

## Geostatistics in Soil Agrochemical Studies

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Received July 28, 2000

**Abstract**—The application of geostatistical techniques for the processing of soil agrochemical data is considered. A concise review of basic geostatistical concepts is presented. Methods for calculating isotropic and anisotropic variograms, their characteristics, and some models of variograms are discussed. Principles of data interpolation using the kriging procedure are elucidated.

### INTRODUCTION

The structural organization of soil cover indicates the presence of a regular component in the natural variability of soil properties. It is known that, as for most of the natural media, quantitative parameters of soil properties within small areas are frequently more similar than those of remote sites. This fact is confirmed in small- and large-scale mapping of soil properties and is represented on maps as areas with similar parameter values.

Although the existence of a regular component of natural variation and its dependence on natural pedogenic factors are well proven, this fact is not always taken into consideration, especially for processing of the results of active experiments. The analysis of results with classical statistical methods is based on the absence of spatial correlation between the values of parameters analyzed in the testing sites. All data are considered equivalent and independent. To decrease the initial variation of soil properties during long-term experiments, a number of known methods are used: an increase of the size of statistical sample, taking mixed samples, the analysis of average samples, and the establishment of replicate experiments with the randomized block design. However, unaccounted variations in the soil cover sometimes cause discrepant results of field experiments even within a given soil type.

In the last decades, an approach based on the study of the regular variation component, rather than on the removal of interfering variation, has been developed and applied for processing the results obtained for various natural objects [9, 13–15, 17]. Kozlovskii pioneered its application in soil science [4, 5]. In this approach, a regular component characterized by a certain spatial structure and a random component are distinguished in the spatial variation of soils. The random component includes the variation caused by both experimental errors and affecting factors that cannot be stud-

ied under specific experimental conditions (e.g., if they act at short distances).

Statistical processing of natural objects with the spatial structure of variation can be performed using geostatistics, or spatial statistics. This method also allows one to characterize the regular component of variation and to interpolate data.

In the last 10–20 years, the method has found a wide application for characterizing soil objects. The use of the method in soil science was analyzed in the works of Burgess and Webster [10, 11], Webster and Burgess [30], Burgess *et al.*, [12], Oliver and Webster [24], Webster [29], Stein *et al.*, [27], and Dobermann *et al.*, [16]; *Geoderma* no. 62, 1994, was fully devoted to this problem. Analogous Russian works are few in number, which is partially associated with the difficulties in purchasing the software necessary for geostatistical processing of data. Ivannikova and Mironenko [3] and Gummatov *et al.*, [2] (Institute of Physico-Chemical and Biological Problems of Soil Science, Russian Academy of Sciences, Pushchino), as well as Samsonova *et al.*, [8] (Faculty of Soil Science, Moscow State University), considered the use of geostatistical techniques in soil science. The authors of this paper reported some applications of geostatistical methods for characterizing soil and agrochemical parameters [6, 7].

The aim of this work is to expound the basics of geostatistics. In addition, we dwell on basic concepts, the understanding of which is necessary for the interpretation of results obtained by means of modern geostatistical software. A detailed description of mathematical apparatus is beyond the scope of this paper; we refer interested readers to the corresponding original works. We attempt to show that the application of geostatistics is readily accessible for soil scientists without a strong background in mathematics, in spite of the seeming complexity of its theory.

## OUTLINES OF GEOSTATISTICS FUNDAMENTALS

Principles of geostatistics are most thoroughly expounded in the classical work of Webster [28]. A Russian description of its mathematics can be found in the works of Ivannikova and Mironenko [3] and Gummatov *et al.*, [2].

Geostatistics is based on the theory of regionalized variables developed by Matheron [20, 21] on the basis of empirical relations, which Krige, a South African geologist, applied for predicting the gold reserves in placers [18, 19]. According to this theory, a regionalized variable (i.e., a spatially distributed variable), along with the random, local, unorganized variation component, includes a regular variation component, which has a spatial structure. It should be noted that the theory of regionalized variables is an outgrowth of the theory of random functions, a fundamental branch of mathematics. The theory of regionalized variables is intended for solving specific mathematical problems, namely, the structural description of the spatial variation in natural materials and the development of an optimal tool for data interpolation and interpretation of the results.

