Bernoulli **1(4)**, 1995, 301–319

How reliable are contour curves? Confidence sets for level contours

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We present a method to add confidence limits to level curves, drawn on a map of a Gaussian random surface, measured with or without error on a regular or irregular grid. The method is based on the conditional level crossing intensity measure for non-stationary Gaussian fields.

Keywords: Level crossings; surface reconstruction; Gaussian field; random field; first passage density; Rice's formula

1. Introduction

1.1. Surface reconstruction

Surface interpolation and surface reconstruction are central problems in computer graphics. A related problem is that of finding level curves of a more or less unknown surface. For example, when dealing with spatial data measuring a pollutant concentration, one may want to construct level curves or isolines corresponding to fixed levels of concentration. In computer vision the level curves may correspond to boundaries between separate image elements. The topic of the present paper is how well such constructed level curves agree with the true isolines or element boundaries.

Several algorithms exist for construction of level curves, which work on regularly or irregularly spaced data. The basic idea is first to interpolate the surface between the measured points, and then to find the exact level curves for the interpolated surface by a curve tracing algorithm. Thus, the confidence of the level curves is entirely dependent on how well the surface has been reconstructed, based on available data. Surface interpolation is often considered as a numerical problem, where computational efficiency is just as important as surface smoothness and other surface characteristics.

In order to evaluate the accuracy of level curves, one also has to have some idea of how well the measured values represent the true surface. This means that one must model the surface as a random field between the measured points. There is an extensive literature on statistical techniques for smoothing and interpolation of spatial data. Many of these techniques have been developed in a geostatistical context, in which spatial dependence was recognized at an early stage. Cressie (1991) gives a quite complete survey of statistics for spatial data, as its title suggests. As far as the authors can see, however, the accuracy of level curves seems to have received no attention in the theoretical literature, even if it should be of considerable interest from a practical point of view.

Related to the level curve problem is that of finding the location of the peaks, or local maxima, in the unobserved surface. Of course, the natural estimates of the peaks are the peaks in the

reconstructed surface, but there is no reason to believe that the true surface and the reconstruction have their maxima at exactly the same location.

The reconstruction, smoothing and interpolation of a partially observed surface is of course dependent on the postulated model structure, as well as on its parameters, and neither of these is generally known from first principles. The parameters can be estimated by any suitable statistical technique, but the model structure needs to be established from more basic knowledge. The aim of this paper is to present a numerically accurate method to calculate confidence limits for level curves in a reconstructed field when the underlying model is assumed to be differentiable and Gaussian. The suggested technique can be combined with any standard statistical techniques for estimation and reconstruction of spatial data based on the Gaussian distribution; the particular estimation methods used in the examples are by no means the only or even preferred ones.

It should be emphasized that the method is closely tied to the Gaussian assumption. However, it is not restricted to homogeneous fields, although its dependence on the correlation structure is explicit. It can therefore be used to calculate alternative solutions dependent on hypothesized correlation structures and parameter values, including assumed measurement errors.

1.2. Level curves and crossing intensities

In this paper we present a method to find the precision of calculated contours in terms of confidence bands which possess a calculable probability of confining the true but unknown contour.

We assume that the surface $\xi(t)$ has been measured, possibly with a random error, at a finite number of points which need not be regularly spaced. In general, the surface is then interpolated or reconstructed by some numerical technique; for general references, see Cressie (1991) and papers cited therein for a statistical approach or Grimson (1983) and Szeliski (1990) for more computer vision oriented aspects. A level set for a level u is the set of points t at which $\xi(t) = u$. However, for our purposes an alternative but equivalent definition is technically more suited. A level set is the union of all *level crossings* when one follows a section of the surface along straight lines in the parameter plane.

In order to state the confidence in the calculated level curves we regard the unknown surface as a random field with a certain conditional distribution, given the observed points. The reconstruction and its level curves should be our best guess, given the observed data. The true field, however, is described only in terms of its statistical distribution around this best guess. The level crossings on a line section are then estimates of the locations of the true level crossings for the unknown surface. The accuracy of these estimates can be given in terms of a conditional *level crossing intensity* for the unobserved field along the straight-line section. This intensity can then be used to evaluate the confidence of the calculated contour.

Surface reconstruction from a statistical viewpoint is discussed in Section 2, while crossing and first crossing intensities are described in Section 3. These are then used in Section 4, with examples in Section 5, to define confidence bands for level curves.

1.3. Some notation

In the stochastic setting, we think of the surface $\{\xi(t), t \in \mathbb{R}^2\}$ as a Gaussian random field, with

average, or expected, height 0, $E[\xi(t)] = 0$. The regularity of the field is described by the covariance function,

$$r(s,t) = \mathrm{cov}[\xi(s), \xi(t)], \qquad \text{for } s, t \in \mathbb{R}^2.$$

This means that the height at a point t is a Gaussian random variable with distribution $N(0, r(t,t))$, and that the correlation between points s and t is $r(s,t)/\sqrt{r(s,s)r(t,t)}$. For generality we also allow for a random measurement error, that is, the observed values are

$$\xi_{\mathrm{obs}}(t) = \xi(t) + \epsilon(t),$$

where the $\epsilon(t)$ are independent Gaussian variables with mean zero and variance σ_ϵ^2. The Gaussian assumption, both for the field itself and for the observation errors, is essential for the numerical computations of crossing intensities later in this paper.

In general, the correlation structure of $\xi(t)$ can take any form, but in order to have some basis for the analysis we will assume that the field is homogeneous, and even isotropic, that is, the covariance function $r(s,t)$ depends only on length of the vector $t - s$. We also assume that the variance is constant and equal to 1.

Isotropy is a rather restrictive assumption, which it may not be possible to satisfy in all image reconstruction problems. For other types of problem, such as level curves in geographical maps, it may well be a reasonable assumption, in particular since there exist techniques to transform the geographical map to make the correlation structure more isotropic; see, for example, Guttorp *et al.* (1992). However, the method we propose is by no means restricted to the isotropic case, not even to the homogeneous case, but can be applied to all types of covariance structures.

The assumption of isotropy simplifies the correlation structure considerably, and in that case the covariance function is always of the form

$$r(t) = \int_{x=0}^{\infty} J_0(x\|t\|)\, \mathrm{d}G(x), \tag{1}$$

where $J_0(x)$ is a first-order Bessel function,

$$J_0(x) = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k!)^2},$$

and $G(x)$ is a bounded non-decreasing function. There are no other restrictions on $G(x)$, and all functions of the form (1) can be the covariance function for an isotropic field. Explicit and simple isotropic covariance functions are

$$r(t) = \sigma^2 \exp(-a^2\|t\|^2) \tag{2}$$

$$r(t) = \sigma^2(1 + \|t\|^2/b^2)^{-\beta}.$$

This and other basic facts about random fields can be found, for example, in Cressie (1991, Section 2.5) and in Wong (1971) and Adler (1981). In the examples we shall use a discrete version of the general form (1) and the Gaussian covariance (2). When no confusion can arise, we shall sometimes write $r(d)$ for the correlation at distance d, that is to say, $r(t) = r(\|t\|)$.

