Influence Functions in Semivariogram Estimation: A Comparative Study

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Spatial data is analyzed in three stages of 1) estimating the variograms, 2) fitting a model for the estimated variograms and 3) predicting the value at unknown location based on the information at known locations (kriging). Recently, it has become a subject of interest to detect influential observations in these stages. Choi and Tanaka (1999) have derived influence functions in the above three stages and have proposed sensitivity analysis procedure. So far influence functions have only been derived for variograms by Gunst and Hartfield (1996). The present article makes a comparison of the performances between those influence functions for variograms derived by Choi and Tanaka (1999) and by Gunst and Hartfield (1996). A real numerical example is given to discuss the validity or usefulness of those influence functions.

Keywords: Stationary spatial data, Influence function, Sample variogram, Median-polish residual

1 INTRODUCTION

Analysis of spatial data is carried out in three stages: (1) estimating variograms, (2) fitting variogram models to the estimated variograms and (3) predicting the value at a specified location using the fitted variogram model. It is very important to detect influential observations which can affect any stage of the above analysis. In case there are influential observations in the data set, they may affect the first stage of the spatial data analysis, i.e., estimating variograms. And incorrectly estimated variograms may affect the following stages. Observations influential to variogram estimation can give rise to the wrong results in kriging (the third stage) which is one of the major purposes of spatial data analysis. On account of these, the problem of detecting influential observations has recently become a subject of interest in spatial statistics and many studies in this field have been performed. For example, Basu et al. (1997) discuss that the presence of influential observations can cause seriously distorted results in estimating variograms by showing four examples such as spikes, excitation crest pattern, shifting the entire variogram upwards, and linear trend. Moreover, they propose graphical and quantitative influence diagnostics for detecting influential observations. Gunst et al. (1997) describe some alternative robust estimators including trimming fixed percentages, robust M-estimator for location, and preliminary test estimators in estimating variogram in case of the presence of influential data and compare their performances by using simulation. Genton (1997) proposes a highly robust estimator for the scale when there exist some outliers in the data set. Gunst and Hartfield (1996) derive influence functions for the sample and robust variogram estimators. Choi and Tanaka (1999) also derive influence functions related to the three stages in the above spatial analysis and discuss the usefulness of the derived influence functions.

The major aim of this article is to compare the influence function derived by Choi and Tanaka (1999) with that derived by Gunst and Hartfield (1996) for sample variogram and to examine their relationship. We use the term "CT-method" and "GH-method" for the methods of Choi and Tanaka (1999) and of Gunst and Hartfield (1996), respectively. As a tool for analyzing spatial data, the software S-Plus is used with its spatial module S+SpatialStats.

Now we briefly explain the contents of this article. At first, we introduce the outline of spatial statistics related to spatial prediction in Section 2. In Section 3, after the concept of influence function is explained, influence functions in CT-method and GH-method are derived and compared, i.e., the CT-method is discussed in Section 3.1, the GH-method is dealt with in Section 3.2 and the comparison of both methods is conducted in Section 3.3. In Section 4, a real numerical example is analyzed to compare the performances of these influence functions. Concluding remarks are made in the last Section.

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2 OUTLINE OF SPATIAL STATISTICS FOR SPATIAL PREDICTION

Spatial data can be considered as a realization of a stochastic process \( Z(s) \), i.e.,

\[
\{z(s) : s \in D \subseteq R^d \}
\]

where \( s \) indicates a location in \( D \) and \( R^d \) is a \( d \)-dimensional Euclidean space. Most often \( d \), the dimension of the space, is 1, 2, or 3. The basic form of spatial data can be expressed as \( (z_i, s_i) : i = 1, \ldots, n \), where \( z_i \) is the \( i \)-th observation of a phenomenon of interest at location \( s_i \). In spatial data analysis, it is assumed that the observed data have the following structure:

\[
z(s) = m(s) + e(s),
\]

where \( m(s) \) denotes a large-scale variation called drift or trend and \( e(s) \) a small-scale variation. The latter term is a fluctuating random component with zero expectation like random variation or measurement error within region. Sometimes assumptions are made about the stationary of the process. In particular, when the mean and variance of the first difference of the stochastic process \( Z(s) \) satisfy

\[
E(Z(s + d) - Z(s)) = 0, \quad \text{Var}(Z(s + d) - Z(s)) = 2\gamma(d), \quad s, s + d \in D,
\]

