DISCRETE GEOMETRIC DEVIATIONS OF FREE-FORM SURFACES AS A SPATIAL PROCESS

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Summary

Coordinate measurements are the source of digital data in the form of coordinates of the measurement points with a discrete distribution on the measured surface. The geometric deviations of free-form surfaces are determined (at each point) as normal deviations of these points from the nominal surface (the CAD model). Different sources of errors in the manufacturing process result in deviations of different character, deterministic and random. Geometric deviations of 3D free-form surfaces may be treated as a spatial process, and spatial data analysis methods can be applied in order to conduct research on the relationships among them. The article presents a discussion on a spatial process of deviations, theoretic bases for testing spatial dependence of measurement data, as well as the results of tests on simulated geometric deviations involving testing their spatial autocorrelation with the use of the Moran's *I* statistics.

Keywords: free-form surface, coordinate measurements, geometric deviations, spatial process, spatial autocorrelation

Odchyłki geometryczne powierzchni swobodnych jako proces przestrzenny

Streszczenie

Pomiary współrzędnościowe są źródłem danych cyfrowych – współrzędnych punktów pomiarowych o dyskretnym rozkładzie na mierzonej powierzchni. Odchyłki geometryczne powierzchni swobodnych wyznacza się w każdym punkcie jako odchyłki normalne tych punktów od powierzchni nominalnej (modelu CAD). Różne źródła błędów w procesie wytwarzania powodują powstawanie odchyłek o odmiennym charakterze, deterministycznym i losowym. Odchyłki geometryczne powierzchni swobodnych 3D można potraktować jako proces statystyczny przestrzenny. Stosować więc można metody analizy danych przestrzennych do badań zależności między nimi. Przedstawiono dyskusję nad modelem statystycznym odchyłek i podstawy teoretyczne ustalania przestrzennej zależności danych pomiarowych. Omówiono wyniki badań symulowanych odchyłek geometrycznych – określono ich przestrzenną autokorelację, stosując statystykę *I* Morana.

Słowa kluczowe: pomiary współrzędnościowe, powierzchnia swobodna, odchyłki geometryczne, proces przestrzenny, autokorelacja przestrzenna

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1. Introduction

The coordinate measurement technique consists in determining the coordinate values of measurement points located on the surface of an object. As a result of the measurement, a set of discrete data is obtained in the form of the coordinates of the measurement points. From the point of view of CAD/CAM techniques, the most important feature of coordinate measurement is providing data concerning the object's geometry in the digital form.

Machine parts composed of free-form 3D surfaces are more often designed. Such parts are shaped by surfaces, which cannot be described with simple mathematic equations. In designing, producing and measuring of free-form surfaces, CAD/CAM techniques are applied. The accuracy inspection consists in digitalizing the workpiece under research (coordinate measurement with the scanning method), followed by comparing the obtained coordinates of the measurement points with the CAD design (model). The values of geometric deviations of the free-form surface, or normal deviations of measurement points from the nominal surface, may be calculated by previously determining the deviation components in the X, Y, Z directions [1-3]. Software of coordinate measurement machines automatically performs such calculation for each measurement point in the UV scanning option.

Geometric deviations of free-form surfaces are attributed to many phenomena that occur during the machining, both deterministic and random in character. These phenomena with theirs consequent machining errors can be described in space domain. In machining workpieces including free-form surfaces a multi-axis machining is applied. Different combinations of machining parameters may produce variations in the final product surface quality. In coordinate measurements of free-form surfaces, spatial data is obtained which provide information on the processing and on geometric deviations in the spatial aspect. Deterministic deviations are spatially correlated, a lack of spatial correlation indicates their spatial randomness. Calculating the values of geometric deviations solely does not provide much information, neither with regard to the surface properties nor to the course of the machining process. Deviations of random values may be spatially correlated which is reflected in their determined distribution on a surface and is indicative of the existence of a systematic source in the course of processing.

The present article suggests treating geometric deviations of 3D free-form surfaces as a spatial process and applying methods of analysing spatial data to research on them since spatial analysis of data makes it possible to determine the similarities and differences between the specified areas and also to quantify spatial dependencies. Testing spatial dependencies aims at demonstrating whether spatial dependence exists or not, and if it does, then what its range and structures are [4].

