

Inference on errors in industrial parts: Kriging and variogram versus geometrical product specifications standard

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(Article begins on next page)

1                   **INFERENCE ON ERRORS IN INDUSTRIAL PARTS:**  
2                   **KRIGING AND VARIOGRAM VS**  
3                   **GEOMETRICAL PRODUCT SPECIFICATIONS STANDARD**

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ABSTRACT. This paper focuses on the inference on the errors in manufactured parts controlled by using measurements devices. The characterization of the part surface topographies is core in several applications. A broad set of properties (tribological, optical, biological, mechanical, etc.) depends on the micro and macro geometry of the parts. Moreover, parts usually show typical deterministic geometric deviation pattern, referred to as manufacturing signatures, due to the specific manufacturing processes and process set-up parameters adopted for their production. In several situations, the measurements may also be affected by systematic errors due to the measurement process, that might be caused, for example, by a poor part alignment during the measurement process. Measurement techniques and characterization methods have been standardized in the International Standard ISO 25178, defining parameters characterizing the surface topography and supplying methods and formula adapt to deal with this issue computationally. In the present paper, we consider a type of spatial dependence between measured values at different points that suggest the use of the variogram to identify patterns in the parts. We offer a comparison, based on a real set of measures, between the latter approach and the conventional as a test of the efficient performance of our findings.

10                   1. INTRODUCTION

11                   The surface topography of components draws its origin both by processing conditions  
12                   and by process parameters.<sup>1,2</sup> From a geometrical perspective and according to Leach,<sup>3</sup>  
13                   the surface topography (simply surface) of a component is its overall surface structure,  
14                   consisting of the form (the underlying shape) and the texture, that is, what remains after  
15                   removing the shape. Being intertwined with the manufacturing process, often the surface  
16                   bears a systematic pattern which is unique and distinctive of the process: the so-named  
17                   manufacturing signature.<sup>4,5</sup> Experts estimate that 10% of component failures depend on

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18 an imperfect realization of topographical specifications.<sup>3</sup> Consequently, measuring and  
19 characterizing the surface topography is core to understand and qualify manufacturing  
20 processes, to support the process optimization and ultimately to enable the identification  
21 of deviations from the in-control state.

22 In the last few years, the industry has targeted the design of surface topography to  
23 engineer the functionality of products and increase their quality and performances. To-  
24 pographies can control a wide range of functional properties,<sup>6,7</sup> because most relevant  
25 physical phenomena, involving the exchange of energy and information, take place on the  
26 surfaces. Structured surfaces and texturing are relevant in several fields: biomedicine,  
27 where the micro-fluidics devices texturing aims to control and trigger the release of drugs  
28 in the patients based on physiological signals;<sup>8</sup> robotics and manufacturing, which ex-  
29 ploits texturing surfaces of handling components of robots to enhance the grip on objects  
30 to support the increasing human-machine interactions;<sup>9</sup> automotive for achieving a sig-  
31 nificant reduction of both fuel consumption and pollutant emission by texturing engine  
32 components.<sup>10,11</sup> Thus, the increasing demand for enhanced performances pulled funda-  
33 mental research in electronics, energy, IT, optics, tribology, and other fields to enable  
34 surface functionalization.

35 All these applications require flexible and fast quality inspections relying on thorough,  
36 accurate and specific characterization methods, to meet customers demands, within the  
37 framework of Industry 4.0, and to deal with big data and interconnected cyber-physical  
38 systems.<sup>12-14</sup> To this aim, surfaces measurement requires dense sampling through appro-  
39 priate technology.<sup>15</sup> Nowadays, new optical technologies are available to overcome the  
40 limitations of conventional inspection technologies based on contact probes (Coordinate  
41 Measuring Machines CMM) and contact stylus instruments.<sup>3,16</sup> CMM may require too  
42 long times, hence high costs, to achieve an adequate sampling density. In some cases, the  
43 physical dimension of the probe forbids the measurement of statistically representative  
44 samples of the surface.<sup>16,17</sup> Efficient surface modelling is a base requirement to cope with  
45 the challenges of surface characterization in the modern manufacturing of Industry 4.0,<sup>18</sup>  
46 where free-form surfaces,<sup>19</sup> additive manufacturing surfaces,<sup>20,21</sup> and other non-standard  
47 features appear.<sup>22-24</sup> Different geometrical features, properties and scales might be tar-  
48 geted depending on purposes and surface technology. In this paper, the interest is focused  
49 on the height and width of features, in order to control the texture regularity, in terms  
50 of periodicities and isotropy.

51 Recently, literature has developed statistical modelling based on Kriging methods to  
52 aid inspection designers to overcome constraints and to enhance the informativeness of  
53 the measurement without increasing costs. In the following, we offer a review of this  
54 Kriging application.

55 1.1. **History.** Pedone *et al.*<sup>25</sup> contains a first attempt to use Kriging modelling for  
56 the online design of inspection plans operated by CMM. The probing of a few point  
57 only leads to the assessment of nominal dimensions and shape, with benefits on the  
58 economy of the inspection process. The inspection plan as a sequential experiment to  
59 be designed online has shown the trade-off between accuracy and costs, exploiting an  
60 updating of the Kriging model iteratively, according to the new incoming data, and using  
61 the predictions from the updated model for selecting the next point to inspect. The paper  
62 discussed two case studies about the verification of form tolerances, straightness and  
63 roundness. Subsequently, Vicario *et al.*,<sup>26</sup> have considered flatness tolerance verification,  
64 while Pistone and Vicario,<sup>27</sup> discussed the improvement of wafer inspection strategies.

65 Later on, Ruffa *et al.*<sup>28</sup> addressed the comparison between conventional and Kriging-  
66 based inspection strategies, from the perspective of measurement uncertainty. Ascione  
67 *et al.*<sup>29</sup> outlined adaptive inspection methods for coordinate measurement system based  
68 on Kriging modelling. Other authors have exploited the capability of Kriging models to  
69 detect geometrical and dimensional errors. Kolios *et al.*<sup>30</sup> developed predictive models for  
70 the reliability of cutting tools. Song *et al.*<sup>31</sup> detect a geometrical deviation in additive  
71 manufacturing processes for polymers and Wang *et al.*<sup>32</sup> outlined corrective models for  
72 this building strategy. Kriging models are of use also in the assembling to detect, and  
73 later correct, non-linear assembling errors for compliant<sup>33</sup> and composite materials.<sup>34</sup>

74 The Kriging modelization requires detecting and, consequently, modelling the correla-  
75 tion between measured responses. However, the choice of the most suitable class of cor-  
76 relation models, amongst the several available options, is not trivial. Several researchers,  
77 mostly geo-statisticians, favour the use of the variogram, or semi-variance diagram, in  
78 the choice of the correlation function. It is very informative about spatial dependence,  
79 showing the averaged square difference in the response values between a pair of measure-  
80 ment points separated by a given distance. Moreover, the variogram is equivalent to the  
81 correlation function for stationary processes, as frequently occurs (see Cressie<sup>35</sup>).

82 This finding suggested further investigations on the relationship between variogram  
83 and correlation, see Pistone and Vicario.<sup>36,37</sup> In the former case, the authors considered  
84 Gaussian vectors with constant variance. They showed how to parametrize the distribu-  
85 tion with the variogram and, conversely, how to characterize all the Gaussian distribution  
86 with a given variogram. In the latter, they discuss the constraints imposed on the set of  
87 parameters defining the variogram.

88 Recently, Ruffa *et al.*<sup>38</sup> and Vicario *et al.*<sup>39,40</sup> discussed the effectiveness of using  
89 variogram in other practical situations. Finally, a relevant paper is Vicario and Pistone,<sup>41</sup>  
90 whose main points provide the base the content of this paper.

91 **1.2. State of art.** Complex interactions between materials and manufacturing tools  
92 during the process can affect the surface texture, ultimately introducing manufacturing  
93 signatures. In most mechanical processes, such as machining or additive manufacturing,  
94 the process is repetitive and periodic. This situation results in a periodic texture and  
95 a spatial correlation between measured surface points. From here, the suggestion to  
96 use the variogram to investigate an existing surface topography correlation and infer  
97 geometrical properties of the surface. In Vicario and Pistone,<sup>41</sup> the authors, exploiting  
98 simulative approaches, analyzed the variogram in the presence of both a noticeable trend  
99 in the model and anisotropy. If the manufacturing process is anisotropic, the variogram  
100 depends on both distances and direction. Contrary to some common beliefs, even for  
101 the most refined surfaces, the assumption of isotropy can fail. These features may show  
102 evidence of technological signatures or CMM systematic errors. The paper mentioned  
103 above represents a contribution to the adoptions of graphical tools in the quality control  
104 of the variability in spatial data.

105 Now in this paper, the authors aim to prove that Kriging and variogram are ade-  
106 quate tools for quantitative characterization of surfaces. They provide a comparison with  
107 methods in the Standard, and theoretically support their findings in several practical  
108 case studies, one of which is presented in detail. Section 2 introduces the protocol rec-  
109 ommended by the Standard for the characterization of the surface topography and the  
110 basic of Kriging. The use of Kriging prediction requires the computation of the weights  
111 assigned at measured points and this essential step depends on a suitable correlation  
112 model. Section 3 discusses variogram as an informative tool in fitting a model of spatial

113 correlation. Section 4 provides the implementation of the two approaches of Section 2:  
 114 a case study based on real measurements illustrates the methods, with a comparison of  
 115 the respective performances. A final discussion concludes the paper.

116 2. SURFACE TOPOGRAPHY CHARACTERIZATION: STANDARD PROTOCOL AND  
 117 KRIGING MODEL

118 **2.1. Standard characterization and protocol.** A wide set of different technologies  
 119 have been developed to enable surface topography measurements.<sup>15,16</sup> Amongst the  
 120 most widely used technologies for measuring surfaces, we mention contact probes (for  
 121 example CMM and contact stylus instruments<sup>15</sup>), optical probes (Point autofocus instru-  
 122 ments<sup>42,43</sup>), and surface topography optical instruments (like focus variation microscopes  
 123 or coherence scanning interferometers<sup>15</sup>). They measure a cloud of points, resulting in a  
 124 set of surface heights as a function  $z(x, y)$  of plane coordinates  $(x, y)$ . The heights rep-  
 125 resent the departures of the measured topography from an arbitrary reference horizontal  
 126 plane, usually the cartesian plane  $z = 0$  representing the mean height.