\( Z(\cdot) \) is said to be intrinsically stationary. Here \( 2\gamma(d) \) is called the variogram and \( \gamma(d) \) the semivariogram. Furthermore, if \( 2\gamma(d) = 2\gamma(||d||) \), it is said that the variogram \( 2\gamma(\cdot) \) is isotropic. If \( 2\gamma(d) \) depends on the direction of \( d \) as well as the distance \( ||d|| \), it is anisotropic. Although it is possible to think the covariance function or correlation function as measure of dependence, variogram is most often used in spatial statistics. For simplicity, we use the term variogram instead of semivariogram where there is no confusion.

The first stage of variogram analysis is to estimate the variogram \( \gamma(d) \) using the observed data. When we can assume that the variogram is isotropic, an estimator for the variogram called sample variogram can be computed by

\[
\hat{\gamma}(d) = \frac{1}{2N_d} \sum_{i=1}^{n} (z_i - z_j)^2,
\]

where \( N(d) \) is the set of all pairs with Euclidean distance \( d \), \( N_d \) is the number of distinct pairs in \( N(d) \), and \( z_i \) and \( z_j \) are data values at spatial locations \( i \) and \( j \), respectively. In S-Plus, we can calculate the sample variogram by using the variogram function, which has some optional arguments such as lag, nlag, tol.lag, tol.azimuth and maxdist. Practically, in order to calculate the variogram value using equation (4), we select first the nominal lag distances \( \text{"d"} \), then we calculate the variogram values by regarding pairs with distance within \( \text{"d + lag.tol"} \) as the pairs in \( N(d) \). When the variogram is anisotropic, the directional sample variogram is computed using the same formula by replacing \( d \) by vector \( d \).

The next stage of variogram analysis is to fit a variogram model which explains best the dependence (autocorrelation structure) of the underlying stochastic process. Most variogram models contain parameters including those which represent the nugget effect, sill, and range. There have been proposed so far several models(functions) such as spherical, Gaussian, exponential, power and linear models.

The third stage of the analysis is to estimate or predict as well as possible the value at an arbitrary position based on the observations at \( n \) known positions. When it can be assumed that the mean structure \( m(s) \) is constant, a kriging method called ordinary kriging is used for this purpose assuming a linear predictor as

\[
Z^*(s_0) = \sum_{i=1}^{n} w_i Z(s_i).
\]

It is a best linear unbiased prediction method under the assumption that the stochastic process underlying the observations is second-order stationary, i.e.,

\[
E(Z(s_i)) = \mu, \quad \text{Cov}(Z(s_i), Z(s_j)) = C(s_i - s_j),
\]

for any \( i, j \). For unbiasedness, the weights must satisfy \( \sum_{i=1}^{n} w_i = 1 \). By minimizing the prediction variance \( E(Z(s_0) - Z^*(s_0))^2 \) under the equality constraint on the weights, we obtain the following system of equations:

\[
-\sum_{i=1}^{n} w_i \gamma(s_i - s_j) + \gamma(s_0 - s_i) - \mu = 0, \quad i, j = 1, \ldots, n, \quad \sum_{i=1}^{n} w_i = 1,
\]
where μ is a Lagrange multiplier. If the variogram γ(s_i - s_j) and γ(s_0 - s_i) are known, the optimal weights {w_ij} can be obtained by solving the above equations. In practical data analysis we usually do not know these variograms, but we can estimate them if the fitted variogram model is available.