Methods to estimate the covariance function by means of observed data are discussed in Section 6; see also Cressie (1991).

2. Surface reconstruction from finite data

2.1. Surface reconstruction

Surface reconstruction from statistical principles can be made under more or less specific distributional assumptions. The least-squares reconstruction, based only on first and second moments, is also optimal under Gaussian assumptions. In geostatistics, surface reconstruction from observed data goes under the name of kriging, and there exist several methods that take care of different applications due to the presence of local trends, estimation bias, and smoothness requirements; see Cressie (1991) for an exhaustive account. Here we summarize the facts we need for the level curve studies.

Assume that the field has been observed at a finite number of points, $\{t_k, k = 1, \dots, n\}$, with coordinates $t_k = (t_{k1}, t_{k2})$, and denote the observed value at the point t_k by $x_k = x(t_k)$. If the field is observed with independent observation errors, $x(t_k)$ is an observation of $\xi(t_k) + \epsilon(t_k)$, where $\epsilon(t_k)$, $k = 1, \dots, n$, are independent random variables with mean zero and variance σ_ϵ^2. When there are no observation errors, $x(t_k)$ is simply an observation of $\xi(t_k)$.

Write

$$T = (t_1, \dots, t_n)^{\mathrm{T}}, \quad x(T) = (x_1, \dots, x_n)^{\mathrm{T}}$$

for the two-column matrix of observation locations and the column vector of observed data, respectively. Similarly, write $\xi(T) = (\xi(t_1), \dots, \xi(t_n))^{\mathrm{T}}$ for the n-dimensional random variable of the field at T, and $\epsilon(T) = (\epsilon(t_1), \dots, \epsilon(t_n))^{\mathrm{T}}$ for the observation errors; that is, $x(T) = \xi(T) + \epsilon(T)$.

Let $\Sigma_T = (r(t_i - t_j) + \sigma_\epsilon^2 I$ denote the covariance matrix of $x(T)$ and write

$$r_T(s) = (r(s - t_1), \dots, r(s - t_n))^{\mathrm{T}} = \operatorname{cov}[\xi(T) + \epsilon(T), \xi(s)]$$

for the column vector of covariances between the observed values $x(T)$, and any field values $\xi(s)$.

The general formulation of the surface interpolation or reconstruction problem is to find a function $\{\xi^*(t), t \in \mathcal{A}\}$, in a given class of functions defined over a set $\mathcal{A} \subset \mathbb{R}^2$, which optimizes some distance and smoothness measure over $\mathcal{A}$.

The following statement is a reformulation of a well-known property of the multivariate Gaussian distribution.

Theorem 1 The best reconstruction of a Gaussian field ξ, over the whole of $\mathbb{R}^2$, given the data $x(T)$, is the conditional expectation

$$m_T(t) = E[\xi(t) \mid \xi(T) + \epsilon(T) = x(T)] = r_T(t)^{\mathrm{T}} \Sigma_T^{-1} x(T), \tag{3}$$

that is, the function $\xi^*(t)$, $t \in \mathbb{R}^2$, of $x(T)$ that minimizes

$$E[\{\xi(t) - \xi^*(t)\}^2], \qquad \text{for all } t \in \mathbb{R}^2,$$

is given by the conditional expectation, $\xi^*(t) = m_T(t)$.

Further, the conditional field $\{\xi(t), t \in \mathbb{R}^2 \mid \xi(T) + \epsilon(T) = x(T)\}$ is a non-homogeneous Gaussian field with mean $m_T(t)$ and covariance function

$$\begin{aligned} r_T(x,t) &= \operatorname{cov}[\xi(s), \xi(t) \mid \xi(T) + \epsilon(T) = x(T)] \\ &= r(s-t) - r_T(s)^{\mathrm{T}} \Sigma_T^{-1} r_T(t). \end{aligned} \tag{4}$$

The statistical uncertainty around the reconstruction is measured by the reconstruction error, $\xi(t) - m_T(t)$, and has covariance function $r_T(s,t)$. In particular, its variance at the point t is $r_T(t,t)$. For future use, we introduce the notation $\{\eta_T(t), t \in \mathbb{R}^2\}$ for a non-homogeneous Gaussian field with mean 0 and covariance function $r_T(s,t)$.

Remark *Smoothing reconstruction*
Most surface interpolation algorithms treat the interpolation or reconstruction problem as an optimization problem that minimizes the distance between the observed data and the reconstruction, under some additional penalty on the lack of smoothness of the reconstruction. The squared distance between data and reconstruction is then simply

$$d(\xi^*, x(T)) = \|\xi^*(T) - x(T)\|^2 = \sum_{k=1}^{n} (\xi^*(t_k) - x_k)^2.$$

There exist in the literature several smoothness measures. A method that should be compared to the statistical reconstruction is the *thin plate spline* model, where the lack of smoothness is measured by local surface curvature,

$$s(\xi^*) = \int\int_{t \in \mathcal{A}} \{\xi^*_{11}(t)^2 + 2\xi^*_{12}(t)^2 + \xi^*_{22}(t)^2\} \, \mathrm{d}t, \tag{5}$$

where the subscripts indicate partial derivatives. The continuous optimization problem is then to find the ξ^* that minimizes the function

$$d(\xi^*, x(T)) + \lambda s(\xi^*)$$

for some fixed constant λ. This can be solved by replacing the integral in (5) by an appropriate sum of second differences over a discrete set of points. The quadratic optimization problem can then be solved explicitly and the solution is linear in $x(T)$; see, for example, Szeliski (1990) for details.

2.2. Examples

Example 1 *Simulated data*
In Section 4 we shall propose a method to analyse level curves on a reconstructed field. To illustrate the method we shall study some artificial Gaussian isotropic fields, observed at irregularly spaced points over a square $\mathcal{A} = [0,2] \times [0,2]$. The covariance function shall be of the isotropic form (1) with the non-decreasing function G piecewise constant with a finite number of jumps,

$$r(t) = \sum_{i=1}^{M} g_i J_0(r_i \|t\|). \tag{1'}$$

Table 1. True and estimated values of g_i in (1') for Example 1.

Location	*True weights*	*Estimated weights*	
r_i	g_i	$n = 5$	$n = 20$
2	2	1.70	1.11
3	4	3.98	0.00
4	2	0.00	5.79

We let the function G have jumps at three distinct points ($M = 3$); see Table 1. The true correlation function is shown in Fig. 1.