127 Measurement techniques and characterization methods have been standardized in the  
 128 ISO 25178.<sup>44</sup> Several areal height parameters and spatial parameters for describing,  
 129 respectively, the statistical distribution of the surface height and the spatial orientation  
 130 of the texture are on hand of the users. In the following, we provide a summary of  
 131 the main, and most widely adopted, parameters and tools used to characterize surfaces  
 132 according to the Standard ISO 25178-2:2012 protocol.<sup>45</sup>

133 Amongst the most widely adopted height parameters, we mention the *arithmetic mean*  
 134 *height*  $S_a$  and the *root mean square height*  $S_q$ , respectively,

$$S_a = \frac{1}{\text{meas}(A)} \iint_A |z(x, y)| dx dy,$$

135 and

$$S_q = \sqrt{\frac{1}{\text{meas}(A)} \iint_A z^2(x, y) dx dy},$$

136 where the definition domain  $A$  is the domain where the measured points are sampled and  
 137  $\text{meas}(A) = \iint_A dx dy$ .

138 It should be noted that the terms used in the ISO Standard sometimes differ from those  
 139 used in Statistics. If  $z(x, y)$  is the deviation from a reference value, and the normalized  
 140 integral is intended as the expectation with respect to the uniform probability on  $A$ , then  
 141  $S_a$  is the absolute deviation,<sup>46</sup> and as such, it is a measure of the dispersion of the heights.  
 142 This parameter is the metric used to quantify the roughness of the texture, which is  
 143 relevant for tribological application, coupling tolerances and aesthetic purposes.<sup>47,48</sup> The  
 144 parameter  $S_q$  is a standard deviation and is more informative than  $S_a$  both in terms  
 145 of statistical meanings and physical relationship; in fact, it is linked to surface energy  
 146 and optical properties.<sup>49,50</sup> Since these two statistical moments cannot fully described  
 147 topographies, the knowledge of the surface height range is further required for sufficiently  
 148 characterizing the amplitude of the height variability. To this aim, the *maximum height*  
 149 *of the surface height*  $S_z$  is the most used parameter, to be used with caution since a  
 150 drawback may be its sensitiveness to isolated and not significant peaks and pits.

151 Occasionally, the textures can exhibit imprints as anisotropy and/or periodicity, either  
 152 due to a product functionalization or to manufacturing signatures. Detection and quan-  
 153 tification of these defects are core for components functionality assessment and for process  
 154 quality control. According to the Standard, the spatial parameters are the best suited for

155 this analysis. They include the *autocorrelation function*  $f_{\text{ACF}}$ , the *autocorrelation length*  
 156  $S_{al}$ , the *texture aspect ratio*  $S_{tr}$ , and the *surface texture direction*  $S_{td}$ .

157 According to the ISO 25178-2:2012 the definition of  $f_{\text{ACF}}$  is

$$(1) \quad f_{\text{ACF}}(\tau_x, \tau_y) = \frac{\iint_A z(x, y)z(x - \tau_x, y - \tau_y) dx dy}{\iint_A z^2(x, y) dx dy},$$

158 for all  $\tau_x$  and  $\tau_y$  such that  $(x - \tau_x, y - \tau_y) \in A$  for some  $(x, y) \in A$ . Notice that, for each  
 159 given  $(\tau_x, \tau_y)$ , the integration domain in the numerator is restricted to compatible  $(x, y)$ .

160 The other two parameters are defined by

$$S_{al} = \min\{\sqrt{\tau_x^2 + \tau_y^2} : f_{\text{ACF}}(\tau_x, \tau_y) \leq s\},$$

161 and

$$S_{tr} = \frac{p_{min}}{p_{max}},$$

162 where  $p_{min} = S_{al}$  and  $p_{max} = \max\{\sqrt{\tau_x^2 + \tau_y^2} : f_{\text{ACF}}(\tau_x, \tau_y) \leq s\}$ .

163 The autocorrelation function is bounded between  $-1$  and  $+1$  and assumes the maxi-  
 164 mum value  $+1$  at  $\tau_x, \tau_y = 0$ .

165 The autocorrelation length  $S_{al}$  is the horizontal distance of  $f_{\text{ACF}}$  which has the fastest  
 166 decay to a specified value  $s$ , with  $s \in [0, 1]$ . The shape of  $f_{\text{ACF}}$  and the distance of  
 167 decay below a threshold  $s$  can support the identification of periodic structures and of  
 168 anisotropy. Opposite, if the spatial correlation is not a feature of the topography, it  
 169 will decrease towards zero for increasing distances from the considered point. Moreover,  
 170 the analysis of the autocorrelation decay in different directions can also identify the  
 171 anisotropic pattern. Thus,  $S_{al}$  and  $S_{tr}$ , whose definition exploits the  $f_{\text{ACF}}$ , are designed  
 172 to characterize the isotropy of the surface synthetically: the former measures the extent  
 173 of the surface (auto-)correlation, being the distance at which a portion of the surface is  
 174 significantly different from the original location, and the latter quantifies the severity of  
 175 the anisotropy. In fact, if the two correlation distances  $p_{min}$  and  $p_{max}$  are sufficiently  
 176 similar, the surface can be considered isotropic, being  $S_{tr}$  the ratio between the smallest  
 177 and largest distance of decay to  $s$ . Provided that  $S_{tr} \in [0, 1]$ , the surface is considered  
 178 isotropic, if  $S_{tr} > s$ . The threshold  $s$  is conventionally<sup>51</sup> set to 0.2 based on experts  
 179 opinions on empirical practices without any formal rationale; clearly, the value of  $S_{al}$  and  
 180  $S_{tr}$  depends on the choice of  $s$ .

181 In the case of anisotropy, the direction of the anisotropy, i.e. the main pattern, is  
 182 orthogonal to the direction of  $S_{al}$  and is quantified, as an angle, by the *surface texture*  
 183 *direction*,  $S_{td}$ , assessed from the Fourier spectrum of the surface, in polar coordinates, as  
 184 the angle at which the spectrum has the maximum amplitude.

185 To this extent, the Fourier transform of  $z(x, y)$  allows computing the spectrum of the  
 186 surface heights, i.e. the frequency-dependent amplitudes of  $z(x, y)$ , whose most typical  
 187 representation makes use of the Power Spectrum Density (PSD). The analysis of ampli-  
 188 tude peaks of the spectrum enables the identification of the main harmonics, identifying  
 189 the main frequency of the periodic pattern. Real surfaces typically show one of the main  
 190 peaks at very low wavelengths: the amplitude of this peak is related to the random  
 191 variation of  $z(x, y)$ , according to signal theory.<sup>3,52</sup> In general, adequate pre-processing is  
 192 necessary to filter the wavelengths that are not relevant to the objectives of the charac-  
 193 terization.

194 The ISO Standard characterization of a surface according to the mentioned parameters  
 195 has been conceived to provide a quick, synthetic although conventional characterization.

196 This approach has inherent limitations, mostly linked to the statistical robustness and  
 197 the significance in the detection and the characterization of an existent anisotropy.

198 **2.2. Kriging.** The concept of using Kriging methods in the research works mentioned  
 199 in Section 1 to characterize surface topographies was prompted by their ability to make  
 200 accurate predictions of a response basing on a limited set of spatial data and the rea-  
 201 sonable assumptions that response values spatially close are much more alike than more  
 202 distant values. This applies to Kriging methods as they consist in a spatial interpolation  
 203 based on the correlation structure between the observations. In the following, Kriging  
 204 methods are introduced in the essential parts, to outline their use in the comparison in  
 205 Section 4. They rely on an optimality criterion that aims at minimizing the mean squared  
 206 prediction error (MSPE) of the linear combination of observations, under the constraints  
 207 of unbiasedness.

208 The ordinary Kriging model assumes that the observed values are realization of a  
 209 Gaussian random field  $Z(\mathbf{x})$  plus an unknown constant term  $\beta$ :

$$Y(\mathbf{x}) = \beta + Z(\mathbf{x}) ,$$

210 where  $Z(\mathbf{x})$  denotes the value of the spatial field in the point  $\mathbf{x} = (x_1, \dots, x_n)^T$  of the  
 211 design space  $\chi_q \subset \mathbb{R}^q$ . In the case study in Section 4,  $Z(\mathbf{x})$  is the height function  
 212 introduced in the sub-section 2.1 ( $q = 2$ ,  $\mathbf{x} = (x, y)$ ) and its realizations are the measures  
 213 obtained by measuring the surface points with respect to an horizontal reference plane  
 214 at height  $\beta$  (usually  $\beta=0$ ) . Moreover, the Gaussian random field is assumed to have  
 215 zero mean and stationary covariance over the design space  $\chi_q$ , i.e.  $\mathbb{E}(Z(\mathbf{x})) = 0$  and  
 216  $\text{Cov}(Z(\mathbf{x}_i), Z(\mathbf{x}_j)) = \sigma_Z^2 R(\mathbf{h}; \boldsymbol{\theta})$ ,  $i, j = 1, \dots, n$ , where  $\sigma_Z^2$  is the process variance and  $R$   
 217 is the spatial correlation function depending only on the displacement vector  $\mathbf{h}$  between  
 218 any pair of points in  $\chi_q$  and on a vector parameter  $\boldsymbol{\theta}$ . If the value of the auto-covariance  
 219 function  $C(\mathbf{h})$  depends only on the length  $\|\mathbf{h}\|$  of the vector  $\mathbf{h}$ , then the stochastic  
 220 process is isotropic; opposite, the process is anisotropic. This property is vital in the  
 221 characterization of the surface topography we deal with in Section 4.