3. INFLUENCE FUNCTIONS

Influence functions quantify the influence of each observation on an estimator. Here, we discuss influence functions derived by Choi and Tanaka (1999) and by Gunst and Hartfield (1996). Before discussing these influence functions, we first give the definition of influence functions, that is, TIF (Theoretical Influence Function), EIF (Empirical Influence Function) and SIF (Sample Influence Function). We can define the EIF as the influence function based on the derivative in ε and the SIF is the influence function based on the difference of the perturbed and unperturbed samples. The TIF (Theoretical Influence Function) is defined as

$$TIF(x; θ) = \lim_{ε→0} [θ((1 - ε)F + εδ_x) - θ(F)]/ε,$$

where δ_x is the cdf of a unit point mass at x and θ = θ(F) is a parameter which is expressed as a functional of the cumulative distribution function (cdf) F of random variables x. The TIF for θ is the derivative of the function θ(ε) = θ((1 - ε)F + εδ_x) with respect to ε evaluated at ε = 0. As sample versions, we consider the EIF and SIF. The EIF is obtained by replacing cdf F for F in the definition of the TIF. That is, the EIF at the x = x_i (i = 1, ..., n) is given by

$$EIF(x_i; θ) = \lim_{ε→0} [θ((1 - ε)F + εδ_x) - θ(F)]/ε.$$

The SIF, which is obtained by omitting “lim” and setting ε = 1/(n - 1) in EIF, is expressed as

$$SIF(x_i; θ) = (1/(n - 1))(θ(0) - θ),$$

where the subscript (i) means the omission of the i-th individual. Generally speaking the SIF is the most valid measure, because the effect of each observation is evaluated by actually omitting the observation. But usually it is time-consuming to compute. The EIF is introduced as a substitute for the SIF. In the present paper we study if the derived EIF in spatial statistics can be used instead of the SIF.

3.1 INFLUENCE FUNCTIONS IN THE CT-METHOD

Introduce weights w_ij for pair (i, j), which is constrained as ∑w_ij = 1, as follows to derive the influence function in sample variogram.

$$w_ij = \frac{\hat{w}_{ij}}{\sum_{N(d)} \hat{w}_{ij}} = \begin{cases} \frac{1}{N_d + N_{d,i^*} - 1}, & (i, j) \in N(d; i^*), \\ \frac{1}{N_d + N_{d,i^*}}, & \text{otherwise}, \end{cases}$$

where N(d; i^*) is the set of pairs containing z(s_i) and having distance d, N_d,i^* is the number of pairs in N(d; i^*), and w_ij is defined as

$$\hat{w}_{ij} = \begin{cases} 1 + ε, & (i, j) \in N(d; i^*), \\ 1, & \text{otherwise}, \end{cases}$$

using a perturbation parameter ε. It is easily verified that the first derivative of an arbitrary statistic with respect to ε evaluated at ε = 0 is a constant times the EIF (see, e.g., Tanaka and Zhang, 1999). In CT-method this derivative is called “influence function”. Unperturbed weights w_ij are 1/N_d for all pairs.

Using w_ij, we can represent the perturbed sample variogram as

$$v_ε(d) = \sum_{N(d)} \{\hat{w}_{ij}/\sum_{N(d)} \hat{w}_{ij}\} \{z(s_i) - z(s_j)\}^2/2$$

$$= \sum_{N(d,i^*)} \frac{1 - ε}{N_d + N_{d,i^*} - 1} \{z(s_i) - z(s_j)\}^2/2 + \sum_{N(d,i^*)} \frac{1 - ε}{N_d + N_{d,i^*} - 1} \{z(s_i) - z(s_j)\}^2/2$$

$$= \sum_{N(d,i^*)} \frac{1}{N_d} (1 - ε)(1 + N_{d,i^*}/N_d)^{-1} \{z(s_i) - z(s_j)\}^2/2$$