The literature states that the Moran's I statistic are used in the majority of cases in order to test the existence of spatial autocorrelation. Cliff and Ord [5] justify that choice. Identifying spatial correlation of measurement data proves the existence of a systematic, repetitive processing error. In such a case, the spatial modelling methods suggested by Cliff and Ord [5], as well as by Kopczewska [6], may be applied to fitting a surface regression model describing the deterministic deviations. The first step in model diagnosing is to examine the model residuals for the existence of spatial autocorrelation. The Moran's I test is also used for this purpose.

2. Characteristics of discrete geometric deviations

Geometric deviations are attributed to many factors. Different sources of errors in the manufacturing process leave traces on the surface, and geometric deviations are a cumulated effect of the influence of these sources. Deviations may be divided into three components: shape deviations, waviness, and roughness [7]. The components connected with the shape deviations and waviness are surface irregularities superimposed on the nominal surface, resulting in a smooth surface and most often deterministic in character. The component connected with random phenomena, including the surface roughness, is irregularity of high frequency. The actual surface is the effect of superimposition of the shape deviations, waviness and roughness on the nominal surface. The contribution of random phenomena on the surface depends on the type of processing. The literature data indicate that after the finish milling process, values of random geometric deviations of the surface are greater than these of the deterministic deviations.

Shape deviations are caused, among others, by deviations of machine tool ways, deviations of the machine tool parts, and improper fixing. The surface waviness results from, among others, geometric deviations or tool movement deviations, and vibrations of the machine tool or the processing tool. Roughness is a result of the shape of the tool blade and the tool's **longitudinal** feed or in-feed as well as of vibrations at the workpiece-tool contact.

In coordinate measurements, the coordinates of a finite number of points on the surface of the workpiece are determined. The aim is to determine a smooth surface superimposed on the nominal surface. However, in the measurement process, the random component and the deterministic component overlap each other. In consequence, the spatial coordinates sampled at each measurement point include two separate components. The component connected with the deterministic deviations represents the smooth surface trend and is spatially correlated. The random component, on the other hand, is weakly correlated and is considered to be of a spatially random character. A surface constructed on measurement points is therefore more complex than a nominal surface.

3. Geometric deviations as a spatial process

Geometric deviations of 3D surfaces constitute a spatial process. Between the observations (deviations values) there may be interrelations not only in the adjacent neighbourhood but also of further span.

Spatial statistics are based on a few assumptions, the most important of which is stationarity. Weak stationarity where the mean and variance are constant, and autocorrelation depends solely on the distance between the researched areas, is sufficient [8]. The notion of stationarity is decisive in spatial models.

When limiting one's interest to a single observation set, it has to be assumed that the μ (expected value) and the V (variance) are determined by a smaller number of parameters than the n observation number. Such a structure allows for modelling the Y_i observation values depending on the neighbouring sites. The main conception of specifying such models is *spatial stationarity* from which it results that the mean of Y_i is the same for every i, and that Y_i and Y_j depend upon each other only by virtue of their relative positions, not on their absolute locations [5]. If a process is both stationary and independent of the direction, it is called an isotropic process.

Various forms of non-stationarity, such as: anisotropy, trends, periodicity, or clustering, may appear in the process. Estimation of parameters and functions of spatial processes requires decomposing the process into elements of low frequency (trends, gradients) as well as of higher frequency (local dependencies and noises). Processes can be classified as *reactive* or *interactive* ones. Reactive processes are governed exclusively by external factors, while interactive processes show mutual influences and dependencies between observations within a defined neighbourhood.

If the main influence is reaction, a *regression model* is suitable, while predomination of interaction effects suggests the need for applying a *model with a spatially dependent covariance structure*. In practice, it might be necessary to adjust a regression model and later to check the errors, model residuals, for spatial dependence; in the other case, fitting a model combining regression and spatial interactions may be needed. Spatial dependence may thus appear at two levels – firstly, at the error level, which is called spatial autocorrelation of the error, and secondly, there might appear spatially correlated observations of the variable under research.