222 Let now  $\mathbf{Y}^n = (Y(\mathbf{x}_1), \dots, Y(\mathbf{x}_n))^T$  the vector of the observed values of the spatial field  
 223 in the  $n$  sampled points  $\mathbf{x}_i$ ,  $i = 1, \dots, n$ , and  $Y_0 = Y(\mathbf{x}_0)$  the value in a new unsampled  
 224 point  $\mathbf{x}_0$ . The most popular prediction criterion is based on the minimization of the Mean  
 225 Squared Prediction Error (MSPE), where the MSPE of  $\hat{Y}_0 = \hat{Y}_0(\mathbf{Y}^n)$  is:

$$(2) \quad \text{MSPE}(\hat{Y}_0, F) = \mathbb{E}_F \left[ (\hat{Y}_0 - Y_0)^2 \right]$$

226 where  $F$  is the joint distribution of  $(Y_0, \mathbf{Y}^n)$ . The predictor in eq. (2) is unique, linear  
 227 unbiased and the best one (BLUP) of  $Y(\mathbf{x}_0)$ . If the joint distribution  $F$  of  $(Y_0, \mathbf{Y}^n)$   
 228 is multivariate normal as in the ordinary Kriging, the MSPE in eq. (2) is equal to the  
 229 conditional expectation of  $Y(\mathbf{x}_0)$  given  $\mathbf{Y}^n$ :

$$(3) \quad \hat{Y}_0 = \beta + \mathbf{r}_0^T \mathbf{R}^{-1} (\mathbf{Y}^n - \beta \mathbf{1})$$

230 with  $\mathbf{1} = [1, 1, \dots, 1]^T$ ;  $\mathbf{R}$  is the correlation matrix with  $r_{ij} = R(\mathbf{x}_i - \mathbf{x}_j)$  ( $i, j$  range  
 231 from 1 to  $n$ ) and  $\mathbf{r}_0 = [R(\mathbf{x}_0 - \mathbf{x}_1), \dots, R(\mathbf{x}_0 - \mathbf{x}_n)]^T$  the correlation vector. The predictor  
 232 in eq. (3) minimizes the MSPE in eq. (2). Considering the interpolatory property of  
 233 Kriging, MSPE is zero at the sampled points and it perfectly reflects the Kriging principle:  
 234 it is large when  $\mathbf{x}_0$  is away from the sampled points, small when it is close to them. Such  
 235 a behaviour expresses a measure of uncertainty of predictions, making possible to provide  
 236 confidence intervals of the predictions.

237 It follows that:

$$(4) \quad \text{MSPE}(\hat{Y}_0) = \sigma_Z^2(1 - \mathbf{r}_o^T \mathbf{R}^{-1} \mathbf{r}_o + \mathbf{c}_o^T (\mathbf{1}_T \mathbf{R}^{-1} \mathbf{1})^{-1} \mathbf{c}_o^T)$$

238 with  $\mathbf{c}_o^T = 1 - \mathbf{1}_T \mathbf{R}^{-1} \mathbf{r}_o$ . The expression eq. (4) takes into account that  $\beta$  parameter is  
 239 replaced by its generalized least squares estimator  $\hat{\beta}$ . Moreover, the unknown parameter  
 240 vector  $\boldsymbol{\theta}$  in  $R(\mathbf{h}; \boldsymbol{\theta})$  can be estimated by maximum likelihood. It has to be highlighted that  
 241 eq. (4) underestimates prediction variance as it does not account for the extra variability  
 242 transmitted to  $\mathbf{r}_o$ ,  $\mathbf{R}$  and  $\beta$  by  $\boldsymbol{\theta}$ .

243 Concerning the correlation modelling in predicting the values of  $Y$  in unsampled points  
 244 and in evaluating the MSPE in the predicted points, there are two approaches: the first  
 245 one uses a spatial correlation function chosen within some parametric function families,  
 246 driving this choice by some underlying phenomenon to model, choosing the parameter(s)  
 247 in order to fit best the model;<sup>53</sup> the second approach, proposed by Matheron<sup>54</sup> exploits  
 248 the variogram, defined as:

$$\gamma(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{2} \mathbb{E}((Z(\mathbf{x}_i) - Z(\mathbf{x}_j))^2)$$

249 Variogram may also be expressed in terms of the model covariance:<sup>36</sup>

$$\gamma(\mathbf{x}_i, \mathbf{x}_j) = \text{Cov}(Z(\mathbf{x}_i), Z(\mathbf{x}_i)) + \text{Cov}(Z(\mathbf{x}_j), Z(\mathbf{x}_j)) - 2 \text{Cov}(Z(\mathbf{x}_i), Z(\mathbf{x}_j))$$

250 Kriging method was originally intended as a model, to be used in Geostatistics, of the  
 251 physical randomness of the quantity of interest. Later a different interpretation of the  
 252 same method has been devised to treat Computer Experiments, where the traditional  
 253 notion of randomness is not applicable.<sup>55</sup> In such a case, for each given covariance, the  
 254 method produces an interpolation of the given values even if the covariance lack of any  
 255 physical interpretation. The Kriging approach, within this framework, can thus be seen  
 256 as a method to augment the density of sparse, i.e. not densely sampled, measurement.  
 257 The resulting surface can then be characterized according to the standard method.

258 The elicitation of a given covariance, together with the corresponding Gaussian distri-  
 259 bution, corresponds then to the choice of a Bayes prior. Such a choice is made according  
 260 to the qualitative type of the surface of interest. In this paper, we follow this approach,  
 261 with the addition of a special method for the choice of a covariance based on the use of  
 262 variograms. The following Section 3 will be devoted to present and discuss in details the  
 263 properties of the variogram.

### 264 3. VARIOGRAMS

265 In this section, we present some facts about variograms and their estimation. We aim  
 266 to illustrate how variograms can be used both to evaluate characteristics of the measured  
 267 surface and to suggest a convenient covariance to be used for Kriging interpolation. The  
 268 presentation is original in that it considers a definition that applies to both systematic  
 269 and random sampling of the locations to be tested.

270 **3.1. Matheron's variogram.** Let  $Z = (Z(\mathbf{x}))_{\mathbf{x} \in A}$  be a real random field, where the  
 271 set of locations  $A$  is endowed with a quasi-distance  $d$ . A quasi-distance is a symmetric  
 272 relation that satisfies the triangle inequality. If, moreover,  $d(\mathbf{x}, \mathbf{y}) = 0$  implies  $\mathbf{x} = \mathbf{y}$ ,  
 273 then  $d$  is a distance. In most applications we consider,  $A$  is either a planar connected  
 274 graph, for example, a grid, or a plane real domain. In the first case, a distance could be a  
 275 length on the graph. In the second case, the most common distance is  $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|$   
 276 for some norm on 2-vectors.



277 Recall that the random field  $(Z(\mathbf{x}))_{\mathbf{x} \in A}$  is *intrinsically stationary* if  $\frac{1}{2} \mathbb{E}((Z(\mathbf{x}) - Z(\mathbf{y}))^2)$   
278 depends only on the difference  $\mathbf{h} = \mathbf{x} - \mathbf{y}$  through a *variogram function*  $\gamma$ , namely,  
279  $\mathbb{E}((Z(\mathbf{x}) - Z(\mathbf{y}))^2) / 2 = \gamma(\|\mathbf{h}\|)$ . If, moreover, the variogram function depends on  $\|\mathbf{h}\|$   
280 only, it is said to be *isotropic* (for that norm). See, for example, §2.2.1 of Cressie's  
281 monograph.<sup>35</sup> The previous definitions are inspired by the theory of stationary processes,  
282 where the stationarity is the invariance with respect to action of the translation group or  
283 of some other transformation group.

284 If both stationarity and isotropic intrinsic stationarity holds, with  $\sigma^2 = \text{Var}(Z(\mathbf{x}))$ , it  
285 is

$$\gamma(\|\mathbf{h}\|) = \frac{1}{2} \mathbb{E}((Z(\mathbf{x}) - Z(\mathbf{x} + \mathbf{h}))^2) = \sigma^2 - C(\mathbf{h}) ,$$

286 hence, the auto-correlation function  $C(\mathbf{h})$  is a function of the norm. This variogram  
287 methodology is extensively used in Geostatistics and in Kriging modellization, see, for  
288 example, the monograph by Cressie.<sup>35</sup> In the original applications as discussed by Krige,  
289 and in many current applications, the variogram is assumed to be monotonic and bounded  
290 to express the idea of a correlation fading out when the distance increases. *We do not*  
291 *make this assumption here.* For a deep mathematical discussion of variograms from  
292 the point of view of Harmonic Analysis see Sasvari<sup>56</sup> and Gneiting et al.,<sup>57</sup> whilst an  
293 exposition of the relevant mathematics of the Gaussian case can be found in Pistone and  
294 Vicario.<sup>36</sup>

295 Now, we consider a variation of the standard setting, in that we assume, more generally,  
296 that the variogram depends on a quasi-distance  $d$ ,

$$\frac{1}{2} \mathbb{E}((Z(\mathbf{x}) - Z(\mathbf{y}))^2) = \gamma(d(\mathbf{x}, \mathbf{y})) .$$

297 This assumption accommodates the instances where the points of  $A$  are identified by a  
298 non-numeric label. In this case, we say that the process is *d-isotropic*.

299 The empirical estimator of the variogram studied by Matheron<sup>54</sup> is based on a *sampling*  
300 *plan*  $A_s$ , a finite subset of  $A$ . This estimator uses the values on  $A_s$  of a realization  $\omega$  of  
301 the random mechanism to compute an estimate of  $\gamma$  at all possible non-zero values  $\theta$  of  
302 the pseudo-distance on  $A_s$ , namely,

$$(5) \quad \tilde{\gamma}(\omega; \theta) = \frac{1}{2 \#\{\mathbf{x}, \mathbf{y} \in A_s \mid d(\mathbf{x}, \mathbf{y}) = \theta\}} \sum_{\{\mathbf{x}, \mathbf{y} \in A_s \mid d(\mathbf{x}, \mathbf{y}) = \theta\}} |Z(\mathbf{x})(\omega) - Z(\mathbf{y})(\omega)|^2 .$$

303 The Matheron estimator can be extended to all possible values of the distance by any  
304 interpolation or fitting method.

305 Clearly, as a random variable depending on the random sample  $\omega$ , this estimator is  
306 unbiased and consistent under independent copies of the random field and a given fixed  
307 sampling plan. If the design is itself random, then unbiasedness and consistency will  
308 depend on proper assumptions on the device generating the sampling plan.

309 Another point of view is possible, that is, to consider the sample  $\omega$  as fixed and the  
310 sampling plan random. This point of view is actually more adapted to the present set-up.  
311 In fact, the measurement error is small if compared with the variability of the surface  
312 itself.

313 Let us discuss more in detail the argument above in order to derive an interesting  
314 generalization of the estimator of eq. (5). Given the sampling plan  $A_s$ , consider the set of  
315 all non-diagonal couples  $\widetilde{A_s \times A_s} = \{(\mathbf{x}, \mathbf{y}) \in A_s \times A_s \mid \mathbf{x} \neq \mathbf{y}\}$ . If the number of sampled  
316 points is  $\#A_s = n$ , then the number of non-diagonal couples is  $n(n - 1)$ .