$$+ \sum_{N(d,i^*)} \frac{1}{N_d} (1 + N_{d,i^*}/N_d)^{-1} \{z(s_i) - z(s_j)\}^2/2,$$
where $N(d, i^*)$ indicates the complement of $N(d, i^*)$ in $N(d)$. And it can be expanded in Taylor series as

$$v_i(d) = v(d) + \frac{N_{d,i^*}}{N_d} \left[ \sum_{N(d,i^*)} \frac{1}{2N_{d,i^*}} (z(s_i) - z(s_j))^2 - v(d) \right]$$

$$- \epsilon^2 \left( \frac{N_{d,i^*}}{N_d} \right)^2 \left[ \sum_{N(d,i^*)} \frac{1}{2N_{d,i^*}} (z(s_i) - z(s_j))^2 - v(d) \right] + \cdots. \tag{14}$$

Thus the influence function is given by

$$v^{(1)}(d; s_i^*) = \frac{N_{d,i^*}}{N_d} \left[ \sum_{N(d,i^*)} \frac{1}{2N_{d,i^*}} (z(s_i) - z(s_j))^2 - v(d) \right]. \tag{15}$$

It is noted that the first and second terms in the bracket are the sample variograms based on all pairs and on the pairs related to the $i^*$-th observation, respectively. CT-method has two features. First, the coefficient $N_{d,i^*}/N_d$ means the influence of $i^*$-th observation depends on the proportion of pairs that include the $i^*$-th observation. That is, if there are many pairs of observation related with $i^*$, the observation may be influential. Second, the first term in the bracket can be recognized as described above, $i^*$-th observation is influential, when the variogram based on the pairs related with $i^*$ is much different from that based on all pairs.

### 3.2 INFLUENCE FUNCTIONS IN THE GH-METHOD

Under the assumption that $F$ is a distribution of a stationary random field generating the bulk of the data and $G$ is a distribution with a single influential observation of magnitude $\mu + \delta_m$ at location $s_m$, Gunst and Hartfield (1996) derived the following influence function for the sample variogram (4):

$$IF_{S}(s_m) = \frac{N_m}{2N_d}\delta_m^2, \tag{16}$$

where $N_d$ and $N_m$ have similar meanings as $N_d$ and $N_{d,i^*}$ in the previous section. Equation (16) gives the theoretical influence function. In practical data analysis parameters in equation (16) must be estimated. In the CT-method it is described that $\delta_m$ is estimated by its median-polish residual as the magnitude of the shift at location $s_m$. They, also, derive the expectation of the sample variogram (4) when there exist a single influential observation at location $s_m$,

$$E{\gamma(d)} = \gamma(d) + \frac{N_m}{2N_d}\delta_m^2. \tag{17}$$

In equation (17), they note that the second term of this equation is the same as the value of the influence function and influence function can be thought of as the asymptotic bias in sample variogram estimator.

### 3.3 COMPARISON OF THE CT- AND GH-METHODS

The influence functions described as in the following equations in the CT- and GH-methods.

1) EIF in the CT-method:

$$v^{(1)}(d; s_i^*) = \frac{N_{d,i^*}}{N_d} \left[ \sum_{N(d,i^*)} \frac{1}{2N_{d,i^*}} (z(s_i) - z(s_j))^2 - v(d) \right], \tag{18}$$

2) EIF in the GH-method:

$$IF_{S}(s_m) = \frac{N_m}{2N_d}\delta_m^2. \tag{19}$$

Here, as the notations in both methods do not coincide with each other, we replace $m$ with $i^*$ and $N_m$ with $N_{d,i^*}$ in the GH-method.