In classical manuals of geostatistics, the basic concepts are explained in terms of the theory of random functions. However, soil scientists are more accustomed to concepts of mathematical statistics; i.e., they describe the objects under study by statistical parameters rather than by the probability distribution function of random variables, among which all soil parameters can be considered. In this context, we attempted to find statistical analogues for the basic concepts of the theory of random functions. In addition, we considered the typical algorithms for calculating the parameters used in modern computer programs on geostatistics.<sup>1</sup>

*Random variable and random function.* Random variable,  $Z(x)$  is a variable that can take some value in the result of the experiment, this value being unknown a priori.

All values of the general population (in more habitual terms of classical statistics) of any soil parameter on the territory under study (pH,  $C_{org}$ , heavy metals, etc.) can be considered random variables. The random variable obeys the distribution law, which relates its possible values with the corresponding probabilities. The value of the random variable in a given experiment is called the realization of the random variable. In our case, this is the value of a soil parameter in some testing site within a massif, which is considered as the unified general population of testing sites on the territory under study.

A set of random variables  $Z(x)$  characterizing the changes of a parameter in some region as depending on

the argument is called *random function*  $z(x)$ . In geostatistics, only spatial coordinates  $(x, y)$  are considered as arguments, although different arguments can be used for other problems; e.g., time is an argument in the study of the seasonal dynamics of soil properties. As a result of the experiment (in our case, of soil survey), the random function takes a specific form called *the realization* of random function.

Another basic concept of the theory of random functions essential for geostatistics is *the concept of stationarity of the second order*. Characterization of a random function requires data on a sufficiently large number of its realizations. Results of a single soil survey are generally available in real soil studies, which seemingly gives no way for characterizing the distribution of a random function. However, this problem can be solved in the presence of the stationarity of the second order in the distribution of the property studied.

The stationarity of the second order includes:

(1) The constancy of the statistical expectation value (which can be estimated by the arithmetic mean value) for the whole territory studied

$$E\{z(x)\} = \mu = \text{const.} \quad (1)$$

In practice, this implies the absence of a trend (i.e., of a pronounced directional change in the arithmetic mean) on the territory studied;

(2) The constancy of spatial covariation  $C(h)$  for every pair of random values  $\{z(x); z(x+h)\}$ , its dependence only on the distance between points, and its independence from the spatial location of points

$$C(h) = E\{[z(x) - \mu][z(x+h) - \mu]\}. \quad (2)$$

As applied to soil studies, this implies that, regardless of the location of testing sites on the territory studied, the mean product of the deviations of soil parameters from the statistical expectation (or the arithmetic mean) in the sites separated by lag  $h$  is a constant value.<sup>2</sup> The stationarity of the second order can be considered as the repetition of the function in space; therefore, it is possible to replace the totality of its realizations by the single realization described for a sufficiently representative territory. In this case, the variance of random function  $z(x)$  is finite and can be calculated as

$$C(0) = E\{[z(x) - \mu]^2\}. \quad (3)$$

If the condition of stationarity of the second order in the distribution of the variable studied is not obeyed (e.g., in the presence of a trend), simple mathematical transformations can result in stationarity in some cases. The simplest transformation is the removal of the trend of the  $N$ th order followed by the analysis of residues for which the stationarity is obeyed.

Let us consider *the basic statistical parameters* used in geostatistics. Along with the mathematical mean and

<sup>1</sup> Definitions are drawn from the Venttsel manual *The Theory of Probability* [1], where the basic concepts of the theory of random functions are explained in simple and understandable terms; therefore, the manual can be recommended for a wide audience of soil scientists.

<sup>2</sup> The simplest case of the so-called isotropic realization is considered.

the sampling variance, *semivariances* and *semivariogram* are such parameters.

*Semivariance*  $\gamma(h)$  is the following quantity:

$$\gamma(h) = 1/2E\{[Z(x_i) - Z(x+h)]^2\}, \quad (4)$$

or, when the variogram is calculated from the results of measurements in separate sites,

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [Z(x_i) - Z(x+h)]^2, \quad (5)$$

where  $N(h)$  is the number of pairs of sites being spaced  $h$  apart, and  $x$  is the spatial coordinate.