317 For each fixed realization  $\omega$  we have a couple of functions, both defined on  $\widetilde{A_s \times A_s}$ ;  
 318 namely we have the  $n(n-1) \times 2$  table

$$\begin{array}{c|cc} \widetilde{A_s \times A_s} & \Gamma & \Delta \\ \hline (\mathbf{x}, \mathbf{y}) & \frac{1}{2}(Z(\mathbf{x})(\omega) - Z(\mathbf{y})(\omega))^2 & d(\mathbf{x}, \mathbf{y}) \end{array}$$

319 and we look for a model to interpolate the column  $\Gamma$  as a function of the column  $\Delta$ . The  
 320 scatter plot of the table is called *variogram cloud* and any regression method could be  
 321 used to produce an estimate of  $\gamma$ .<sup>35,41</sup> The plot of the variogram cloud in a proper scale  
 322 will provide us with a neat summary statistics of the data, see Figures 7 and 8 below.

323 The Matheron's solution is the computation of mean value for each distance value,  
 324 that is, it is a conditional expectation. Namely, if we consider the uniform probability  
 325 function on  $\widetilde{A_s \times A_s}$ ,  $s(\mathbf{x}, \mathbf{y}) = 1/n(n-1)$ , then

$$\tilde{\gamma}(\omega; \theta) = \frac{1}{2} \mathbb{E}_s (|Z(\mathbf{x})(\omega) - Z(\mathbf{y})(\omega)|^2 | d(\mathbf{x}, \mathbf{y}) = \theta) .$$

326 The conditional expectation above defined for each realization of the original random  
 327 field model depends on the sampling plan only.

328 The idea to consider generic sampling measure originally arose in the discussion of the  
 329 application of the Kriging methodology to random fields of the form  $(F(\mathbf{x}) + Z(\mathbf{x}))_{\mathbf{x} \in D}$ ,  
 330 where  $(Z(\mathbf{x}))_{\mathbf{x} \in D}$  is intrinsically stationary and  $F$  is a deterministic function.<sup>41</sup> If the  
 331 deterministic part  $F$  is prevalent to the random part  $Z$ , then the Matheron variogram  
 332 tells more about the features of  $F$  than about the correlation structure of  $Z$ . The effects  
 333 of the deterministic trend and the correlation are confounded in the variogram and could  
 334 be difficult to evaluate which one prevails, by inspection. Nonetheless, the tool is useful in  
 335 two ways. If the deterministic effect is assumed to be prevalent, a proper model, suggested  
 336 by the shape of the variogram, can be introduced in the Kriging model via a term  $\beta(\mathbf{x})$   
 337 in order to compute residuals representing the  $Z(\mathbf{x})$  term. Or, in the other case, the  
 338 variogram can be used to evaluate the correlation in a Kriging model with constant  $\beta$ .

339 In the following section, we discuss the first case, and we show how to define the variogram  
 340 of a deterministic function  $F$ . This plan requires a generalization of the Matheron  
 341 estimator in a way that ignores (provisionally) the effect by the random field and focusses  
 342 on the randomness that comes from the sampling design.

343 **3.2. Empirical variogram or G-variogram.** This section is a review of the properties  
 344 of the variogram re-defined as follows.

345 **Definition 1.** Let  $A$  be a domain endowed with a semi-distance  $d$  and  $\nu$  a symmetric  
 346 probability measure on  $A \times A$ . Given a bounded response function of interest  $F: A \rightarrow \mathbb{R}$   
 347 and  $(X, Y) \sim \nu$ , the empirical variogram, or G-variogram, of  $F$  with respect to  $\nu$  is a  
 348 regular version  $\gamma_F$  of the conditional expectation of  $\frac{1}{2}(F(X) - F(Y))^2$  given  $d(X, Y)$ , that  
 349 is,

$$\mathbb{E}_\nu \left( \frac{1}{2}(F(X) - F(Y))^2 \middle| d(X, Y) \right) = \gamma_F(d(X, Y)) .$$

350 In the definition above, the joint distribution  $\nu$  is intended to give a theoretical model  
 351 of the sampling plan. The simplest case is independent sampling as it is the case in  
 352 Matheron estimator.

353 Expansion of the square gives

$$\gamma_F(d(X, Y)) = \frac{1}{2} \mathbb{E}_\nu (F(X)|d(X, Y)) + \frac{1}{2} \mathbb{E}_\nu (F(Y)|d(X, Y)) - \mathbb{E}_\nu (F(X)F(Y)|d(X, Y)) ,$$

354 where the two first terms in the right-hand side are equal because  $\nu$  is symmetric. Notice  
 355 that the last term, without the minus sign, is similar to the autocorrelation function (1)  
 356 when the sampling measure is uniform on the set  $\{(\mathbf{x}, \mathbf{x} + \boldsymbol{\tau})\}$ .

357 The G-variogram function is defined only on the support of the semi-distance  $d$  under  
 358 the distribution  $\nu$ . By polarization, a bi-linear non-negative definite joint G-variogram  
 359  $\gamma_{G,F}$  can be defined. Instead, the definiteness of the G-variogram function could be  
 360 considered only in particular cases, precisely when the set of possible distances is a semi-  
 361 group.

362 We conclude this discussion by observing that the use of a quasi-distance appears in  
 363 applications where the directional G-variogram is the index of interest.<sup>41</sup> For example,  
 364  $d((x_1, y_2), (x_2, y_2)) = |x_1 - x_2|$  allows to bring to light variations in one direction, here  
 365 the first coordinate direction. This case is of high practical interest as when anisotropy  
 366 occurs. Both the toy examples and the case study below present an instance of such a  
 367 feature.

368 **3.3. General properties of the variogram.** Here is a list of simple general properties  
 369 of the G-variogram that show how the features of  $F$  affect  $\gamma_F$ .

370 (1) The effect of an affine transformation is, see p. 72 of Cressie,<sup>35</sup>

$$\gamma_{\alpha F + \beta} = \alpha^2 \gamma_F .$$

371 (2) If the sampling joint distribution is symmetric,  $(X, Y) \sim (Y, X)$ , we have

$$\begin{aligned} \gamma(d(X, Y)) &= \\ &= \frac{1}{2} \mathbb{E} (F(X)^2 | d(X, Y)) + \frac{1}{2} \mathbb{E} (F(Y)^2 | d(X, Y)) - \mathbb{E} (F(X)F(Y) | d(X, Y)) \\ &= \mathbb{E} (F(X)^2 | d(X, Y)) - \mathbb{E} (F(X)F(Y) | d(X, Y)) . \end{aligned}$$

372 Notice the similarity with the stationary random field case. In particular, assum-  
 373 ing independence,

$$\mathbb{E} (\gamma(d(X, Y))) = \mathbb{E} ((F(X) - F(Y))^2) = \text{Var} (F(X)) .$$

374 (3) The maximal variation of  $F$  at comparable distances is an important feature of  
 375 the response function. Precisely, if  $F$  is  $d$ -Lipschitz, that is,

$$|F(x) - F(y)| \leq \|F\|_{\text{Lip}} d(x, y)$$

376 and  $\|F\|_{\text{Lip}} = \min_{x \neq y} |F(x) - F(y)| / d(x, y)$ , then

$$\begin{aligned} \gamma(d(X, Y)) &= \frac{1}{2} \mathbb{E} (|F(X) - F(Y)|^2 | d(X, Y)) \leq \\ &= \frac{1}{2} \mathbb{E} (\|F\|_{\text{Lip}}^2 d(x, y)^2 | d(X, Y)) = \frac{\|F\|_{\text{Lip}}^2}{2} d(x, y)^2 , \end{aligned}$$

377 that is, the graph of  $\gamma$  as a function of the distance  $t = d(x, y)$  is bounded by a  
 378 parabola,  $\gamma(t) \leq \frac{1}{2} \|F\|_{\text{Lip}}^2 t^2$ .

379 (4) In general, the *interaction variogram* can be defined by

$$\mathbb{E} ((F_1(X_1) - F_1(X_2))(F_2(X_1) - F_2(X_2)) | d(X_1, X_2)) = \gamma_{1,2}(d(X_1, X_2)) ,$$

380 so that, with obvious notations,

$$\gamma_{1+2}(t) = \gamma_1(t) + \gamma_2(t) + \gamma_{1,2}(t) .$$

381 In order to appreciate the potential interest of the methodology, we discuss some toy  
 382 examples below. Note that we will plot the variograms in the scale  $\sqrt{2\gamma}$ . In fact, the  
 383 Lipschitz inequality computation above suggests plotting in a scale which is linear in the  
 384 distance.

385 **3.4. 1d examples.** Let us consider the simple case, where, with no restriction of gener-  
 386 ality, the metric space is the unit interval,  $A = ]0, 1[$ , endowed with the standard distance  
 387  $d(x, y) = |x - y|$ . Assume the sampling random variables  $X$  and  $Y$  are IID with uniform  
 388 common distribution on  $A$ .

389 The distribution of the conditioning random variable  $d(X, Y) = |X - Y|$  has a trian-  
 390 gular density  $t(\rho) = 2(1 - \rho)$  if  $0 < \rho < 1$ , and  $t(\rho) = 0$  otherwise.

391 The variogram  $\gamma$  is characterized by the master equation

$$\int_0^1 \int_0^1 \frac{1}{2} |F(x) - F(y)|^2 \Phi(|x - y|) \, dx dy =$$

$$\int_0^1 \int_0^1 \gamma(|x - y|) \Phi(|x - y|) \, dx dy = \int_0^1 \gamma(\rho) \Phi(\rho) t(\rho) d\rho ,$$

392 where the last integral is the result of the change of variable  $\rho = |x - y|$  and  $\Phi$  is any  
 393 measurable function such that the integral exists. Because of the symmetry, the first  
 394 integral is

$$\int_{0 < x < y < 1} |F(x) - F(y)|^2 \Phi(y - x) \, dx dy =$$

$$\int_0^1 \left( \frac{1}{2(1 - \rho)} \int_0^{1-\rho} |F(v) - F(\rho + v)|^2 \, dv \right) \Phi(\rho) t(\rho) \, d\rho ,$$

395 where  $u = x - y$  and  $v = x$ .

396 In conclusion, the variogram is

$$(6) \quad \gamma(\rho) = \frac{1}{2(1 - \rho)} \int_0^{1-\rho} |F(v) - F(\rho + v)|^2 \, dv .$$

397 Let us consider a few typical cases, illustrated in Figure 1 and Figure 2. All the graphs  
 398 in this section are done with the Wolfram Mathematica suite.