In some examples we shall assume that the covariance function is completely known, but we shall also estimate it from data by means of a cross-validation method; see Section 6. In the examples, we shall consider both a difficult case with few observed data ($n = 5$), and a better-defined case with many observations ($n = 20$). In the estimation, we shall use the true locations, r_i, and estimate only the weights g_i. The observations are made without observation error ($\sigma_\varepsilon^2 = 0$), and this is also assumed known, and is used in the estimation of the covariance function.

Figure 1 also shows the estimated cross-validated covariance functions; estimated data for the weights g_i can be found in Table 1. Of course, one should not expect the coefficients to be correctly estimated from only $n = 5$ or $n = 20$ data points.

The field is reconstructed by means of the conditional expected fields, calculated as in Theorem 1, and the level curves reconstructed by the MATLAB routine `contour`. The reconstructed fields, with the covariance function known or estimated, are shown in Figs 2–3, for $n = 5$ and $n = 20$ observations, and the corresponding level curves in Fig. 4.

The level curves calculated from the true and the estimated covariance functions are rather close to each other in these examples. As we shall see in later examples, the uncertainties imposed by the

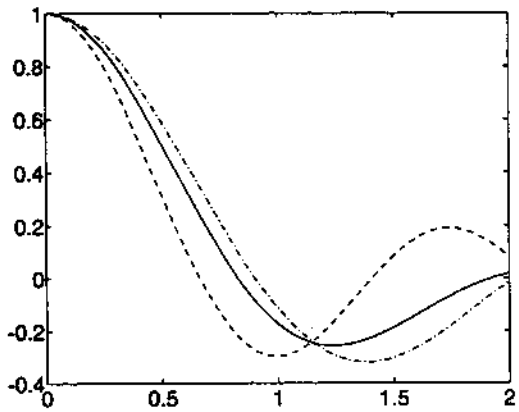

Figure 1. True (solid) and estimated (dash-dotted, $n = 5$; dashed, $n = 20$) correlation functions for the field in Example 1.

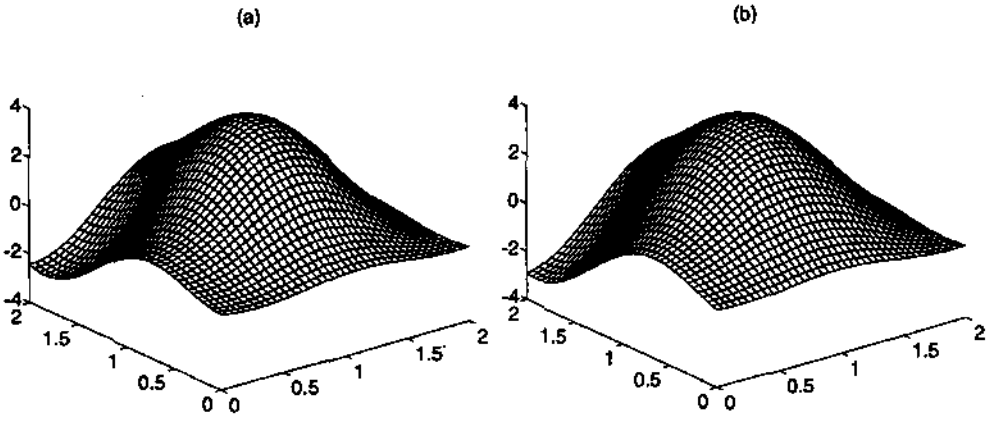

Figure 2. Reconstructed field in Example 1; $n = 5$. (a) True covariances. (b) Estimated covariances.

estimation can still be large compared to the inherent uncertainty about the true field, at least when the observations of the field are made with extra random error.

Example 2 *Ozone data*

We shall now illustrate the method on data where we have no prior knowledge of distribution or correlation structure. We take the publicly available ozone data from the built-in data set in S-PLUS, consisting of the medians of the daily maxima of ozone concentration (in parts per billion, ppb) for June–August, 1974, at 41 measuring stations in north-eastern USA; see Becker *et al.* (1988). Figure 5 shows the data, after subtraction of the mean, together with contour lines on the

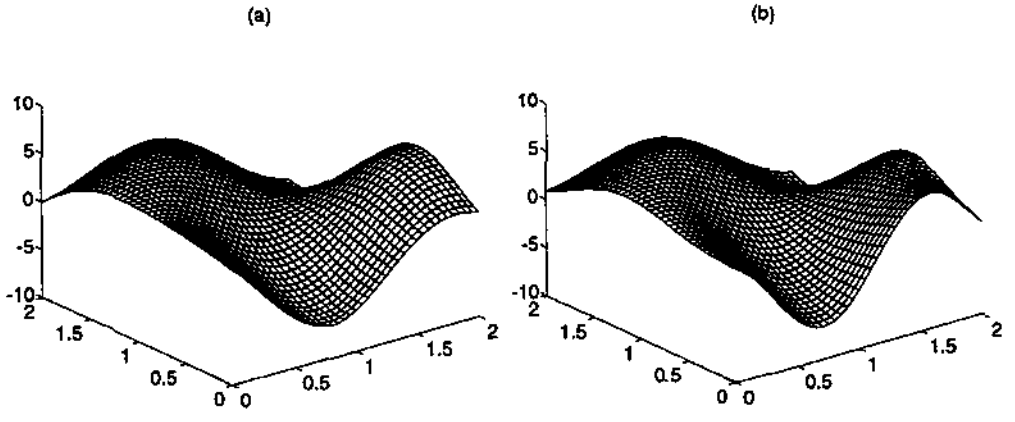

Figure 3. Reconstructed field in Example 1; $n = 20$. (a) True covariances. (b) Estimated covariances.

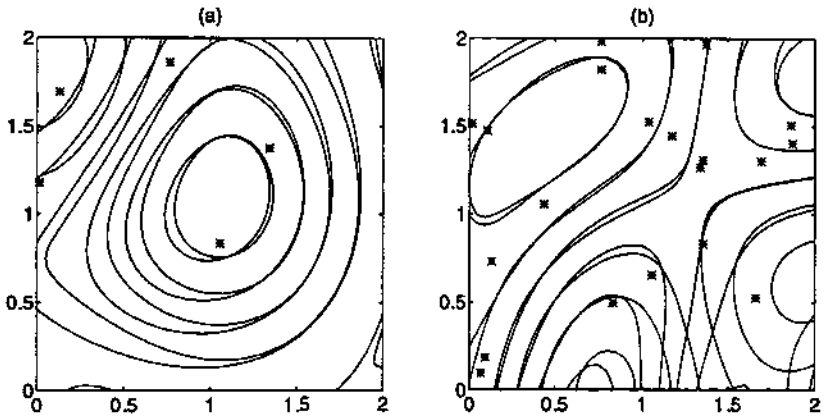

Figure 4. Observation points and contour curves in Example 1, (a) $n = 5$, (b) $n = 20$, with true and estimated covariances.