Geometric deviations appear only as the result of complex external influence, i.e. they constitute the first of the processes mentioned above – *a reactive spatial process*. The presence of spatial autocorrelation in such processes may be connected with the appearance of trends (or gradients) in data. The right procedure in such situations is to determine a regression model with the mean as the input variable function. Such a process is non-stationary for the mean but stationary for the covariance structure. In the case of geometric deviations of a surface, we are interested in a spatial surface model including trends or gradients (the trend surface), which might be a basis for forming conclusions on systematic processing errors and later for eliminating such errors or/and correcting the processing programme. The appropriate model here is a *spatial error model*, since according to the physical nature of the analysed process, as it was described above, geometric deviations constitute a reactive process [6]. Such a model assumes spatial autocorrelation of the residuals.

Spatial modelling, using spatial estimation methods, aims at improving model specification. The adequacy of a model is checked with tests for spatial autocorrelation in the model residuals. The model needs to have such a form as to eradicate a trend and not regional variability. The existence of spatial autocorrelation in the observed residuals is demonstrative of a bad specification of the model. A general (matrix) form of a *spatial error model* is as follows [6, 9]:

$$Z = \beta X + u, \quad u = \lambda W + e \tag{1}$$

where: X – independent variable matrix, β – regression coefficient vector, u – model residuals, λ – spatial autocorrelation parameter, W – spatial weight matrix (Section 4), e – random independent errors, model residuals.

In spatial error models, it is researched whether $\lambda = 0$ or whether there is no spatial autocorrelation. To this end, Moran's I test is used (Section 4.1).

4. Measuring spatial autocorrelation

Autocorrelation is a characteristic of data obtained from a process that is articulated in one or more directions and describes the error structure of the data.

Spatial autocorrelation refers to systematic spatial changes. In general, positive autocorrelation means that the observed feature values in a selected area are more similar to the features of the contiguous areas than it would result from the random distribution of these values. In the case of negative spatial autocorrelation, the values in the contiguous areas are more different than it would result from their random distribution. A lack of spatial autocorrelation means spatial randomness. The values observed in one area do not depend on the values observed in the contiguous areas, and the observed spatial pattern is as much probable as any other spatial pattern.

In order to test the existence of spatial dependence, global and local Moran's and Geary's statistics for a given variable are applied. A spatial autocorrelation measure may be used in a number of ways: for testing the existence of spatial autocorrelation and population characteristics, determining the autocorrelation degree or the distance beyond which observations are independent, for determining a theoretical model suitable for the observed spatial structure, or finally for concluding on the spatial process. The spatial effects range may be researched by means of analysing the lag in the spatial process, and the structure of spatial dependence – by testing and selecting weighting matrices defined according to different criteria. Structure of weights describe Cliff [5] and Kopczewska [6]. First-order autocorrelation is measured as a function of nearest neighbours; higher-order autocorrelation is measured as a function of more distant neighbours along the defining directions.

A measure of spatial interaction requires a few assumptions in the form of a W weighting scheme. Taking interaction as a function of proximity leads to the simplified concept of a bounded neighbourhood of spatial influence, $W = \sum_j \sum_i w_{ij}$, where i and j are spatial indices. The next simplification is the assumption of spatial interactions symmetry within the neighbourhood, $w_{ij} = w_{ji}$. Putting together the concepts of spatial weighting, local neighbourhood deviations, and regional variance, the measure of spatial autocorrelation was formulated [5, 6, 8].

The literature data state that the Moran's I statistic is used in the majority of cases; it can be applied to analysing spatial data of both normal and unknown (randomisation) probability distribution [5, 6].

In adapting methods of spatial statistics, concerning research on spatial autocorrelation, to research on geometric deviations, the following need to be determined: ε_i – geometric deviation at each measurement point, $\bar{\varepsilon}$ – arithmetic mean of geometric deviations at n – measurement points, w_{ij} – weighting coefficients, elements of weighting matrices reflecting spatial relations between ε_i and ε_j.

A spatial weighting matrix defines the structure of the spatial neighbourhood. The matrix measures spatial connections and is constructed in order to specify spatial dependence. One of the possible dependence structures is assumed, e.g. neighbourhood along a common border, neighbourhood within the adopted radius or within the inverse of distance. In research on geometric deviations, it is most suitable to make the spatial interrelations dependent on the distance between the measurement points, in particular on the inverse of the minimum straight-line distance.

As a result of scanning, the coordinates (as well as geometric deviations) of the points distributed on the surface along a regular grid are obtained. The distance between the i-th and j-th point, according to the Euclidean metric, is as follows:

$$d_{ij} = \left[\left(x_i - x_j\right)^2 + \left(y_i - y_j\right)^2 \right]^{\frac{1}{2}} \tag{2}$$

where: x_i, y_i – i-th point coordinates, x_j, y_j – j-th point coordinates, d_{ij} – distance between the i-th and j-th measurement point.