399 *Affine F.* If  $F$  is affine,  $F(x) = ax + b$ , then

$$\gamma(\rho) = \frac{1}{2(1 - \rho)} \int_0^{1-\rho} a^2 \rho^2 \, dv = \frac{1}{2} a^2 \rho^2 .$$

400 This example clearly supports the choice to plot  $\sqrt{2\gamma}$  instead of  $\gamma$  itself.

401 *A bound on F.* If  $|F| \leq k$ , then  $\frac{1}{2} |F(x) - F(y)|^2 \leq 2k^2$ . If  $F$  is Lipschitz,  $|F(x) - F(y)| \leq$   
 402  $a|x - y|$ , then  $\gamma(\rho) \leq \frac{1}{2} a^2 \rho^2$ , see Item (3) in the list of properties above. If moreover  
 403  $F(0) = 0$ , then  $F \leq |a|$ , and the bound is  $\min(a^2 \rho^2, a^2) = a^2 \rho^2$ .

404 *Bended F.* Consider  $F(x) = 4hx(1 - x)$  or  $F(x) = 1 - x^2$ . In such cases, the computation  
 405 and the qualitative analysis are both simple. See Figure 1

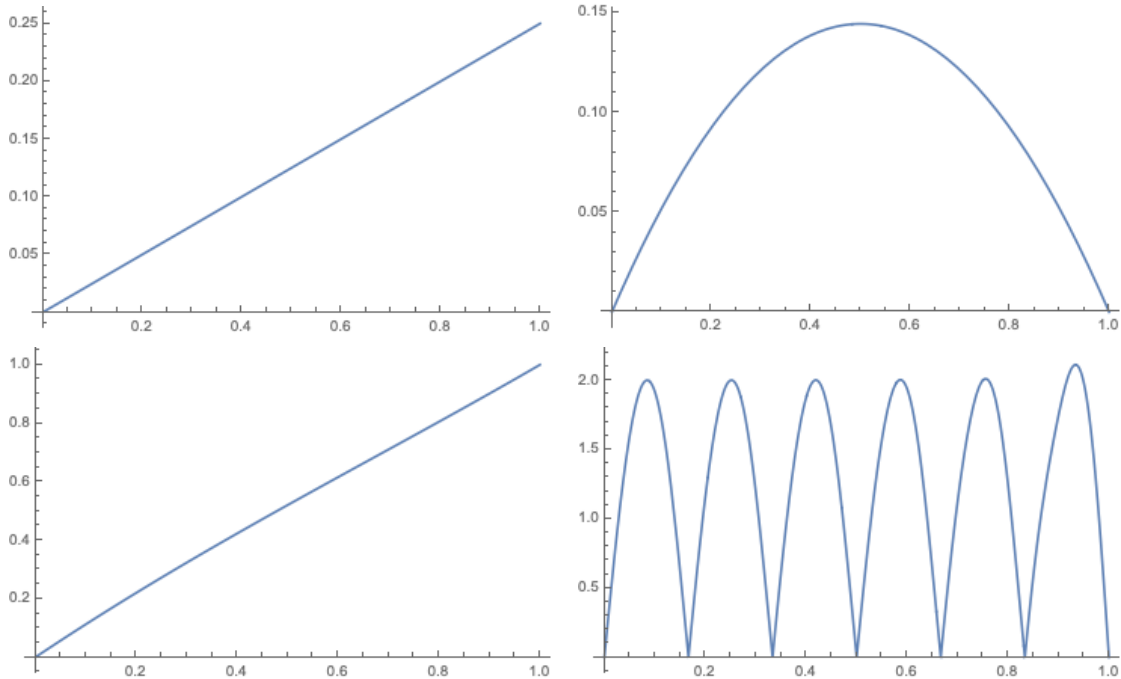


FIGURE 1. Examples of G-variograms  $\gamma_F$ . The four cases show how the shape of  $F$  is reflected in the shape of  $\gamma_F$ . The cases of  $F$  are, left to right, top to bottom: Affine function  $F(x) = 1 + \frac{1}{4}x$ ; Parabolic bump  $F(x) = x(1 - x)$ ; Parabolic bend  $F(x) = 1 - x^2$ ; Sine function  $F(x) = \sin(6(2\pi)x)$ .

406 *Periodic  $F$ .* Let us consider a periodic function,  $F(x) = \sin(k(2\pi)x)$ . In this case,

$$\begin{aligned} (F(v) - F(u + v))^2 &= \left( \sin\left(\frac{2\pi}{k}v\right) - \sin\left(\frac{2\pi}{k}(u + v)\right) \right)^2 \\ &= \left( \sin\left(\frac{2\pi}{k}v\right) - \sin\left(\frac{2\pi}{k}u\right)\cos\left(\frac{2\pi}{k}v\right) + \sin\left(\frac{2\pi}{k}v\right)\cos\left(\frac{2\pi}{k}u\right) \right)^2 \end{aligned}$$

407 *Superposition.* Let us consider the case of superposed functions. The variogram of  $F_1 + F_2$   
 408 appears to be difficult to understand in terms of the separate variograms because there is  
 409 an interaction term:

$$\gamma_{1+2} = \gamma_1 + \gamma_2 + \gamma_{1,2} ,$$

410 where  $\gamma_{1,2}$  is defined by the polarised version of the definition of  $\gamma$ . Figure 2 provides two  
 411 examples of superposed affine and periodic shapes with different relative weights.

412 **3.5. Discussion of the examples.** Let us review the purpose of the exercises above.  
 413 The idea is to motivate the use of variograms with sampled points in the characterization  
 414 of surfaces. Consider a response surface on a given real domain  $A$  (usually a rectangle). A  
 415 measurement is available at each testing points  $\mathbf{x} \in A$ . We want to assess the conformity  
 416 of the shape of the response surface to some standard. For example: “is the surface  
 417 bended in some direction?” Or: “Is there a waviness of a type associate to a specific  
 418 technology?” These are possible defects that cannot be specified in a parametric way.<sup>39</sup>

419 A very popular modeling method relies on the assumption that the surface under study  
 420 is the realization of a random field, for example, a Gaussian random field  $(Z(\mathbf{x}))_{\mathbf{x} \in A}$ . In  
 421 such a case, the observed characteristics of the surface will, in fact, depend on the auto-  
 422 covariance of the random field.

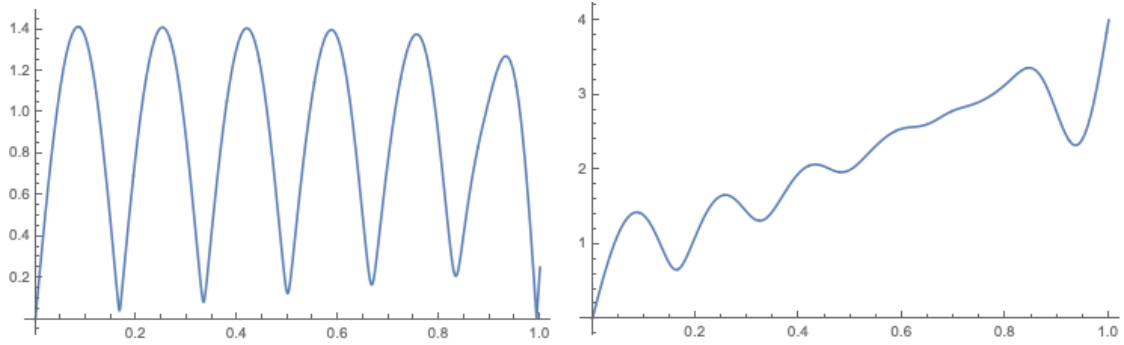


FIGURE 2. Examples G-variogram showing the effect of the superpositions of a linear and a sinusoidal shape:  $F(x) = \frac{1}{4}x + \sin(6(2\pi)x)$  (left) and  $F(x) = 4x + \sin(6(2\pi)x)$  (right).

423 Even if the surface under examination is not random in any physical sense, the examples  
 424 show that one can use the G-variogram to assess some specific features, such as the  
 425 waviness.

426 Moreover, one can perform the prediction of the response at untried points by a  
 427 Bayesian Kriging interpolation based on the elicitation of a covariance. In this case,  
 428 the form of the variogram will suggest the choice of a reasonable and compatible covari-  
 429 ance.<sup>35</sup> That is, knowledge about the variogram provides knowledge about the correlation  
 430 and, in turn, a least square prediction of the response at untried points.<sup>27,36,54</sup> We stress  
 431 that this methodology is not a method of estimation of a correlation, but it is a method  
 432 of elicitation of a Gaussian prior, as it is illustrated in the following section. In fact, the  
 433 empirical variogram is not a bona fide variogram, that is, it does not necessarily satisfy  
 434 the negative-definite condition. For this reason, the associated auto-covariance could be  
 435 negative definite. See, for example, the discussion in Gneiting *et al.*<sup>57</sup> and Stehlik *et*  
 436 *al.*<sup>58</sup> Concerning the latter paper, the authors proved that the probability of choosing a  
 437 negative-definite covariance when dealing with empirical financial data is high. The same  
 438 issue might happen when a sequential design is used in the measurement process, mainly  
 439 when ad hoc software are blindly used to overcome computational features. Therefore,  
 440 possible topics to be investigated are the next-point selection criteria that may look for  
 441 geometric variograms corresponding to positive-definite covariance structure.

442

#### 4. CASE STUDY

443 This section presents a case study to show the effectiveness and the potential of the  
 444 methodologies formerly discussed. A real surface has been densely measured by an areal  
 445 surface topography measuring instrument, achieving a very large set of data ( $10^6$  mea-  
 446 sured points) and the characterization of surface topography has been carried out ac-  
 447 cording to the Standard protocol, as presented in Section 2.1. Then, considering only a  
 448 very small subset (0.4%) of the measured data, a larger number of the surface points has  
 449 been predicted using Kriging and variogram. The set of the predicted points was used for  
 450 characterizing the surface according to the standard protocol. The comparison between  
 451 the parameters obtained according the two ways of approaching the problem is in favour  
 452 of Kriging and suggests final considerations.

453 The standard characterization method is applied through the commercial software  
 454 Mountains Map 7.4.

455 **4.1. Materials and Methods.** Modern industry, within the paradigm of Industry 4.0,  
 456 experiences a constant increase in the demand for flexibility and customization of prod-  
 457 ucts.<sup>18</sup> This has led to the development of innovative manufacturing strategies in the  
 458 production processes to satisfy customer requirements. Additive Manufacturing (AM)  
 459 outstands other solutions for its capability to optimize the design of components and the  
 460 material and energy consumption.<sup>59</sup> Due to its flexibility in a wide range of application,  
 461 we focus on the Fused Deposition Modelling (FDM), i.e. an additive process for poly-  
 462 meric material. The component is manufactured by fusing a wire of material, deposited  
 463 layer-by-layer raster scanning the layer cross-section of the part. Figure 3(a) represents  
 464 a schematic view of the process; Figure 3(b) shows the manufactured specimen with a  
 465 benchmark geometry.