Now let us consider the expectation of the influence function $v^{(1)}(d; i^*)$ derived by the CT-method. Since Gunst and Hartfield (1996) derive their influence function assuming the so-called location shift model, we shall assume the same model, i.e.,

$$z(s_i) = \begin{cases} \mu + \delta_{i^*} + \epsilon_{i^*}, & i = i^*, \\ \mu + \epsilon_i, & i \neq i^*, \end{cases} \tag{20}$$
where \(\{\epsilon_i\}\) are random variables taken from a stationary random field, that is, we assume that \(\epsilon_i\)'s have a constant variance and the correlation between \(\epsilon_i\) and \(\epsilon_j\) is a constant for any pair \((i, j) \in N(d)\). For a pair in \(N(d,i^*)\),

\[
E[(z(s_i) - z(s_j))^2] = E[(\epsilon_i^* + \epsilon_i - \epsilon_j)^2] = E[\epsilon_i^2 + 2\epsilon_i^*(\epsilon_i - \epsilon_j) + \epsilon_i^2 + \epsilon_j^2 - 2\epsilon_i\epsilon_j] = \delta^2_d + 2\sigma^2_{\epsilon}(1 - \rho),
\]

where \(\rho\) is the correlation coefficient of a pair with lag \(d\) and \(\sigma^2_{\epsilon}\) is variance of \(\epsilon_i\)'s. For pairs which aren't in \(N(d,i^*)\), the term \(\delta^2_d\) disappears.

The expectations of the first and second terms in \([ \ ]\) in equation (18) are obtained as

\[
\frac{1}{2N_{d,i^*}}\{N_{d,i^*}\delta^2_d + N_{d,i^*}2\sigma^2_{\epsilon}(1 - \rho)\} = \frac{1}{2}\delta^2_d + \sigma^2_{\epsilon}(1 - \rho),
\]

\[
\frac{1}{2N_d}\{N_{d,i^*}\delta^2_d + N_d2\sigma^2_{\epsilon}(1 - \rho)\} = \frac{N_{d,i^*}}{2N_d}\delta^2_d + \sigma^2_{\epsilon}(1 - \rho),
\]

respectively. Therefore, the expectation of the influence function in the CT-method is given by

\[
E(\psi(1)(d; s_{i^*})) = \frac{N_{d,i^*}}{2N_d}(1 - \frac{N_{d,i^*}}{N_d})\delta^2_d
\]

It is noted that the expected value of the EIF in the CT-method is approximately equal to that of the GH-method if \(N_{d,i^*}/N_d \ll 1\).

**4 NUMERICAL EXAMPLE**

**4.1 DATA**

Data are collected about the locations and the measured observations for permeability (a measure of oil flow) on 104 oil wells in the US Naval Petroleum Reserve No. 1 in California. The data set is taken from Maher, J.C. et al. (1975), Petroleum geology of Naval Petroleum Reserve No. 1, Elk Hills, Kern County, California. The raw data are shown in Appendix A. As the median polish residuals are used for the estimates for \(\{\delta_m\}\) in GH-method, we must transform the raw data into gridded data. Therefore, we use 17 \times 17 low-resolution map gridded for the original data locations and we have to assign data locations to the nearest nodes of the grid. The locations for the raw and gridded data are displayed in Figure 1.

![Figure 1](image-url)
4.2 INFLUENCE ANALYSIS USING THE CT-METHOD

Setting the width of the lags equal to “maxdist/nlag”=5/19, we have calculated the sample variograms. Figure 2 shows the resulting plot of the sample variogram for $d = 0.29, \ldots, 4.99$.

![Figure 2 plot of the sample variograms](image)

Influence functions are calculated to evaluate the sensitivity or stability of sample variograms. Figure 3 indicates the index plots of the EIF for the sample variograms. These figures show the influence of each observation on the variograms for various lags. Looking at these figures, we can find that the $3^{rd}$ observation is influential at almost all lags, and the $16^{th}$, $64^{th}$, $63^{rd}$, $73^{rd}$, $88^{th}$, $89^{th}$ and $93^{rd}$ observations are influential at some lags.

