigation by the authors include consideration of non-constant diffusion-type values at the boundary axes, to exploit exogenous factors accounting for covariable effects, as well as higher-dimension spatial and spatio-temporal formulations. Also, development of validation techniques in this context would be most important for real applications.

Table 3 Estimates of ϕ_0 and \tilde{B} by the two methods considered for 16 simulations of the lognormal diffusion random field (unknown constant mean case)

| Simulation number | ϕ_0^* | \tilde{B}^* | \tilde{B}^{**} |
|-------------------|------------|---------------|------------------|
| 1 | 0.2465 | 1.1328 | 1.2162 |
| 2 | 0.2965 | 1.1060 | 0.6644 |
| 3 | 0.3357 | 0.6264 | 0.4295 |
| 4 | 0.2555 | 1.0045 | 0.8650 |
| 5 | 0.2453 | 0.9928 | 0.5687 |
| 6 | 0.2434 | 1.3253 | 0.5777 |
| 7 | 0.1959 | 0.9338 | 0.3480 |
| 8 | 0.2202 | 0.8337 | 0.5206 |
| 9 | 0.2814 | 0.8788 | 0.4451 |
| 10 | 0.3016 | 1.0578 | 0.9393 |
| 11 | 0.2036 | 1.0823 | 0.2217 |
| 12 | 0.2509 | 0.9359 | 0.6627 |
| 13 | 0.2968 | 0.9008 | 0.3172 |
| 14 | 0.2159 | 0.9217 | 0.6742 |
| 15 | 0.1809 | 0.9993 | 0.5006 |
| 16 | 0.2834 | 0.8746 | 0.7880 |

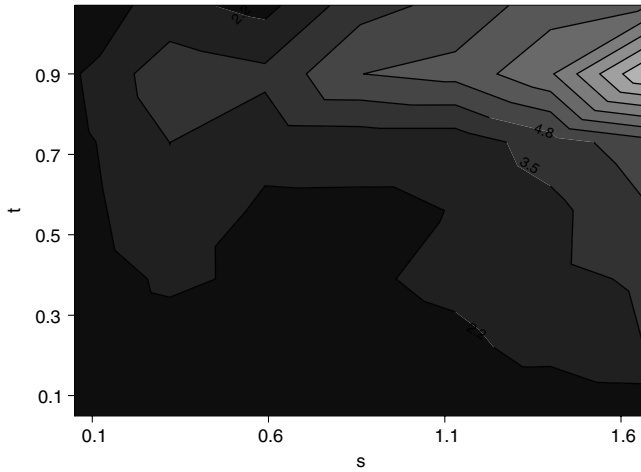


Fig. 3 Contour-level plot of 49 values generated (simulation 1) for the lognormal diffusion random field (unknown constant mean case)

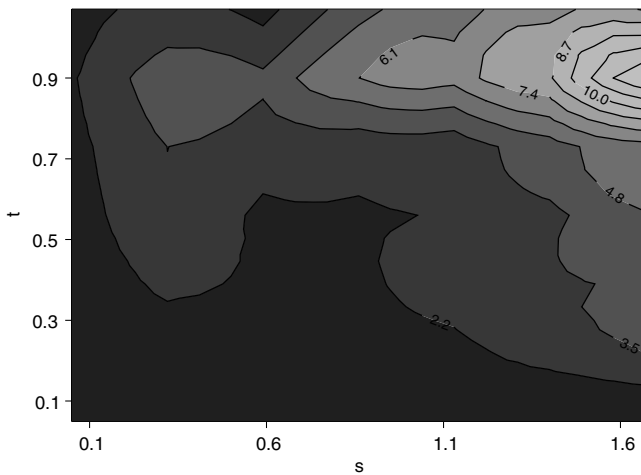


Fig. 4 Contour-level plot of the 361 predictions obtained by ordinary lognormal kriging using the 49 values plotted in Fig. 3

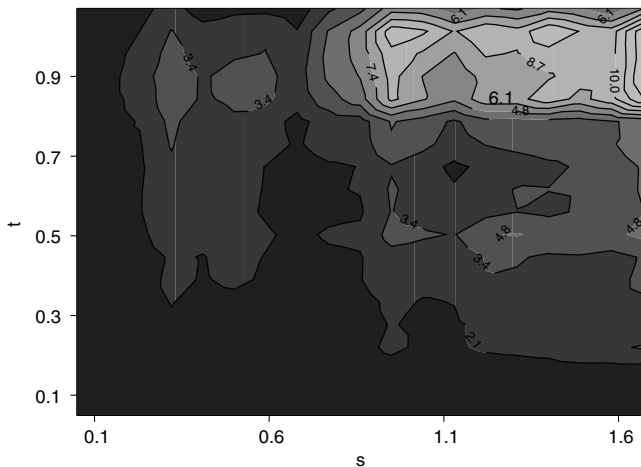


Fig. 5 Contour-level plot of the 361 values (including the 49 values used for estimating \hat{B}) generated (simulation 1) for the lognormal diffusion random field considered

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