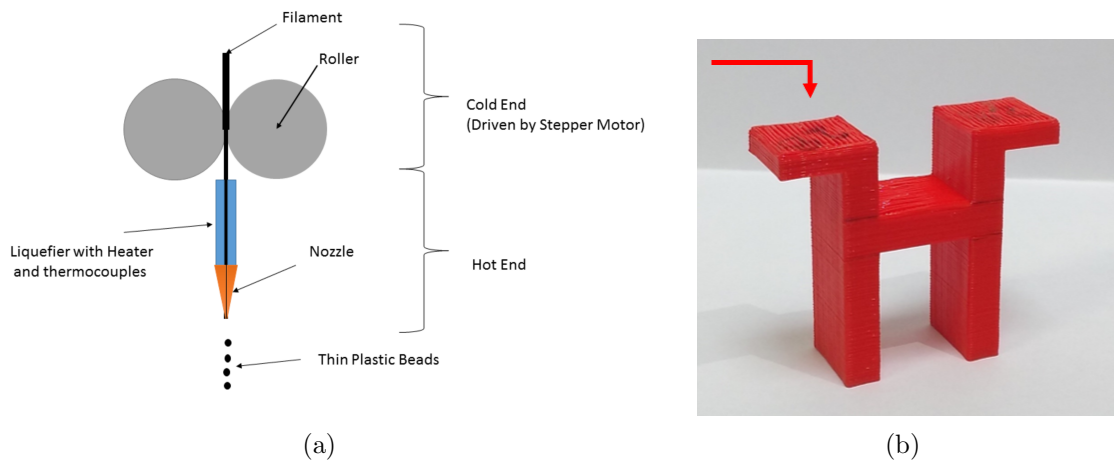


FIGURE 3. (a) Schematic of FDM process and (b) manufactured specimen. The top left surface, indicated by the arrow, has been characterised.

466 The top surface topography of the specimen (indicated by a red arrow) has been mea-  
 467 sured exploiting an area surface topography measuring instrument (Figure 4): Coherence  
 468 Scanning Interferometer (CSI), a Zygo NewView 9000 equipped with a  $20\times$  objective  
 469 and a  $0.5\times$  digital zoom. This instrument provides a high measurement density, with the  
 470 maximum measurement speed, and is a state of the art instrument for the inspection of  
 471 topographies. Thanks to the measurements acquisition capability of the CSI instrument,  
 472 a dense sampling of the surface, with a lateral resolution of  $3.56\ \mu\text{m}$ , was made possible,  
 473 resulting in one million measured points.

## 474 4.2. Results.

475 **4.2.1. CSI measurements.** The surface topography based on the measured points is shown  
 476 in Figure 5, where the manufacturing signature is clearly noticeable as a waviness pattern  
 477 along the  $x$ -axis; also a deviation from planarity can be highlighted, even though at a  
 478 minor extent. The measured topography is consistent with the known manufacturing  
 479 signature of the FDM process, due to the raster scanning approach according to which the  
 480 layers are built; in fact, the signature unfolds in a periodic pattern resembling the adjacent  
 481 deposition of the molten wires of material. Given the high density of the measured points,  
 482 the representation of the surface topography in Figure 5 may be considered faithful to  
 483 the real one. Therefore, the comparison we perform considers that surface as the real  
 484 one and the CSI measurements as the reference to qualify the effectiveness of the Kriging  
 485 method in predicting surface topographies.



FIGURE 4. The CSI Zygo NewView 9000.

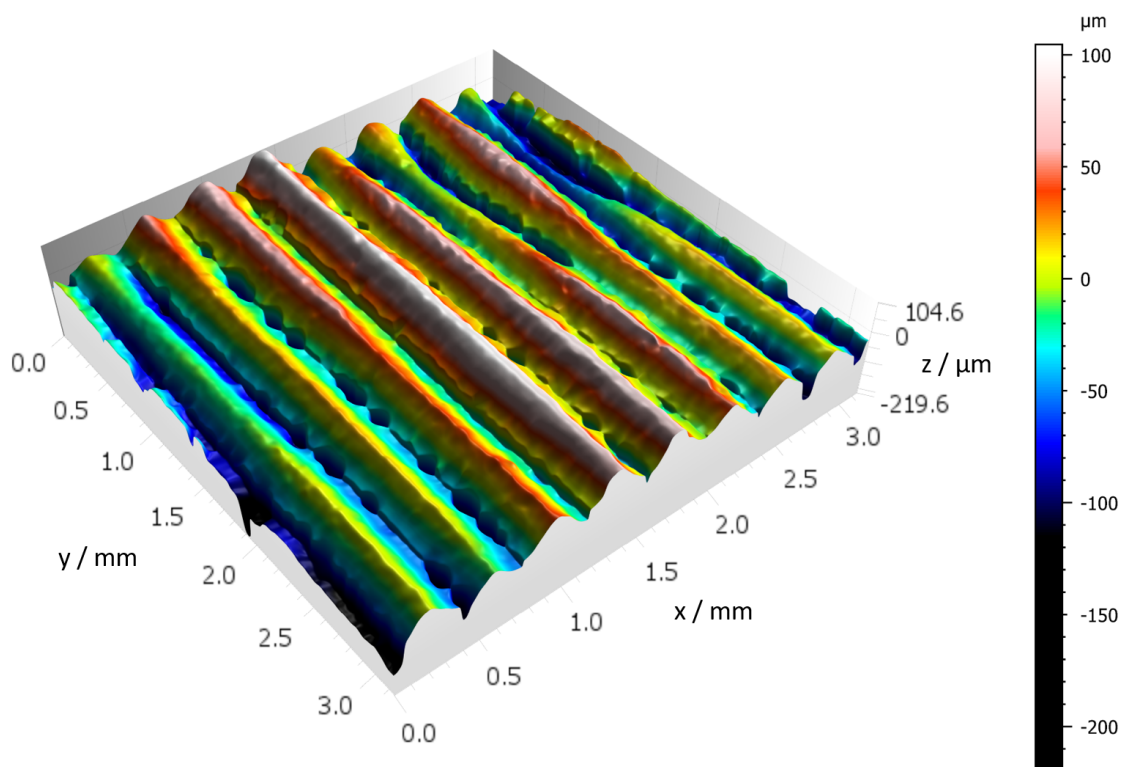


FIGURE 5. 3D plot of the surface topography  $z(x,y)$  measured by the CSI. It may be considered a faithful representation of the real surface topography.

486 To this aim, the main parameters (according to Standard, see Section 2) for the char-  
 487 acterization of the surface texture are computed, using the large data set of CSI measure-  
 488 ments and by means of the commercial software Mountains Map v7.4. As the object of



489 the characterization is the surface texture, the waviness surface, i.e. the S-F surface,<sup>45</sup> is  
 490 considered<sup>i</sup>. The resulting surface texture parameters are in Table 1 and the correspond-  
 491 ing PSD is represented in Figure 6. The first three parameters,  $S_a$ ,  $S_q$  and  $S_z$ , characterize  
 492 the surface heights, highlighting hills and valleys with respect to the reference cartesian  
 493 coordinate plane, set at the average height,  $z = 0$ . The other three parameters,  $S_{al}$ ,  $S_{tr}$   
 494 and  $S_{td}$ , are for the detection of possible anisotropies. The anisotropy of the surface is  
 495 highlighted according to the standard analysis through the isotropy parameter  $S_{tr}$ , that  
 496 relies on the evaluation of  $S_{al}$ .  $S_{tr}$  is 9.5%, definitely less than the conventional threshold  
 497 of 20%, and the texture pattern direction, which describes the direction of the anisotropy  
 498 measured by the parameter  $S_{td}$ , is at  $178^\circ$  (or equivalently at  $-2^\circ$ ) with respect to the  
 499  $x$ -axis. As regards the analysis of the PSD graph, computed as the average of the PSD  
 500 evaluated in all possible directions, it can be noticed the main harmonic i.e. the base  
 501 wavelength, at 0.39 mm. The recognized wavelength is coherent with the surface topog-  
 502 raphy in Figure 5, pointing out the manufacturing signature and its entity. There is a  
 503 second relevant harmonic in close proximity of zero (at 0.027 mm): this feature represents  
 504 the noise content of the surface, due to measurement noise and local random variability  
 505 of the surface.

TABLE 1. Surface texture parameters according to ISO 25178-2:2010, computed on CSI measurement data and by means of the dedicated software MountainsMap

Parameter	$S_a/\mu m$	$S_q/\mu m$	$S_z/\mu m$	$S_{al}/mm$	$S_{tr}$	$S_{td}$
Value	36.1	45.5	326	0.149	9.5%	$178.0^\circ$

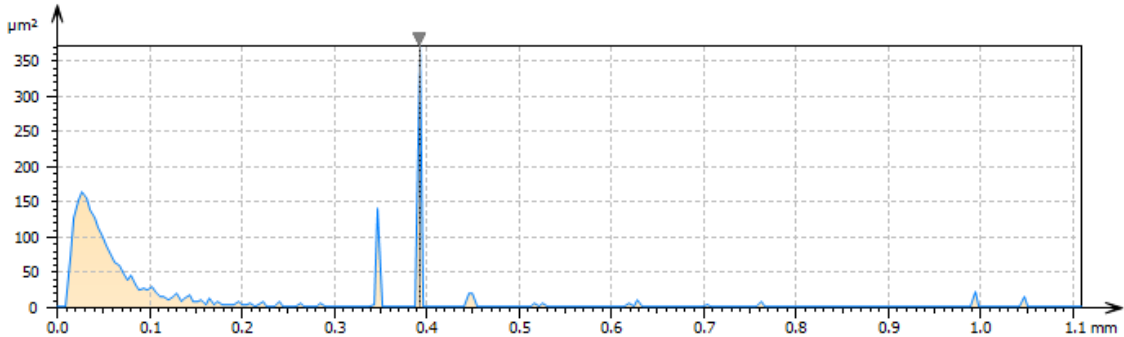


FIGURE 6. Power Spectrum Density of the surface topography according to CSI measurements.