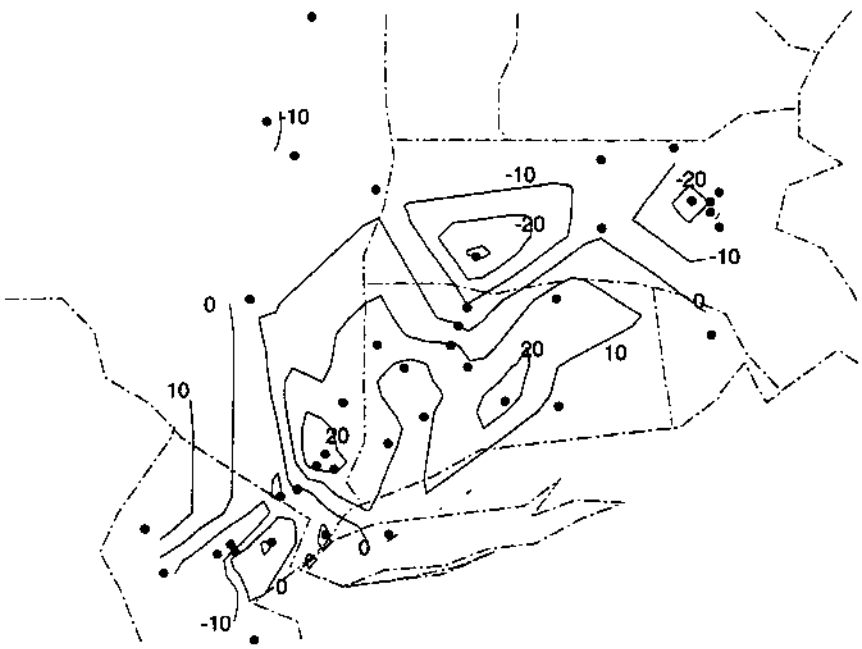

Figure 5. L3evel curves for the variation of ozone concentration in north-eastern USA around the mean value; data in Example 2 from S-PLUS.

linearly interpolated surface, calculated by means of the S-PLUS routines `contour` and `interp`, respectively. Before we estimated the covariance structure, we transformed the coordinate sites (x, y) by an affine transformation to simplify coordinate notation and make the surface more isotropic. The final coordinates were

$$x' = (2x + y + 109.15)/2$$

$$y' = 4(-x + 2y - 154.5)/3.$$

We also deleted three points in the north-eastern part of the region, that is, those with the largest x' coordinate. This left 38 data points for the analysis.

By means of the cross-validation technique described in Section 6 we fitted a covariance structure of the Gaussian type (2), together with an observation error variance σ_ϵ^2. The fitted covariance function was

$$r(t) = \sigma^2 \exp(-a^2\|t\|^2) = 176 \exp(-3.77\|t\|^2),$$

and the estimate of the observation error variance was $\sigma_\epsilon^2 = 17.5$.

3. Directional crossing intensities

3.1. Line sections

Under the statistical model, where the surface is assumed to be a Gaussian (isotropic) field, the conditional mean $m_T(t)$, given by (3), is the best reconstruction of $\xi(t)$, given the observations $\xi(T) + \epsilon(T) = x(T)$. Obviously, a level curve for $m_T(t), t \in \mathcal{A}$, consists of the solutions to the equation $m_T(t) = u, t \in \mathcal{A}$. The true level curve consists similarly of the solutions to the equation $\xi(t) = u, t \in \mathcal{A}$. The difference between the true field and the reconstruction $m_T(t)$ was introduced in Theorem 1, and was denoted by $\eta_T(t) = \xi(t) - m_T(t)$.

Thus, the natural framework of contour confidence intervals is to make probabilistic statements about the level crossings of the field $\{\eta_T(t) + m_T(t), t \in \mathcal{A}\}$, with known mean $m_T(t)$ and covariance function $r_T(s, t)$ given by (4), and describing the conditional distributions of $\{\xi(t), t \in \mathcal{A}\}$ given $\xi(T) + \epsilon(T) = x(T)$. In general, even for Gaussian fields, this is an extremely difficult problem, and no general theory is available that allows us to define the full stochastic properties of random level curves.

However, contour curves can also be constructed by taking sections through the surface. A level contour for the reconstruction $m_T(t)$ is then the union of the solutions of all equations $m_T(t) = u$, when t lies on all the straight lines that can be drawn in $\mathcal{A}$. The true level contour is similarly the union of level crossings for all sections of the unobserved field $\{\xi(t), t \in \mathcal{A}\}$. Thus, the basic question can be reformulated as how well the level crossings of sections of the mean value function $m_T(t)$ represent the level crossings of sections in the true field. Under the Gaussian hypothesis this can be given a satisfactory numerical answer.

Let $\mathcal{L}_0$ be a straight line in $\mathcal{A}$ through a point t_0 making angle θ_0 with one of the axes; that is, points on $\mathcal{L}_0$ are of the form

$$t_0(\tau) = t_0 + \tau(\cos\theta_0, \sin\theta_0), \qquad \tau \in \mathbb{R}.$$

Thus, we define, for fixed (t_0, θ_0), the conditional mean $m_0(\tau)$ along $\mathcal{L}_0$, and the residual around $m_0(\tau)$, $m_0(\tau) = m_T(t_0(\tau))$, and $\eta_0(\tau) = \eta_T(t_0(\tau))$, where $\eta_T(t)$ is the non-homogeneous Gaussian field defined in Theorem 1. The process $\eta_0(\tau)$ has mean 0 and covariance function given by

$$r_0(\tau_1, \tau_2) = r_T(t_0(\tau_1), t_0(\tau_2)). \tag{6}$$

Due to the isotropy of $\xi(t)$, the covariance function $r_0(\tau_1, \tau_2)$ can be considerably simplified. Write $d_k(\tau) = \|t_0 - t_k + \tau(\cos\theta_0, \sin\theta_0)\|$ for the distance between t_k and $t_0(\tau)$. Then, with $r(t) = r(\|t\|)$, as is easily seen, the covariance function for the residual process $\eta_0(t)$ is given by

$$r_0(\tau_1, \tau_2) = r(\tau_1 - \tau_2) - (r(d_1(\tau_1)), \ldots, r(d_n(\tau_1)))\Sigma_T^{-1}(r(d_1(\tau_2)), \ldots, r(d_n(\tau_2)))^{\mathrm{T}}. \tag{7}$$

3.2. Crossing intensity

The crossings of a level u by the section $\xi(t_0(\tau)), \tau \in \mathbb{R}$, have a conditional distribution, given $\xi(T) + \epsilon(T) = x(T)$, which is the same as the distribution of zero crossings by the process

$$\eta_0(\tau) + m_0(\tau) - u, \qquad \tau \in \mathbb{R}. \tag{8}$$

We denote the zerocrossing intensity of (8) by $\mu_0^+(\tau)$, $\mu_0^-(\tau)$, or $\mu_0(\tau)$, depending on whether we are dealing with zero upcrossings, downcrossings, or just crossings, regardless of direction. (That the crossing intensity is $\mu_0(\tau)$ means that the expected number of crossings in any interval $\mathcal{I}$ is $\int_{\mathcal{I}} \mu_0(\tau)\,d\tau$. Thus, the crossing intensity at a specific point is just a measure of how likely it is that there is a level crossing at that point.)