It follows from the above formula that semivariance for each  $h$  is calculated as half of the average square of difference between the parameter values measured at distance  $h$  one from another. As the spatial covariance for any pair of random values spaced  $h$  apart is constant, the semivariance values depend on the distance  $h$  between the sites rather than on their location in space. From Eqs. (2)–(4), it follows that

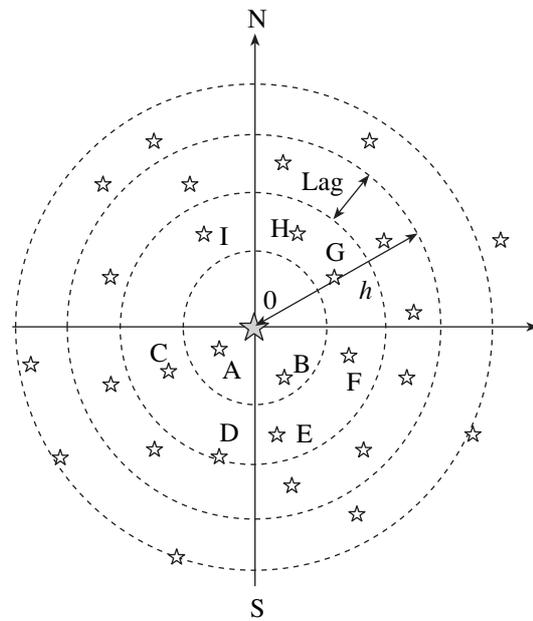
$$\gamma(h) = C(0) - C(h). \quad (6)$$

This ratio relates semivariance  $\gamma(h)$  with covariation function  $C(h)$  and shows that the former composes only a part of the general variance  $C(0)$  for the parameters measured at distance  $h$  one from another. When spatial covariance is absent,  $\gamma(h)$  is equal to variance  $C(0)$ . (This supposition is taken in classical statistics, which considers all elements of the population studied as equivalent and independent ones). Dependence (5) also suggests that semivariance  $\gamma(h)$  is more suitable than variance  $2\gamma(h)$ .

A *semivariogram* or *variogram* (we shall employ the latter term, which finds increasing use in the modern geostatistical literature) represents a dependence of semivariance  $\gamma(h)$  on distance  $h$ ; i.e., it characterizes the dependence of the average square of the difference between the parameter values on the distance between the measuring sites. The variogram is the main characteristic of the spatial structure of natural object variation.

*Isotropic variogram and the principle of its calculation in modern computer programs.* It is known that natural materials are called isotropic if their properties are independent of direction. In some computer programs (e.g., GS+), the variogram characterizing the structure of the parameter variation on the whole testing territory independently of direction is considered an *isotropic* variogram. It should be noted that it is advisable to calculate an isotropic variogram when the spatial distribution of soil parameter values can be considered as independent of direction within the framework of the problem.

To plot an isotropic variogram, all possible pairs of testing sites are considered. The pairs are combined into groups depending on the distance between the sites within the pairs, and half of the average square of dif-



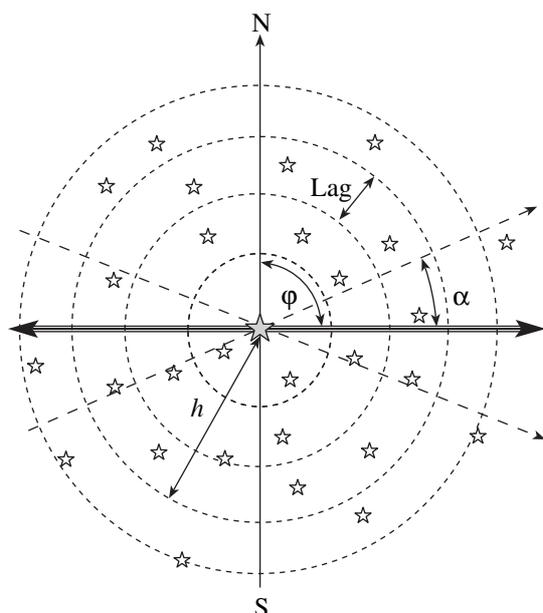
**Fig. 1.** Principle of the calculation of isotropic semivariogram: (0, A, B, ..., I) testing points and ( $h$ ) the lag-fold distance between testing points.

ference between the parameter values, i.e., semivariance, is then calculated for each pair. These semivariance values are used for plotting the variogram.