If it is assumed that the dependence between the data values at the i and j points decreases when the distance increases, this relation can be described in the following way:

$$w_{ij} = d_{ij}^{-k} \tag{3}$$

$w_{ij} = 0$ for $i = j$, k – constant ($k \geq 1$).

The spatial autocorrelation coefficient has the following form co-variance/variance ratio with a weighting scheme based on spatially symmetric interactions:

$$I = \frac{n}{S_0} \frac{\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}\left(\varepsilon_i - \bar{\varepsilon}\right)\left(\varepsilon_j - \bar{\varepsilon}\right)}{\sum_{i=1}^{n}\left(\varepsilon_i - \bar{\varepsilon}\right)^2} \tag{4}$$

where: $S_0 = \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij} \; (i \neq j)$.

The Moran's I statistic has an asymptotically normal distribution (for $n \to \infty$). In order for assessing the Moran's statistics to be correct, the analysed variable must have a constant variance.

The Moran's I statistic indicate whether there is a spatial effect of agglomeration or not. Positive and significant values of the statistics imply the existence of positive spatial autocorrelation, i.e. a similarity of observation in the specified d distance. Negative statistics values mean negative autocorrelation, i.e. diversification of the tested observations and are indicative of the fact that the neighbouring areas are more different than it would result from their random distribution.

After having determined the I coefficient, the null hypothesis of no spatial autocorrelation at the assumed significance level needs to be verified, examples showed Upton and Fingleton in [10]. The distribution moments of Moran's I statistic can be determined both at the assumption that the data (deviations) comes from the normal distribution population and at the assumption that it comes from the population of an unknown probability distribution. When the number of localities is large it is reasonable to use the normal approximation. In the case of assuming the normal distribution, the expected value and the variance depend exclusively on spatial weights. If randomisation is assumed, these moments depend also on the value of the variable under research.

Assuming a normal probability distribution for geometric deviations, the E(I) expected value and the var(I) variance are calculated using the formulae [5, 10]:

$$\mathrm{E}(I) = \frac{-1}{n-1} \tag{5}$$

$$\mathrm{var}(I) = \frac{\left(n^2 S_1 - n S_2 + 3 S_0^2\right)}{(n-1)(n+1) S_0^2} \tag{6}$$

where:

$$S_1 = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \left(w_{ij} + w_{ji}\right)^2 \quad (i \neq j),$$

$$S_2 = \sum_{i=1}^{n} \left(w_{i(.)} + w_{(.)j}\right)^2 ,$$

$$w_{i(.)} = \sum_{j} w_{ij} \ , \ w_{(.)j} = \sum_{i} w_{ji} \ .$$

The expected value (5) of the Moran I statistic approaches 0, which might be interpreted as randomness [5, 6, 10].

5. Theoretical investigations

5.1. Computer simulations

The experiments were performed on a free-form surface with the base measuring 100x100 mm, which model CAD is presented in Fig. 1. A simulation was performed, involving generating random geometric deviations of values ranging from – 0.01 to + 0.01 mm of normal distribution, followed by their virtual superimposition on a CAD model at 1400 points distributed over a regular grid (40 rows and 35 columns). Figure 2 illustrates the spatial plot and the map of simulated geometric deviations with reference to the nominal x and y coordinates.

At the second stage, a deterministic deviation in the form of gradient in the middle area of the model was additionally superimposed on the CAD model (Fig. 3). The deviations values at the respective points amounted from 0.00 to + 0.02 mm. The simulated geometric deviation of spatial systematic distribution was equal to the random deviations scatter. Each of the virtual 1400 measurement points included both a determined and a random component in different proportions.