A crossing intensity in a non-stationary Gaussian process can be calculated explicitly by a generalization of Rice's formula for level crossings, see Cramér and Leadbetter (1967, Chapter 13). It is a function of $m_0(\tau)$ and $r_0(\tau_1, \tau_2)$ as in the following lemma. Define

$$\sigma^2(\tau) = V[\eta_0(\tau)] = r_0(\tau, \tau), \tag{9}$$

$$\gamma^2(\tau) = V[\eta_0'(\tau)] = \left[\frac{\partial^2 r_0(\tau_1, \tau_2)}{\partial\tau_1 \partial\tau_2}\right]_{\tau_1=\tau_2=\tau}, \tag{10}$$

$$\rho(\tau) = \frac{\operatorname{cov}[\eta_0(\tau), \eta_0'(\tau)]}{\gamma(\tau)\sigma(\tau)} = \frac{\left[\frac{\partial r_0(\tau, \tau')}{\partial\tau'}\right]_{\tau'=\tau}}{\gamma(\tau)\sigma(\tau)}. \tag{11}$$

Further, define (omitting the argument τ),

$$\zeta(\tau) = \frac{E[\eta_0' \mid \eta_0 + m_0 = u]}{D[\eta_0' \mid \eta_0 + m_0 = u]} = \frac{m_0' - \gamma\rho(m_0 - u)/\sigma}{\gamma(1 - \rho^2)^{1/2}}. \tag{12}$$

For a proof of the following lemma, see Cramér and Leadbetter (1967, Chapter 13).

Lemma 1 The intensities of a downcrossing, upcrossing, and crossing, regardless of direction, of

the level u by the process $\eta_0(\tau)$ at time τ are given by

$$\mu_0^-(\tau) = \sigma^{-1}\phi\Big(\frac{u-m_0}{\sigma}\Big)\gamma(1-\rho^2)^{1/2}\{\phi(\zeta) - \zeta(1-\Phi(\zeta))\},$$

$$\mu_0^+(\tau) = \sigma^{-1}\phi\Big(\frac{u-m_0}{\sigma}\Big)\gamma(1-\rho^2)^{1/2}\{\phi(\zeta) + \zeta\Phi(\zeta)\},$$

$$\mu_0(\tau) = \sigma^{-1}\phi\Big(\frac{u-m_0}{\sigma}\Big)\gamma(1-\rho^2)^{1/2}\{2\phi(\zeta) + \zeta(2\Phi(\zeta)-1)\},$$

respectively. These functions can all be calculated explicitly from the covariance function, and are thus directly available.

For easy comparison with the first crossing intensity in the next section, we observe that the upcrossing intensity can be expressed as (with $x^+ = \max(x, 0)$)

$$\mu_0^+(\tau) = f_{\eta_0(\tau)}(u - m_0) \cdot E[(\eta_0'(\tau) + m_0'(\tau))^+ \mid \eta_0(\tau) + m_0(\tau) = u]. \tag{13}$$

3.3. First crossing intensity

Lemma 1 gives the intensity with which a level crossing occurs at distance τ from the starting point t_0, with no restriction on the number of crossings between t_0 and $t_0(\tau)$. To make a precise statement about the location of the level curves, we need a more complicated quantity, namely the *first crossing intensity* in an interval $[a, b]$; this is the probability

$$\bar{\mu}_0(\tau)\,\mathrm{d}\tau = P\begin{pmatrix}\eta_0(s) + m_0(s) \text{ has a } u\text{-crossing for some } s \in [\tau, \tau + \mathrm{d}\tau] \\ \text{and } \eta_0(s) + m_0(s) \neq u \text{ for all } s \in [a, \tau]\end{pmatrix},$$

with analogous definitions for $\bar{\mu}_0^+(\tau)$. The first upcrossing intensity can be expressed in analogy with (13) as

$$\bar{\mu}_0^+(\tau) = f_{\eta_0(\tau)}(u - m_0(\tau)) \cdot E[(\eta_0'(\tau) + m_0'(\tau))^+ \chi_u(\tau) \mid \eta_0(\tau) + m_0(\tau) = u], \tag{14}$$

where

$$\chi_u(\tau) = \chi_{\{\eta_0(s) + m_0(s) \leq u \text{ for all } s \in [a,\tau]\}}$$

is the indicator function for the event that τ is the first u-upcrossing point in $[a, b]$.

3.4. Numerical aspects

There do not exist any explicit formulae for the first crossing intensities in (14), but accurate numerical algorithms exist. A collection of such algorithms can be found in the program library CROSSREG, which is a library of Fortran routines for calculation of level crossing and wave characteristic distributions, developed by the authors. The library was presented in Rychlik and Lindgren (1993), which contains a number of examples of its use. The algorithms are available in a MATLAB toolbox, FAT, for analysis of crossing intensities and various other sample path

properties; see Frendahl *et al.* (1993). We have used a FAT routine `firstp.m` to calculate first crossing intensities.

FAT routines approximate the first upcrossing intensity (14) as a conditional expectation where the continuous-time indicator function $\chi_u(\tau)$ is replaced by an indicator function for the finite-dimensional event that $\eta_0(\tau_k) + m_0(\tau_k) \leq u, k = 1, \ldots, N$. The calculations are done by numerical integration of multidimensional integrals.

For large data sets, the direct reconstruction technique and the residual covariance of Theorem 1 may be less useful, since they involve the inversion of large ill-conditioned matrices. The ozone example in Section 2.2 contained 38 data points and was handled without any problems by the routines. For larger data sets the MATLAB routines in FAT provide a check on the residual variances which can be used to reduce the numerical problems. When calculating the conditional crossing intensity at a specific point one only needs to condition on so many surrounding data points that addition of further points does not reduce the residual variances and covariances.

4. Confidence bands for level curves

Figure 4a showed level curves on a reconstruction $m_T(t)$ of an isotropic Gaussian field based on $n = 5$ observations with covariance function as defined in Table 1. Figure 6 shows the level contour drawn at level $u = 0$. The figure also shows a line $\mathcal{L}_0$ perpendicular to the contour through a point $t_0 = t_0(0)$ on the curve, from a point A, $t_0^- = t_0(\tau^-)$ with $m_T(t_0^-) < 0$ to a point B, $t_0^+ = t_0(\tau^+)$ with $m_T(t_0^+) > 0$.

The function $m_0(\tau) = m_T(t_0(\tau))$, which is the best reconstruction of the field along the line is illustrated in Fig. 7. The section through the true field is an unobserved and random Gaussian process with $m_0(\tau)$ as its expected value, and with residual covariance structure given by (6). Figure 7 shows ten realizations of such a random process.