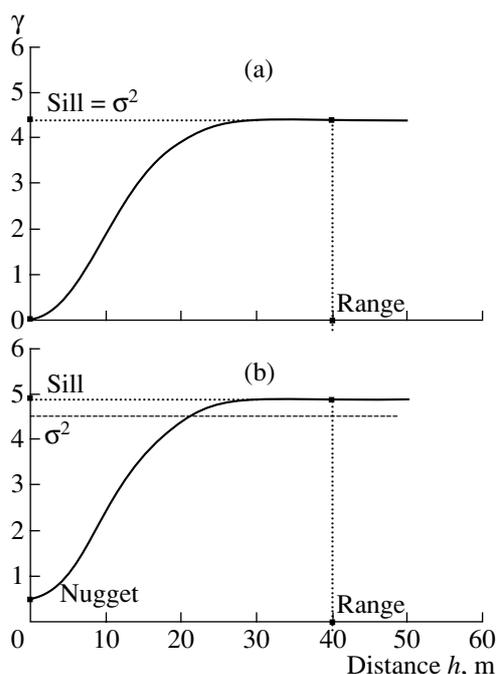
The semivariance values for distances multiple to the unit  $h$  distance (lag) are used to plot variograms. The lag can correspond to the minimum distance between the testing sites or be selected arbitrarily from the problem specification. The average variance values for the lag-fold distances between the sites in a pair (i.e., for  $h = 1, 2, 3$ , etc., lags) are thus obtained. In reality, sampling at exactly lag-fold distances is hardly possible. Therefore, distances lower or equal to the lag are equated to 1 lag; distances between 1 and 2 lags are equated to 2 lags; etc.

The principle of grouping the points for the calculation of an isotropic variogram is illustrated in Fig. 1. To consider all point pairs with the participation of point 0, circles of lag-fold radii with the center in point 0 are drawn. Points A and B are considered removed from point 0 at a distance of 1 lag; points C, D, E, F, G, H, and I are at a distance of 2 lags; etc. If similar circles with lag-fold radii are drawn around all the other points, we obtain all groups of point pairs for calculating an isotropic variogram.

*Calculation of an anisotropic variogram.* The spatial structure of parameter variation is not always isotropic. To determine the variation of a parameter along the directions selected, *anisotropic variograms* are calculated. An example of anisotropic variogram is presented in Fig. 2. The selected direction in space is specified by the values of angle  $\phi$  between the directing vector and axis X (in some programs, the reference point is



**Fig. 2.** Principle of the calculation of anisotropic semivariogram: ( $\star$ ) testing points; ( $\alpha$ ) angle of tolerance; ( $\varphi$ ) angle between the selected direction and the X axis; and ( $h$ ) lag-fold distance between testing points.



**Fig. 3.** Theoretical (a) and (b) real semivariograms:  $\gamma$ —semivariance value;  $\sigma^2$ —sample variance value; Sill— threshold variance; Range—correlation range; and Nugget—nugget variance.

taken on axis  $Y$ ). The so-called *angle of tolerance*  $\alpha$  is laid off to both sides of the vector to determine the spatial sector where the points necessary for the variogram are considered. Thus, points are grouped depending not

only on the distance between them but also on the direction of the vector coupling the points. When the angle of tolerance is equal to  $\pm 90^\circ$ , the anisotropic variogram is transformed into an isotropic one.

*Main parameters of variograms.* Let us consider the *ideal variogram* (Fig. 3a). Its values increase from the origin and tend to some constant value. This value is called threshold variance or sill; for it, semivariance  $\gamma(h)$  is equal to the variance of random function:

$$\gamma(h) = C(0). \quad (7)$$

A variogram attaining a constant level is called a *transitive variogram*. The distance at which semivariance attains a constant value is called the *correlation range* or *range*. Within the range, the parameter values are interdependent, i.e.,  $\gamma(h) < C(0)$ . When distances between the testing sites exceed the range, the parameter values become really independent and equivalent, as is required by classical statistics ( $\gamma(h) = C(0)$ ).

*Real variograms*, including those describing the variation structure of soil parameters, generally do not pass through the origin of coordinates, and their characterization includes a third parameter called the *residual variance* or *nugget variance* (Fig. 3b). Nugget variance represents the unexplained variance for distances shorter than the minimal testing step.