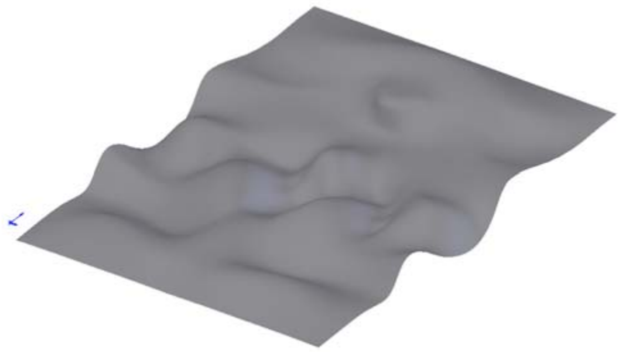

Fig. 1. CAD model of the surface

a) b)

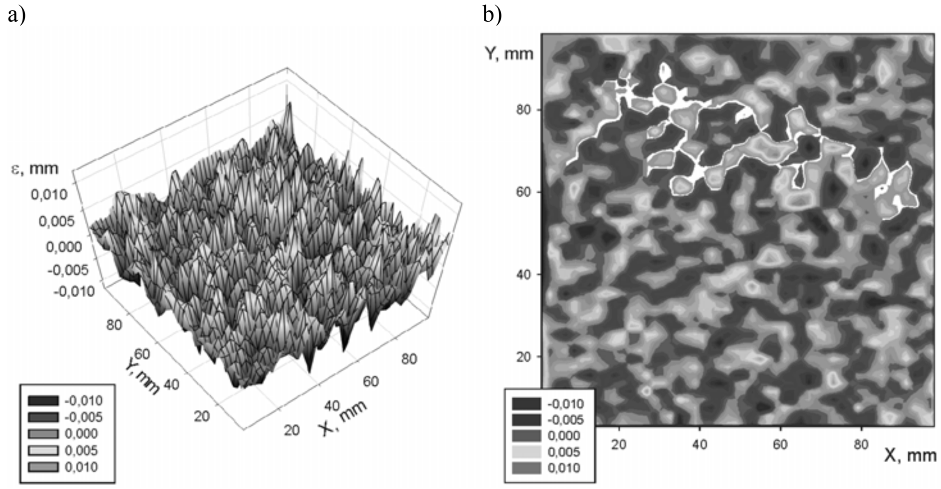

Fig. 2. Simulated random geometric deviations versus XY plane (a) and the map of deviations (b)

The virtual geometric deviations obtained in this way represented a spatial process with a gradient, i.e. non-stationary with regard to the mean but stationary with regard to the variance. Therefore, it was expected that spatial autocorrelation would appear in the case of compound deviations with a gradient, and that there would be no autocorrelation of deviations after eliminating the gradient.

a) b)

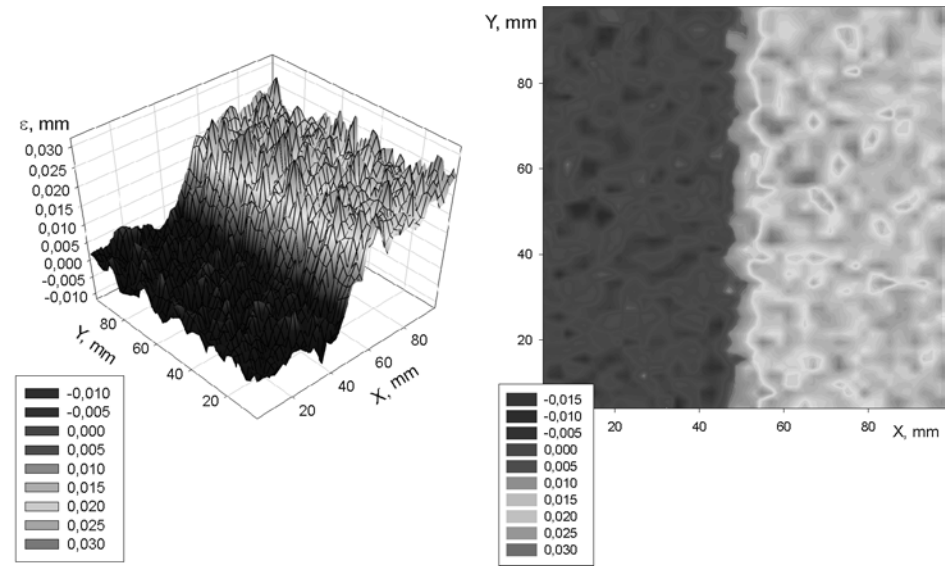

Fig. 3. Simulated compound geometric deviations versus XY plane (a) and the map of deviations (b)