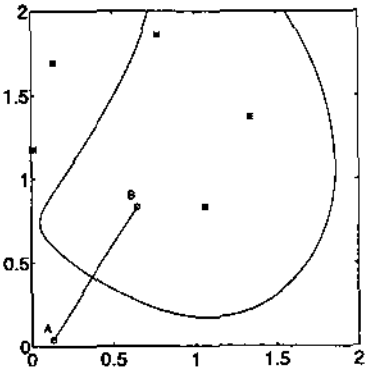

Figure 6. Level curve at level 0 with section AB for Example 1.

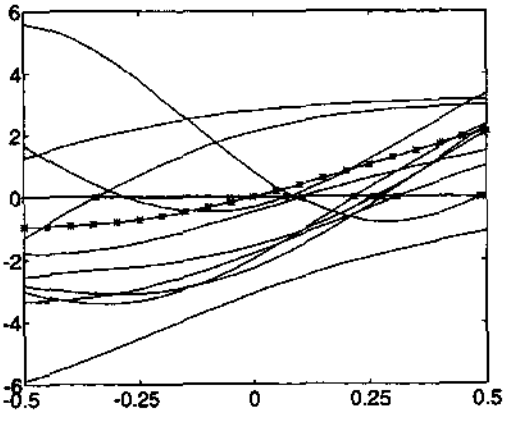

Figure 7. Best reconstruction $m_0(\tau)$ and ten realizations of the field around $m_0(\tau)$ along section AB for Example 1.

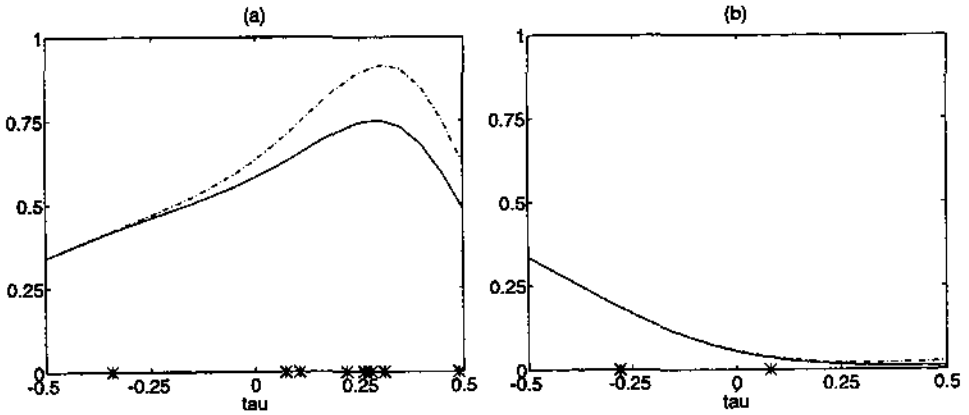

Figure 8. Up- and downcrossing (dash-dotted) and first up- and downcrossing (solid) density across level curve along section AB for Example 1. (a) Shows upcrossings, (b) downcrossings.

We shall take $u = 0$ and study the zero crossings in more detail. The upcrossing intensity $\mu_0^+(\tau)$ and the first upcrossing intensity $\tilde{\mu}_0^+(\tau)$ along the section are shown in Fig. 8a. Figure 8b shows the corresponding downcrossing intensities. As will be seen, the first upcrossing intensity coincides with the upcrossing intensity at the left-hand end of the interval and is strictly smaller at the right-hand end, indicating that the sample function may cross the level several times. The downcrossing intensities are not small in this example, indicating that despite the fact that the reconstruction has an upcrossing, the true field may very well have a downcrossing instead.

We shall now use the first upcrossing intensity to define the confidence level of a section. For an interval I, the integral

$$1 - \alpha = \int_I \tilde{\mu}_0^+(\tau)\, \mathrm{d}\tau,$$

is the probability that there is at least one zero upcrossing by $\eta_0(\tau) + m_0(\tau)$ for $\tau \in I$, which means that the probability is $1 - \alpha$ that a level curve passes through the line segment $\mathcal{L}_0 = \{t_0(\tau); \tau \in I\}$.

Definition 1

A line segment $\tilde{\mathcal{L}}_0^\alpha = \{t_0(\tau); \tau \in I\}$ is a confidence interval with simple confidence level $1 - \alpha$ if

$$1 - \alpha = \int_I \tilde{\mu}_0^+(\tau)\, \mathrm{d}\tau.$$

Simultaneous confidence intervals and confidence levels are defined analogously, as the probability that two or more intervals all contain level upcrossings.

Since the crossing intensity $\mu_0^+(\tau)$ is much easier to calculate than the first crossing intensity $\tilde{\mu}_0^+(\tau)$ one would like to use it in an alternative definition.

Definition 2
A line segment $\mathcal{L}_0^\alpha = \{t_0(\tau); \tau \in I\}$ is an approximate confidence interval with simple confidence level $1-\alpha$ if

$$1-\alpha = \int_I \mu_0^+(\tau)\,\mathrm{d}\tau.$$

The approximate confidence intervals $\mathcal{L}_0^\alpha$ are always contained in the exact intervals $\bar{\mathcal{L}}_0^\alpha$. Consequently, if the location of the level curve is very uncertain, $\mathcal{L}_0^\alpha$ is very wide and there is no need to calculate the more accurate interval $\bar{\mathcal{L}}_0^\alpha$, which in this case is very time-consuming. In the opposite case, when $\mathcal{L}_0^\alpha$ is narrow, unless the process is very irregular, the sample path has no chance of crossing the level more than once, and hence $\mathcal{L}_0^\alpha \approx \bar{\mathcal{L}}_0^\alpha$. In addition, in this case the first passage intensity is easy to compute, and one can easily check the exact coverage probability of $\mathcal{L}_0^\alpha$. The procedure we propose is therefore to use the approximate intervals $\mathcal{L}_0^\alpha$ if they are wide and the exact intervals $\bar{\mathcal{L}}_0^\alpha$ when they are narrow.

The simplest way to construct confidence intervals is to take the normal at a point $t_0 = t_0(0)$ on the level curve and extend it to $\tau = \pm\tau^+$, adjusting τ^+ to give the desired confidence level. The confidence bands in the following examples were constructed in this way, as $\bar{L}_0^\alpha = \{t_0(\tau), -\tau^+ < \tau < \tau^+\}$. The approximate bands $\mathcal{L}_0^\alpha$ are narrower, as noted above.

5. Examples

Example 1 (continued)
We continue the simulated example from Section 2.2 with the covariance function defined in Table 1. Figure 9 shows 50% simple confidence bands for contours at levels $u = 0$ and $u = 2$ based on only $n = 5$ observations. Each section across the band has 50% probability of containing a true level upcrossing. As will be seen, the intervals have to be very wide, except where the level curves pass near an observation point. Of course, this is to be expected with only five observations.