![Figure 3 Index plots of the influence functions for the sample variograms](image)
To summarize these index plots their Euclidean norms are plotted. The resulting index plot is given in Figure 4. It shows clearly that the 3rd observation is more influential than the rest.

![Figure 4](image)

**Figure 4** Index plot of the Euclidean norm of the influence functions for the sample variograms (CT-method)

To detect influential subsets of observations (see, e.g., Tanaka, 1994; Tanaka and Zhang, 1999) we apply principal component analysis (PCA) to the influence functions. The first two principal components (PCs) account for 72% of the total variance. Biplots of PC scores and axes are given in Figure 5. In this figure, we can see that there are some candidates for singly or jointly influential observations. That is, the 3rd observation may be singly influential, and the 88th and 64th may be jointly influential.

![Figure 5](image)

**Figure 5** PCA of the influence functions for sample variograms (CT-method)

To investigate the validity or usefulness of the derived influence functions for the sample variograms a scatter diagram is drawn for the EIF and the SIF, where

\[
EIF = v^{(1)}(d; s_{(i)}) , \quad SIF = v(d) - v_{(i)}(d)
\]
indicating the v-value without the $i^*$-th observation. Since most points are located almost on the 45 degrees line, we can insist that the EIF in CT-method can be used effectively instead of the SIF.

Figure 6 Scatter diagram of the EIF and the SIF for sample variograms at various lags (CT-method)

4.3 INFLUENCE ANALYSIS USING THE GH-METHOD

Figure 7 indicates the index plots of the influence function obtained by the GH-method for the sample variograms, where $\delta_m$'s are estimated by the median polish residuals. Let us investigate the influence of each observation on the variograms for various lags through these figures. In these figures, as in the CT-method, we can find that the 3rd observation is influential at almost all lags. And the 16th, 64th, 65th, 73rd, 88th and 89th observations are influential at some lags. We can find some differences between the results of both methods. Among them, the notable difference is that 93rd can not be found with the GH-method.

Figure 7 Index plots of the influence functions for the sample variograms (GH-method)
We use the Euclidean norms to summarize these index plots of influence functions at various lags. The resulting index plot is given in Figure 8. It shows clearly that the 3rd, 73rd and 65th observations are more influential than the rest.

Figure 8 Index plot of the Euclidean norm of the influence functions for the sample variograms (GH-method)

Now compare this index plot with that by the CT-method. The sets of detected candidates for influential observations are somewhat similar with each other, but we may say that influential observations are more widely spread out in the GH-method than in CT-method.

Scatter diagram is drawn between the EIF and the SIF for sample variograms at various lags in Figure 9, where the EIF is calculated by using equation (19) with $\delta_m$ replaced by the median polish residuals. In these figures it is difficult to find correlation between the EIF and the SIF. Therefore, we can say the influence function derived by the GH-method can't be used as the substitutes for the SIF in influence analysis.

Figure 9 Scatter diagram of the EIF and the SIF for sample variograms at various lags (GH-method)
5 CONCLUDING REMARKS

In the present paper a comparison is made between the influence functions for sample variogram derived by Choi and Tanaka(1999) and by Gunst and Hartfield(1996), theoretically and numerically. Theoretically it is found that the expectation of the empirical influence function(EIF) by Choi and Tanaka(1999) is similar to the theoretical influence function derived by Gunst and Hartfield(1996). To study the validity or usefulness of the sample versions of influence functions we have drawn the scatter diagrams of the empirical influence functions and the sample influence function(SIF), where the SIF is computed by actually omitting each observations. As the results we can say that the EIF by Choi and Tanaka(1999) can be used for detecting influential observations because it has close correlation with the SIF, while the EIF by Gunst and Hartfield(1996) cannot be used for the same purpose because the correlation is not large enough with the SIF.
References


Appendix A: Original data

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