5.2. Tests on spatial autocorrelation of deviations

Tests on spatial autocorrelation of simulated geometric deviations were subsequently carried out. The relationships between the deviations were made dependent on the reciprocal distances determined from the (2) formula. The elements of weight matrices, defining the dependencies between deviations at points i and j were calculated from the (3) formula, assuming the value of the constant as $k = 3$. A fragment of the weight matrix is shown in Fig. 4. Moving successively from the dependence (4) to (6) the I spatial autocorrelation coefficient was determined. The null hypothesis on the lack of geometric deviations autocorrelation was verified, assuming a normal distribution approximation, with the significance level $\alpha = 0.05$ (the upper point of a standard normal distribution $z_\alpha = 1.645$). The computations were performed in the ***R-Gui*** programme. Fig. 5 presents the print screen image with the computation results for compound, deterministic and random geometric deviations and Fig. 6 for random deviations.

In the case of compound deviations the null hypothesis of the lack of spatial autocorrelation was rejected ($I = 0.8471$; $z = 46.3096$; $z_\alpha = 1.645$; $z > z_\alpha$) (Fig. 5). The computation results show a clear positive autocorrelation of geometric deviations. In this case it is possible to predict in approx. 72% the values in the neighbouring points on the basis of the deviation value at any point.

Data Editor

	col1	col2	col3	col4
1	0	0.03797923	0.008843025	0.003329529
2	0.03797923	0	0.1552046	0.01939576
3	0.008843025	0.1552046	0	0.1551272
4	0.003329529	0.01939576	0.1551272	0
5	0.001595682	0.005747631	0.01939705	0.1552256
6	0.0008857658	0.002430481	0.00576541	0.01949205
7	0.0005443191	0.001254297	0.002456029	0.005847414
8	0.0003593307	0.000732981	0.001271661	0.002498982
9	0.0002481433	0.0004616842	0.0007356076	0.001277269
10	0.0001793137	0.0003110757	0.0004660723	0.0007438453

Fig. 4. The top left corner of the *W* matrix

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        Moran's I test under normality

data:  odchylki
weights: wagi

Moran I statistic standard deviate = 46.3096, p-value < 2.2e-16
alternative hypothesis: greater
sample estimates:
Moran I statistic       Expectation          Variance
     0.8471168777      -0.0007147963      0.0003351794
```

Fig. 5. Print screen image of *R-Gui* programme with computation results for compound deviations

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        Moran's I test under normality

data:  odchylki
weights: wagi

Moran I statistic standard deviate = 0.1499, p-value = 0.4404
alternative hypothesis: greater
sample estimates:
Moran I statistic       Expectation          Variance
     0.0020291536      -0.0007147963      0.0003351794
```

Fig. 6. Print screen image of *R-Gui* programme with computation results for random deviations

In the case of deviations of random values, the null hypothesis of the lack of spatial autocorrelation was accepted (I = 0.0020; z = 0.1499; z_α = 1.645; $z < z_\alpha$) (Fig. 6).

An approximately zero value of the I coefficient was obtained, which is indicative of the lack of spatial autocorrelation i.e. of the fact that the deviations observed in one area do not depend on the deviations observed in the contiguous areas.

6. Conclusions

It may be assumed that geometric deviations of free-form 3D surfaces constitute a spatial process. In research on these deviations the statistical methods of spatial data analysis are most suitable, because they allow for obtaining information on spatial interdependence between the deviations values at individual measurement points. These methods may be applied both to analysing raw data, or data obtained directly from measurements, and also to researching residuals from surface regression models in tests of models' adequacy. Detecting a positive spatial autocorrelation is a proof that a systematic geometric deviation (deviations) has (have) appeared, while the character of the deviation (deviations) makes it possible to determine its value (theirs spatial regression model) and to decompose deterministic and random components.

The article presents the results of the experiment involving virtual superimposition of random and determined geometric deviations on a CAD model of a free-form surface. The geometric deviations obtained in this way represented a spatial process with a gradient. Tests on spatial autocorrelation of those deviations were then conducted. The Moran's *I* statistic was applied because it made it possible to quantitatively qualify the spatial dependence of the geometric deviations. In the case of deviations of a compound character, significant spatial autocorrelation of deviations at adjacent points, i.e. the existence of a determined distribution, was observed. After the gradient had been eliminated, the values of the generated random deviations at neighbouring points were of random spatial distribution.

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