For $n = 20$ more reliable statements can be made. Figure 10 shows 95% confidence bands for levels $u = 0$ and $u = 4$. The confidence bands are now quite narrow, except in the outer part of the observation region.

Figure 11 shows the upcrossing density $\mu_0^+(\tau)$ for each section drawn on Figs 9 and 10 with $u = 0$.

A different situation occurs if the true surface is observed with independent observation errors. Figure 12 illustrates this. Here the observation points as well as the observations themselves are exactly the same as in Fig. 10, that is, the observations are made without error, but in the analysis it is assumed that the observation errors are normal with unit variance, $\sigma_\epsilon^2 = 1$. To obtain 50% confidence the bands around the zero level curves have to be very wide. Since real data are very likely to contain observation errors, this indicates that in practice, one should be careful when one interprets level curves based on observed data.

Example 2 (continued)
For the ozone data we used the estimated covariance function

$$r(t) = \sigma^2 \exp(-\alpha^2\|t\|^2) = 176\exp(-3.77\|t\|^2)$$

with an observation error with variance $\sigma_\epsilon^2 = 17.5$. Figure 13b shows 25% and 50% confidence

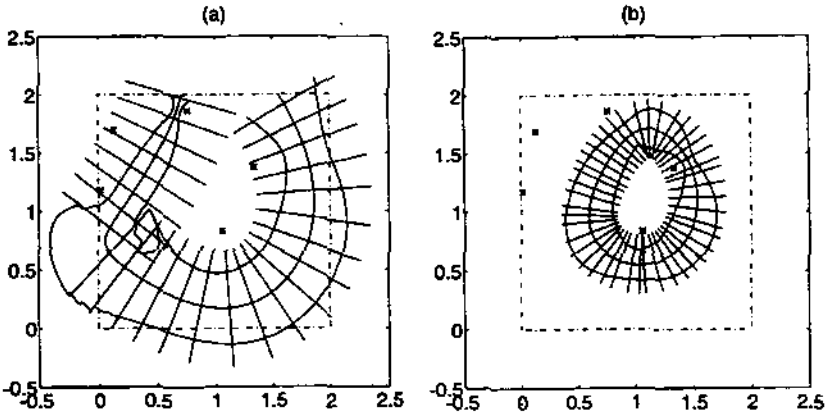

Figure 9. 50% confidence bands in Example 1 for level (a) $u = 0$, (b) $u = 2$; $n = 5$.

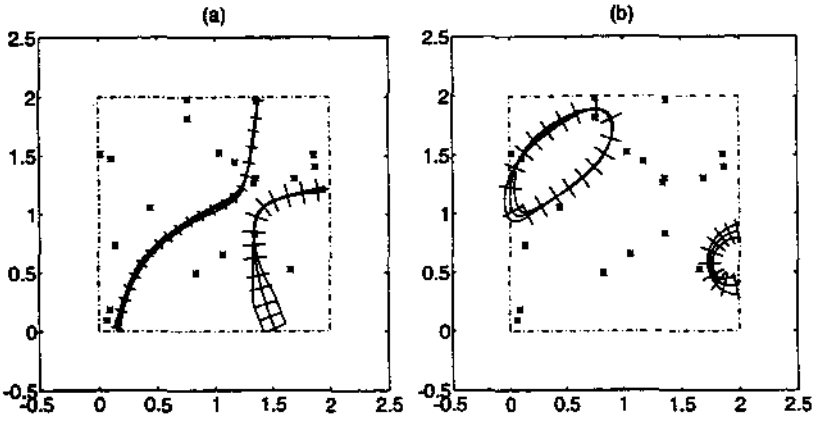

Figure 10. 95% confidence bands in Example 1 for level (a) $u = 0$, (b) $u = 4$; $n = 20$.

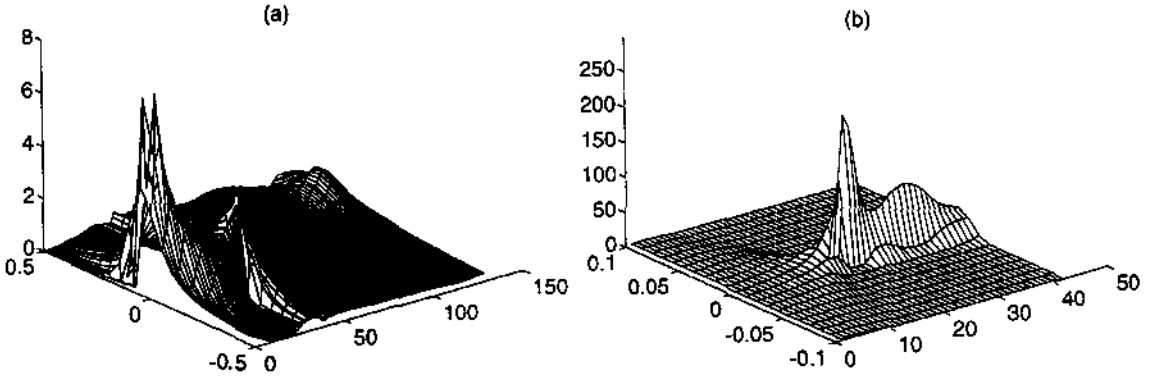

Figure 11. Upcrossing intensities in Example 1 along the zero level curves: (a) $n = 5$; (b) $n = 20$.

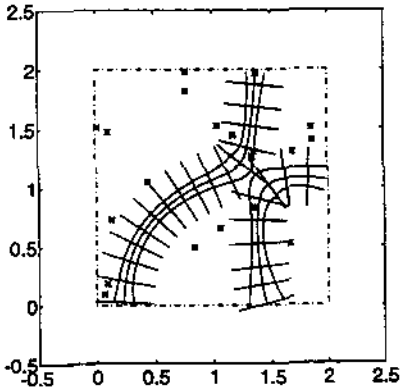

Figure 12. 50% confidence bands in Example 1 for zero level contours when observations are disturbed by observation errors with $\sigma_\varepsilon^2 = 1$; $n = 20$.

bands for a level curve drawn at the mean of the observed ozone values. Note how the band narrows when the level curve passes near observation points. The fact that we have assumed independent observation errors prevents the band from collapsing to zero width at any point. It can also be seen, in Figure 13a, that the linear interpolation performed by the S-PLUS routine `interp` does not make efficient use of the large gradient, for example at the rightmost end of the figure.