The sample variance of parameters under study is generally slightly lower than the sill value. This is explained by the following reason. The sample variance is calculated from the values obtained for all testing sites on the territory studied. In a real experiment, the territory has a finite size, and points within the range generally make a significant contribution to the sample variance and thus decrease it relative to sill. The calculation of the ideal variogram includes no limitation for the territory; therefore, the general variance tends to the sill value.

*Types of variograms.* Calculation of experimental variograms is the first step in the analysis of spatial variation of variables. In the next step, the parameters of theoretical curves are adjusted to the experimental variogram. Adjustment is performed using such methods as calculation of the minimum sum of deviation squares or the maximum determination coefficient and maximum likelihood estimation [23, 26]; calculation of the weighted minimum sum of deviation squares is the most prevalent technique [31]. Because of the mathematical ambiguity in the optimization of experimental data by these parameters, many programs (e.g., GEO-STAT and GEOEAS) imply a visual adjustment performed by users.

One selects several types of variograms characterizing different spatial structures of parameter variation. The main types of variograms, formulas for their description, and processes determining the type of variation are presented in Fig. 4.

More detailed information on variogram types and corresponding functions can be found in publications [23, 28].

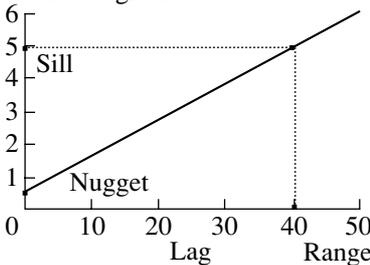
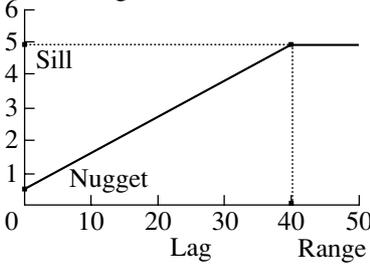
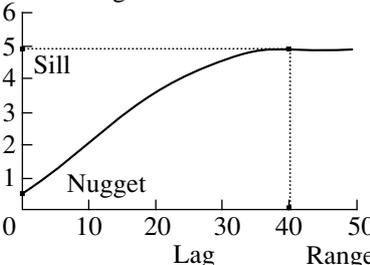
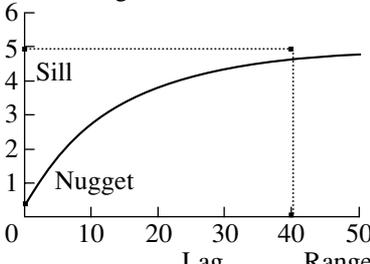
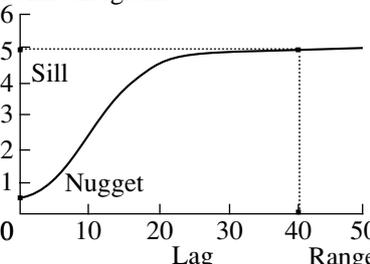
Model/formula/parameters	Graph	Nature (properties)
<p>1. Linear</p> $\gamma(h) = C_0 + C \frac{h}{a},$ <p>(<math>C_0</math>) Nugget; (<math>h</math>) number of lags</p>	<p>Semivariogram</p> 	Intransitive
<p>2. Linear with sill</p> $\gamma(h) = \begin{cases} C_0 + C \frac{h}{a} & h < a \\ C_0 + C & h \geq a, \end{cases}$ <p>(<math>a</math>) correlation range; (<math>C_0 + C</math>) threshold variance (sill)</p>	<p>Semivariogram</p> 	The limiting case of transitive model (sharp inflection)
<p>3. Spherical</p> $\gamma(h) = \begin{cases} C_0 + C \left[ 1.5 \frac{h}{a} - 0.5 \left( \frac{h}{a} \right)^3 \right], & 0 < h \leq a \\ C_0 + C, & h > a \end{cases}$	<p>Semivariogram</p> 	Moving average of randomized process
<p>4. Exponential</p> $\gamma(h) = C_0 + C \left[ 1 - \exp\left(-\frac{h}{r}\right) \right]$ <p><math>a = 3r</math>; <math>\gamma(a) = C_0 + 0.95C</math>, (<math>r</math>) auxiliary parameter</p>	<p>Semivariogram</p> 	Processes of autoregression of the first order (Markov processes); Poisson processes
<p>5. Gaussian</p> $\gamma(h) = C_0 + C \left[ 1 - \exp\left(-\left(\frac{h}{r}\right)^2\right) \right]$ <p><math>a = 3r</math>; <math>\gamma(a) = C_0 + 0.95C</math></p>	<p>Semivariogram</p> 	Gradual approximation to nugget