506 4.2.2. *Variogram and Kriging prediction.* Since we aim at proving the adequateness of  
 507 Kriging methodology in increasing the measurement informativeness of slow and low-  
 508 resolution surface measurement instruments (as CMMs and contact styluses), a sample  
 509 from the dense surface set of points measured using the CSI was randomly extracted to  
 510 be used as input of the Kriging prediction model. The sample size was 4,000 points,  
 511 only the 0.4% of the  $10^6$  measured points; this size is meant both to be representative of  
 512 the low-resolution measurement system, simulating a sparse measurement, and to make

<sup>i</sup>The operators sequence involve an S-operator (i.e. a high-pass filter) with cut-off of  $80 \mu m$ , and an F-operator for levelling

513 the comparison more persuasive. In fact, this scenario may also happen in situations in  
 514 which, after a process optimization requiring thorough expensive characterization (e.g.  
 515 based on optical surface topography instruments) and yield reference information about  
 516 the surface, subsequent cheaper online quality controls may be performed using less ex-  
 517 pensive but slower instruments. The choice of the random sampling is aimed at enabling  
 518 inferences on the statistical distribution and properties of the results.

519 As the first step, the empirical variogram (as suggested in Section 3.1) was computed.  
 520 In Figure 7, the variogram cloud and the (omni-directional) variogram, based on the  
 521 Euclidean distance and according to the Matheron's estimator, are represented.

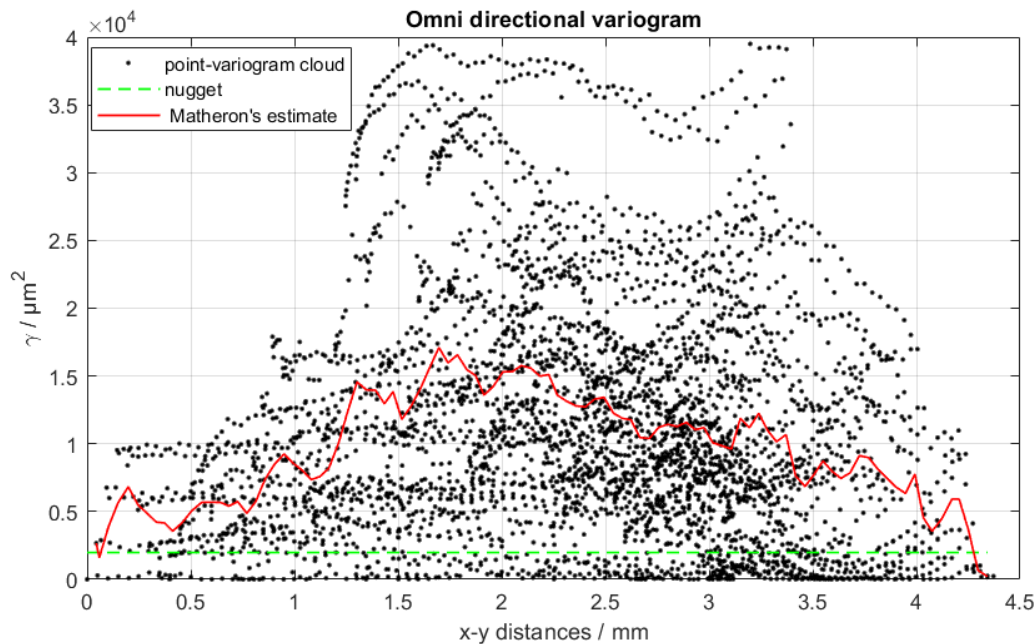


FIGURE 7. Omni-directional variogram cloud and estimated variogram (in red), that suggests the presence of a structured correlation. Its directionality is investigated in Figure 8

522 The variogram exhibits a structured correlation; the behavior due to the sampled points  
 523 significantly and systematically differs from that of a set of points measured on a planar  
 524 surface, without any systematic behavior. In particular, two deviations from planarity  
 525 can be appreciated: a periodic pattern superimposed to a polynomial trend (second-  
 526 order seems suited). Such behavior suggests the presence of a sinusoidal texture and of a  
 527 systematic deviation from planarity that can be generally described by a polynomial of  
 528 at least first order (recall that a quadratic variogram characterizes a linear relationship  
 529 between responses). The variograms along the  $x$ - and  $y$ -axis have been evaluated, to in-  
 530 vestigate the possible presence of anisotropy. These directions have been chosen knowing  
 531 the technological characteristics of the process, which introduces periodicities and struc-  
 532 tured correlations only in orthogonal directions. A pronounced waviness, see Figure 8(a),  
 533 is highlighted by the variogram along the  $x$ - axis; whereas, the variogram along the  $y$ -axis  
 534 in Figure 8(b) does not reveal a departure from the planarity of the surface and there is  
 535 no evidence of any correlation structure. Therefore, the two one-directional variograms  
 536 detect severe anisotropy.

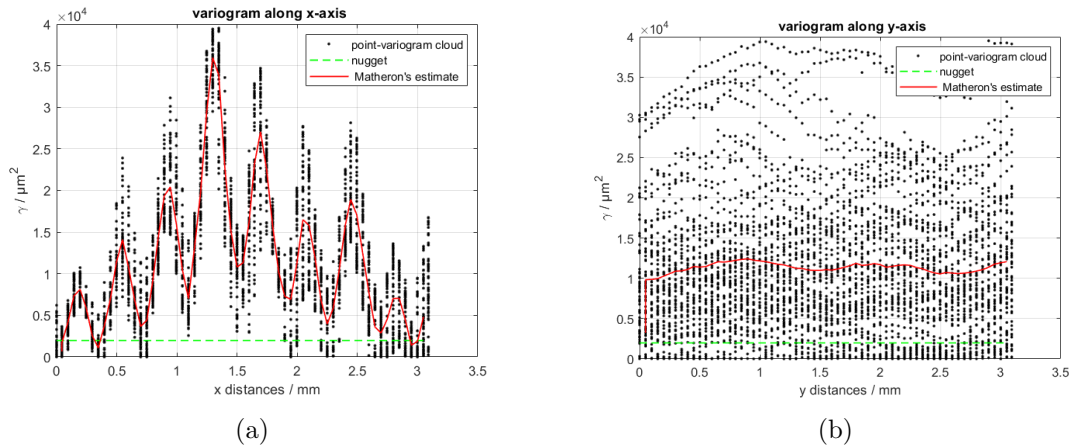


FIGURE 8. Variogram clouds along the (a)  $x$ -axis and (b)  $y$ -axis. In red the correspondent empirical variograms.

537 Relying on these findings, the height of the surface was predicted at 62,500 points  
 538 (representing the 6.25% of the measured points dataset). It should be noted that com-  
 539 putational constraints limited the size of the Kriging prediction set; but it is not so  
 540 small if compared with the starting data set (4,000 points), resulting in about 6.4% the  
 541 percentage of predictor points to predicted ones.

542 Kriking predictions have been computed exploiting the DACE toolbox of MatLab  
 543 2019b, and relying on a supervised procedure to choose the functional form of the spatial  
 544 correlation function. Provided the knowledge of the variogram, a cubic spline function  
 545 has been selected, because, amongst the available ones in the toolbox, it the aptest to  
 546 model a wavy trend. The spatial correlation along the  $y$ -axis was a constant and the over-  
 547 all correlation results from the product of the two.<sup>38</sup> The toolbox, to achieve the Kriging  
 548 prediction, recomputed the spatial correlation based on the sampled points; the model  
 549 caters for anisotropy by differently choosing the spatial correlation function parameters  
 550 for the two spatial directions.

551 The surface topography, obtained with Kriging predictions of the heights, is represented  
 552 in Figure 9. The manufacturing signature due to waviness can still be appreciated along  
 553 the  $x$ -axis direction, despite the poor sampling density. The predicted surface has been  
 554 characterized, considering its points as measured ones, to provide a quantitative compar-  
 555 ison: the surface texture parameters (summarised in Table 2) and the PDS (shown in  
 556 Figure 10), according to the Standard, have been computed.

TABLE 2. Surface texture parameters, of the Kriging-interpolated surface, computed according to ISO 25178-2:2010 by means of the dedicated software MountainsMap.

Parameter	$S_a/\mu m$	$S_q/\mu m$	$S_z/\mu m$	$S_{al}/mm$	$S_{tr}$	$S_{td}$
Value	35.6	44.8	325.5	0.152	10.3%	180.0°

557 Comparing the results in Table 1, based on  $10^6$  measured point with the CSI, with the  
 558 results in Table 2, computed on the predictions based on 0.4% of the mentioned measured  
 559 points, it can be stated that the surface is still correctly characterized as anisotropic with  
 560 the parameter  $S_{tr}$  significantly smaller than 20% and the texture pattern is directed at  
 561  $178.7^\circ$  (i.e.  $-1.3^\circ$ ) with respect to the  $x$ -axis. The main harmonic representing the base

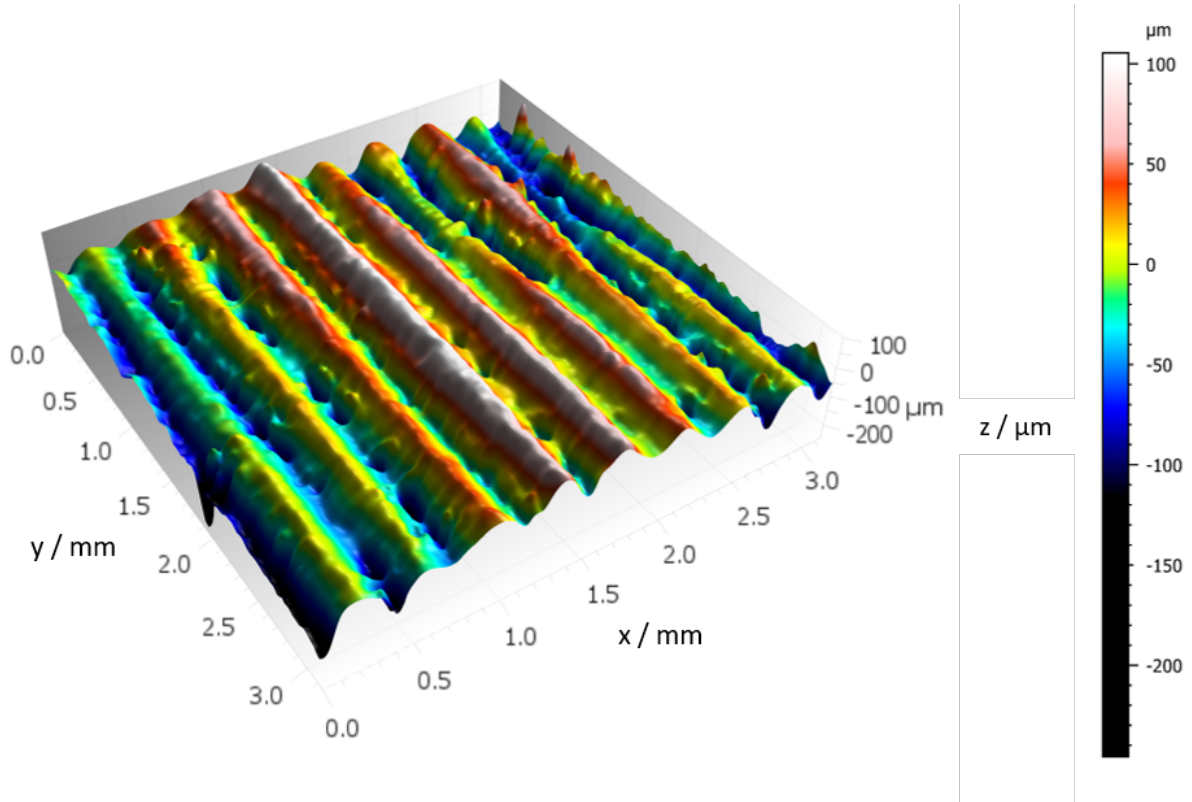


FIGURE 9. 3D plot of the Surface topography  $z(x,y)$  obtained through the application of Kriging. This results has to be compared with Figure 5