6. Estimation of correlation structure

In order to apply the suggested technique, one has to know the covariance function

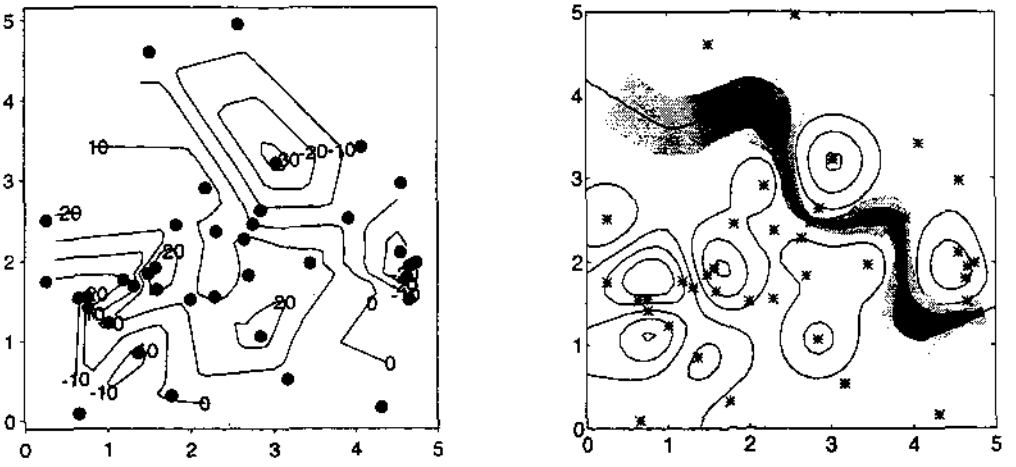

Figure 13. Variation around mean level for Example 2. (a) Level curves after linear interpolation in S-PLUS; (b) level curves after statistical reconstruction with 50% and 25% confidence bands.

$r(t) = \text{cov}\,[\xi(s), \xi(s+t)]$. In practice, one may have to estimate it from data, and this may not be easily done in full generality. If one has repeated measurements on a regular or irregular grid an estimate can be constructed by methods suggested in Guttorp *et al.* (1992) and Loader and Switzer (1992), but in many applications only one replicate is available.

Here we shall exploit the assumed isotropy of the field and construct an estimate from only one single, finite sample of observations of the field. The idea is to use the simple structure (1) of an isotropic covariance function, and estimate the distribution function $G(x)$ in the representation

$$r(t) = \int_{x=0}^{\infty} J_0(x\|t\|)\,\mathrm{d}G(x).$$

Instead of estimating the general $G(x)$, we shall, for example 1, estimate a discrete approximation by letting G be a discrete distribution with mass g_i at points r_i, $i = 1, \ldots, M$. With $g = (g_1, \ldots, g_M)$, write

$$r^*(t; g) = \sum_{i=1}^{M} g_i J_0(r_i\|t\|), \tag{15}$$

where the points r_i can be chosen, for example, as equidistant points from 0 to $r_{\max}$. Both M and r_i are kept constant in the following estimation procedure. The coefficients g_i should be estimated from data, in order to make the field, reconstructed by means of $r^*(t)$, fit the real field as closely as possible.

For the ozone data in Example 2 we fit a covariance function, including observation errors, of the form

$$r^*(t; \sigma, a, \sigma_\epsilon) = \sigma^2 \exp(-a^2\|t\|^2) + \sigma_\epsilon^2 \delta_0(\|t\|). \tag{16}$$

The parameters to be estimated will in both the examples be denoted by θ, $\theta = (g_1, \ldots g_M)$ and $\theta = (\sigma, a, \sigma_\epsilon)$, respectively. To evaluate the reconstruction and find a good estimate we shall use cross-validation, and take as estimate of θ that θ value that minimizes the prediction error when each one of the observations is predicted from the others, using $r^*(t; \theta)$; see Cressie (1991, Section 2.6.4). We shall further impose a variance condition, and require that the estimated covariance function at zero is equal to the observed variance, that is

$$r^*(0; \theta) = \frac{1}{n-1} \sum_{k=1}^{n} (x_i - \bar{x})^2. \tag{17}$$

Let, as previously, the observation points be $T = (t_1, \ldots, t_n)^{\mathrm{T}}$, and denote the observed value at t_k by $x_k = x(t_k)$. Write $x(T) = (x_1, \ldots, x_n)^{\mathrm{T}}$, for the vector of observed data, and let, for $i = 1, \ldots, n$,

$$x_{(i)}(T) = (x_j,\ j \neq i)^{\mathrm{T}},$$

be the vector of observations, except for x_i. Further, let

$$\bar{x}_{(i)} = \frac{1}{n-1} \sum_{k \neq i} x_k$$

be the average of all observations with x_i deleted, and arrange them in a vector

$$\bar{x}_{(\cdot)}(T) = (\bar{x}_{(1)}, \ldots, \bar{x}_{(n)})^{\mathrm{T}}.$$

Now, let θ be any parameter vector in (15) or (16). We can then make the best prediction of x_i given all the other observations, by means of (3). Write

$$\Sigma_{T(i)} = (r^*(t_j - t_k),\ j,k \neq i) \tag{18}$$

for the covariance matrix Σ_T with row and column i deleted, with $r(t)$ calculated from (15) or (16).

A prediction of x_i is then, in view of (3),

$$\hat{x}_{(i)} = \bar{x}_{(i)}(T) + r^*_{T(i)}(t_i)^{\mathrm{T}} \Sigma^{-1}_{T(i)} (x_{(i)}(T) - \bar{x}_{(i)}(T)).$$

Let

$$\hat{x}_{(\cdot)}(\theta) = (\hat{x}_{(1)}, \ldots, \hat{x}_{(n)})^{\mathrm{T}}$$

be the vector of predictions. The dependence on θ is indicated.

Definition 3

The cross-validated estimate of $\theta = (g_1, \ldots, g_M)$ or $\theta = (\sigma, a, \sigma_\epsilon)$ is defined as

$$\operatorname*{argmin}_{\theta_i \geq 0} \|x(T) - \hat{x}_{(\cdot)}(\theta)\|,$$

taken over all θ which satisfy condition (17).

Other estimators are possible, for instance a non-negative least-squares type estimate. With d_{ij} equal to the distance between t_i and t_j, this is defined as (for (15)),

$$\operatorname*{argmin}_{g_i \geq 0} \sum_{i,j} \left((x_i - \bar{x})(x_j - \bar{x}) - \sum_{k=1}^{M} g_k J_0(r_k d_{ij}) \right)^2,$$

the maximum also here taken over all g which satisfy (17).

One could expect that the fact that one estimates the covariance function has a great effect on the interpolated surface, and hence on the level curves. In the simulated examples we have run, the difference between level curves calculated by means of the true and the estimated covariance function, is quite small. This is possibly due to the fact that we have used the cross-validation technique to estimate the covariance function, which automatically gives the best agreement between observed and expected values.

Acknowledgements

The authors are grateful to two referees and the Editors for valuable comments on previous versions of the paper, in particular concerning the practical difficulties with surface reconstruction. The second author was supported in part by the Office of Naval Research under Grant N00014-93-1-0841.

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Received March 1994 and Revised January 1995