Fig. 4. Main models of isotropic variograms.

Model/formula/parameters	Graph	Nature (properties)
6. Hyperbolic $\gamma(h) = \frac{h}{\alpha + \beta h}$ $C = 1/\beta,$ ( $\beta$ ) auxiliary parameter		

Fig. 4. (Contd.)

*Kriging.* The main function of kriging (the procedure takes its name from D.G. Krige) is data interpolation. As opposed to other methods, kriging not only minimizes the error of interpolation but also evaluates it. The kriging principle consists of determining the weights of the variable values in neighboring points in order to estimate the variable value in the target point or spatial domain. The weight of each point is determined from the variogram. The weights are selected to obtain an unbiased estimate of the target value and the minimum variance of the estimate. The closer the specific testing site to the point or domain for which the parameter should be determined, the more substantial its contribution to the target value. It is clear that it is advisable to use only the points within the correlation range.

Theoretical models describing experimental variograms are generally used for kriging rather than the variograms themselves.

Kriging is subdivided into point and block procedures, depending on the size of the area for which the parameter should be estimated. In *point kriging*, the value of a parameter is determined in the target point; in *block kriging*, the average value for some domain (block) is calculated. Point kriging is generally considered as the limiting case of block kriging when the block size is equal to the soil sample. Among other multiple types of kriging, in our opinion, of greatest interest is *disjunctive kriging*, which can study the distribution of a parameter even if it differs from the normal distribution but obeys the condition of stationarity of the second order. This method is used for statistical processing of results when the conventional transformations of the original variable (taking the logarithm or square-rooting) cannot yield a near-normal distribution.

Principles of disjunctive kriging were developed by Matheron [22]. In disjunctive kriging, the population of values of the original variable is subdivided into a series of normally distributed subpopulations, which are then interpolated using the kriging procedure. This method makes it possible to apply conventional statistical

methods to the variables, the distributions of which significantly differ from the normal one. Disjunctive kriging is used, in particular, to calculate the probability that the target variable exceeds certain threshold values (e.g., maximum permissible concentration, acidity or alkalinity levels, etc.). Thus, areas requiring urgent conservation and reclamation measures or regular monitoring can be revealed regardless the distribution of parameter values, which presents an advantage for this method over the ordinary kriging. The theory of disjunctive kriging and examples of its practical application are described in detail previously [25].

*Spatial relationship between variables (covariogram) and cokriging.* The spatial distribution of a property is frequently determined by the distribution of another property, or the distributions of two or several properties depend on the same variation factor. The former case can be exemplified by the dependence of the humus content on the share of the related fine-particle-size fraction; the latter can be illustrated by the migration of soluble  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  along a slope. In this case, *coregionalization* of variables is stated. To estimate the spatial relation between variables, a cross-variogram (or covariogram) is calculated, which represents a product of two variograms. Assuming that two soil properties are measured in each point in Fig. 1, the covariogram value for distance  $h$  between points is calculated as the product of semivariance for all points of one parameter spaced  $h$  apart by the semivariance for all points of the other parameter, also spaced  $h$  apart.

The main idea of *cokriging* consists of interpolation of the values of a variable from the values of the other variable coregionalized with the first variable. Cokriging is applied in order to indicate one property by another property, i.e., in the cases when one property is significantly easier to determine than another property (e.g., because of the expensive analysis of the latter).

In this paper, we attempted to fill a gap in Russian publications concerning geostatistics, as compared to

the global literature on soil science, which has become especially striking in recent times.

We believe that the application of geostatistics significantly increases the potential of data interpretation in soil studies; therefore, acquaintance with this method is necessary for a wide audience of soil scientists.

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