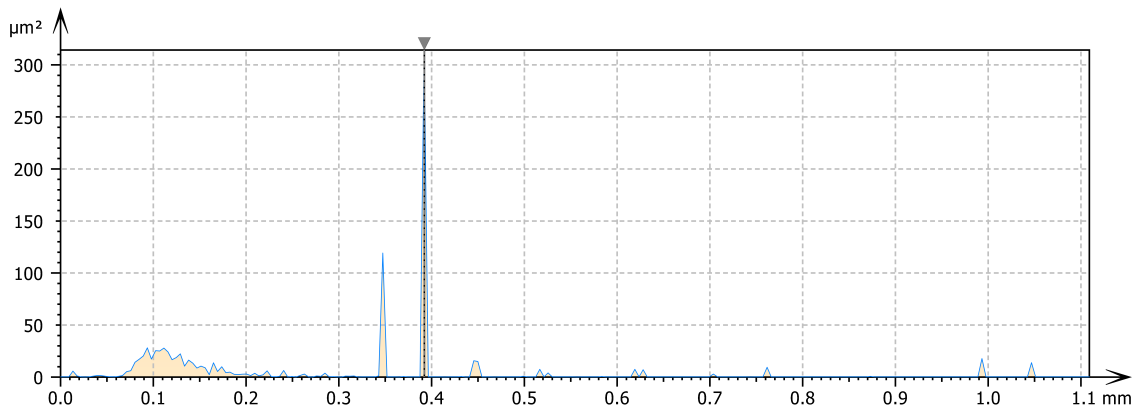


FIGURE 10. Power Spectrum Density of the Kriging-interpolated surface.

562 wavelength is evaluated correctly at 0.39 mm. Due to the interpolation inherent in the  
 563 Kriging, very low scale variation can be only partially captured. In fact, the PSD of the  
 564 interpolated surface shows a peak at 0.1 mm (see Figure 10). This harmonic is near the  
 565 upper bound of the noise frequency of the CSI measured surface (0.027 mm) and shows  
 566 that the procedure based on the Kriging acted as a high-pass filter.

567 A possible way to investigate the nature of the slight differences between the surface  
 568 topography parameters in Table 1 and in Table 2 can be sought in the analysis of the  
 569 interpolation error, shown in Figure 11. Not particular trends can be highlighted, and  
 570 larger errors are at the edges of the investigated domain, which is typical for interpola-  
 571 tion methods.<sup>55,60</sup> Moreover, considering the spectral content of this interpolation error,

572 shown in Figure 12, only one harmonic at 0.021 mm can be noticed, which is not far from  
 573 the noise content of the original dataset, i.e. 0.027 mm.

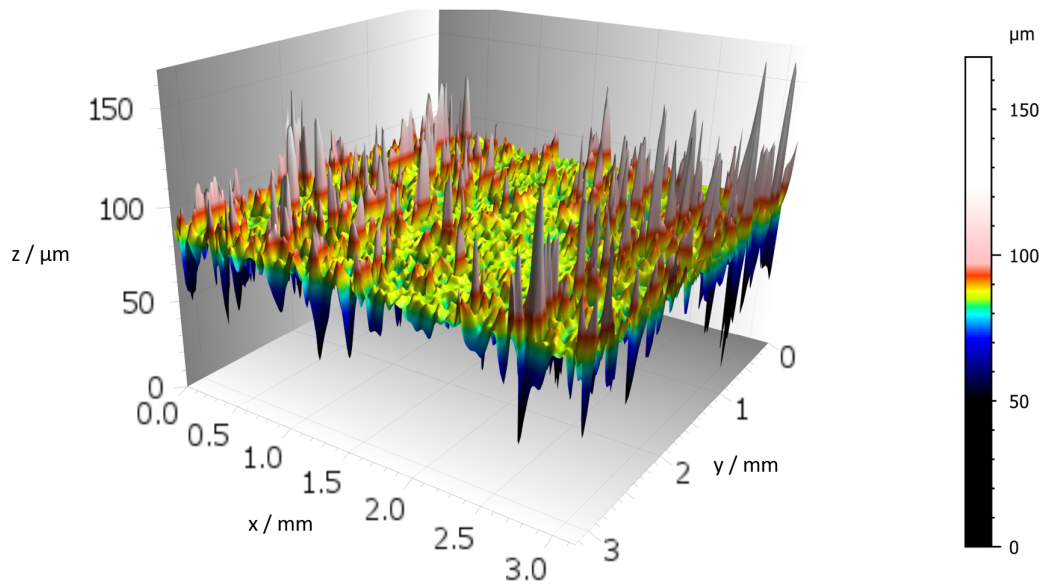


FIGURE 11. Surface topography of interpolation error of the Kriging prediction.

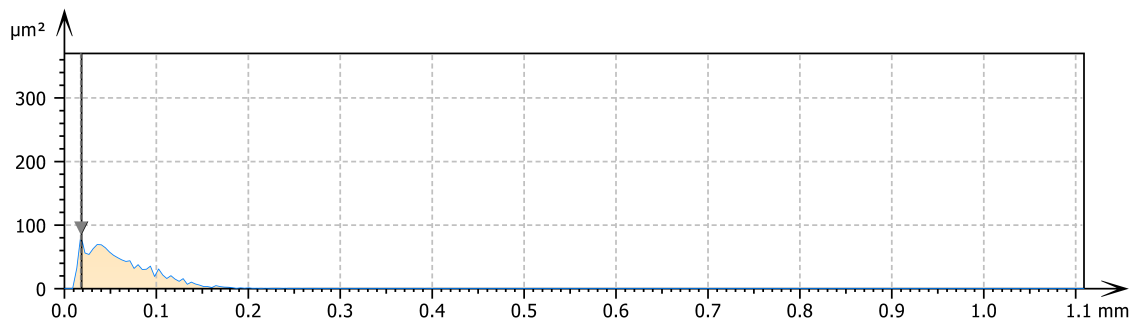


FIGURE 12. Power Spectrum Density of the interpolation error of the Kriging interpolation.

574 The procedure has been repeated 1,000 times, to provide statistical meaningfulness  
 575 to the performed comparison. Each time, a random sample was extracted, the Kriging  
 576 prediction was repeated and, for each prediction, the parameters characterizing the pre-  
 577 dicted surface topography were computed. In Table 3, there are the 2.5% and the 97.5%  
 578 quantiles of the empirical distribution of the parameters. The reference characterization  
 579 values of Table 1 are included in the confidence intervals of Table 3, concluding that the  
 580 differences between the reference characterization values and the ones based on Kriging  
 581 predictions (in Table 2 and formerly discussed) may be considered as not systematic.

582

## 5. CONCLUSIONS AND FINAL REMARKS

583 The issue addressed in this paper is the surface topography form measurement and  
 584 verification. The standards provide several indices in order to detect possible technolog-  
 585 ical errors and signatures in the parts. In this work, we adopted the ordinary Kriging  
 586 model, which proved to be effective in predicting geometrical errors in manufacturing,

TABLE 3. The 2.5% quantile and 97.5% quantiles of the surface texture parameters distribution, evaluated on the Kriging-interpolated surfaces obtained evaluated through the 1000 random independent samples. Computations have been carried out according to ISO 25178-2:2012 by means of the dedicated software MountainsMap

Parameter	$S_a/\mu m$	$S_q/\mu m$	$S_z/\mu m$	$S_{al}/mm$	$S_{tr}(\%)$	$S_{td}(\circ)$
2.5% quantile	35.2	44.4	258.3	0.143	9.5	177.0
97.5% quantile	36.2	45.8	397.4	0.154	11.2	180.0

587 and the variograms for modelling a possible correlation between the sampled points of the  
588 measured surface, according to geostatistic practices for very noisy data. The comparison  
589 between the Standard measurement approach and the Kriging methods was based both  
590 on theoretical insights about the use of the variogram in case of random sampling and  
591 on a case study based on real measurements where random sampling and Kriging predic-  
592 tions are used. The Kriging methodology proved effective in predicting surface textured  
593 patterns, even if it was based on a set of sparse economic measurements. The result of  
594 Kriging interpolation, once characterized according to the Standard procedure, yielded  
595 information consistent with denser and more expensive measurement approaches. The  
596 current challenges of Industry 4.0 for surface texture characterization, hereby including  
597 freeform surfaces and additive surface, require an extremely long time, and hence high  
598 costs, to achieve an adequate and representative measurement by means of traditional  
599 devices. The SMEs would have to purchase extremely expensive new equipment (typi-  
600 cally optical instruments) or to invest a consistent amount of time for quality assessments  
601 using the traditional one, to cope with technological challenges enforced by the current  
602 industrial framework. Thus, the adoption of the empirical variogram in detecting corre-  
603 lation structure as well as Kriging prediction can be considered adequate tools to achieve  
604 informativeness from sparse and cheap set of measurements statistically. Moreover, we  
605 consider our finding as an encouraging preliminary step to be used as a guide for further  
606 developments in detecting anomalies, obtaining definitive practical advantages for SMEs.  
607 Future work shall address the application of these tools for process control. A typical  
608 scenario may be the application of Kriging method for in-line process control with contact  
609 probes based on control limits set on the basis of reference surface topography measure-  
610 ments performed by optical devices. The software implementing the Kriging prediction  
611 can be straightforwardly incorporated into the CMM computer control, and it can run in  
612 real time; being the automation of the Kriging predictions quite inexpensive, it is possi-  
613 ble to predict the surface texture over a tight grid, also providing a quantification of the  
614 uncertainty on the basis of the MSPE.

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