GEOSTATISTICS: PAST, PRESENT, AND FUTURE

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Summary

Geostatistical analyses were first developed in the 1950's as a result of interest in areal or block averages for ore reserves in the mining industry. Today, variogram estimation and spatial prediction (kriging) span all sciences where data exhibit spatial correlation. Theoretical properties of the spatial process are addressed under the distribution-free and likelihood-based perspectives. Strengths and weaknesses of these two dominant methodologies for modeling spatial correlation and predicting responses at unsampled sites and areal units are explored. Examples of hot spot detection and areal prediction show the flexibility of the Bayesian paradigm. Current bottlenecks and future directions in the field of geostatistics are discussed.

1. Introduction

The science of geostatistics has grown tremendously from its mining roots approximately 50 years ago to encompass a wide range of disciplines. Olea (1991, p. 31) defines geostatistics as "the application of statistical methods … for use in the earth sciences, particularly in geology". Geostatistical analyses are employed in fields where the data are viewed as (essentially) point observations and prediction (at unsampled sites or at areal units) is desired. Today, geostatistical studies are conducted with hydrological data (Rouhani and Myers, 1990; Kitanidis, 1996), in mining applications (Kelker and Langenburg, 1997; Schuenemeyer and Power, 2000), air quality studies (Guttorp, Meiring and Sampson, 1994; Krajewski, Molinska and Molinska, 1996), soil science data (Webster and Oliver, 1992; Raspa and Bruno, 1993), biological applications (Ecker and Gelfand, 1999; Ritvo, Sherman, Lawrence and Samocha, 2000), economic housing data (Basu and Thibodeau, 1998; Gelfand, Ecker, Knight and Sirmans, 2003), and constructing environmental monitoring networks (Wikle and Royle, 1999).

One purpose of this chapter is to acknowledge the fundamental contributions of two pioneers in geostatistics, D. G. Krige and G. Matheron, who formulated the underpinnings of geostatistics and kriging approximately 40 years ago. This chapter will not focus much on the history of geostatistics; other authors, in particular, Cressie (1990), have already retraced its history quite well. Rather, this author presents his perspective on the current status of the science of geostatistics. What are the strengths and weaknesses of the dominant methodologies used in undertaking such an analysis? What are the bottlenecks that current researchers are encountering? What is the future for the field of geostatistics?

Mining variables such as deposits of ore are often highly concentrated in veins. When these data are collected at locations or sites at a fixed time, a purely spatial analysis revolves around the tendency for pairs of sites closer in space (distance and possibly orientation) to have more similar responses than that for pairs further apart, i.e., the data exhibit spatial correlation. Predicting block ore grades (prediction of an areal block average) from a sample taken at point support was of primary interest to D. G. Krige in the 1950's. Krige predicted areal gold concentrations in South Africa based on large amounts of data which exhibited strong positive correlation (Cressie, 1990, p. 246). In honor of D. G. Krige's contribution, G. Matheron coined the term *kriging* to refer to (optimal) prediction of responses at unsampled locations. Matheron (1963) is first to publish a detailed exposition on geostatistics and kriging. He recognized that prediction is only one component of the analysis and should not be viewed as the only goal of a geostatistical analysis. As with any statistical analysis, the quality of the geostatistical prediction depends upon how well the postulated model explains the observed data.

In this spirit, two fundamental goals exist in the analysis of clustering or spatially correlated data. First, accurately explain the clustering mechanism, i.e., develop a model for the correlation structure. Second, use this proposed model to predict responses at unsampled locations or at areal units. Standard statistical techniques (such as ordinary least squares regression) fail to incorporate the clustering effect that spatial data tend to exhibit. In fact, many statistical analyses ignore the geographic coordinates altogether in treating the data as an independent and identically distributed sample rather than one (spatially correlated) vector of observations.

At the explanation stage, one needs to accurately model the spatial correlation structure. The primary method of extracting this spatial clustering is through the variogram. The variogram is at the heart of geostatistics. It expresses the variability of pairs of spatially indexed observations as a function of their separation vector. For a particular spatial region $D \subseteq \mathbb{R}^n$, where n is the dimension of the s vector which consists of the geographic coordinates for a particular location. In most practical cases, it is either two or three dimensional; however, in the present chapter it is denoted as an n × 1 vector, one needs to address two basic questions: does the spatial process underlying the observed data in the region exhibit spatial correlation and if so, is this correlation equally strong (at a fixed distance) in every direction? If the answer is yes to both questions, then the spatial process is isotropic. There is an enormous body of literature whose focus is variogram modeling for isotropic spatial processes. Cressie (1993), Wackernagel (1998) and Stein (1999) are excellent current references. Under isotropy, the variogram or the spatial correlation is only a function of the Euclidean distance

between sites. In addition, techniques for studying the most common departure from isotropy shall be discussed.

At the prediction stage, the standard technique of kriging incorporates the association structure (the variogram) to optimally solve a system of linear equations which predict the value at an unsampled location. Kriging produces the best linear unbiased predictor (BLUP) for the unsampled site. It maintains two distinct advantages over other interpolation techniques such as inverse distance weighting. First, standard interpolation techniques do not include any information about the spatial correlation structure. Secondly, kriging allows a prediction variability estimate to assess, under certain conditions, its prediction accuracy. Methodologies for predicting responses at unsampled sites and areal units shall be explored.

The primary modeling decision for geostatistical analyses involves choosing either the parametric family of distributions from which the responses arise or to take a distribution-free approach. While not choosing a sampling distribution for the observed data has certain advantages, it does induce limitations in the resulting statistical inference. Under the parametric or likelihood-based approach, a Gaussian random field is traditionally assumed, partly for convenience and partly for the flexibility that this family offers; however, many environmental responses are binary or positive with right-skewed distributions (such as water pollution concentrations). In the latter case, lognormality is often assumed as a default option, but other transformations to normality can be employed.

This chapter is organized as follows. Section 1 is the introduction. Section 2 outlines the distribution-free geostatistical methodology and examines its strengths and weaknesses while section 3 does the same for the parametric or likelihood-based techniques. Section 4 explores model based prediction of unsampled locations and of areal blocks. Finally, Section 5 outlines some future directions in the field of geostatistics.

2. Distribution-Free Methodology

The observed data, $Y(\mathbf{s}_i)$, $i = 1,...,N$, are collected at N locations or sites $\mathbf{s}_i \in D \subseteq \mathbb{R}^n$. Theoretical assumptions such as ergodicity, stationarity, isotropy, continuity and differentiability of the random field, the population (sampling) distribution, and prior distributions for various components are customarily developed for features of the underlying spatial process, $Y(\mathbf{s})$. These assumptions are needed to validate statistical inference, however, they tend to be difficult to verify given only the observed data.

The first assumption is that of *ergodicity*, which allows inference to proceed using only one (vector) replicate. By making this ergodicity assumption (Zhan, 1999), one uses spatial averages (those formed by averaging responses over sites in the region, *D*) in lieu of probabilistic or ensemble averages (those formed by averaging over multiple (vector) realizations of the spatial process). Unfortunately, the observed data cannot be used to check the validity of the ergodicity assumption (see Myers, 1989, pp. 351-352).

Much of the focus of geostatistics centers on developing models for the correlation structure of the observed data. The concepts of stationarity (both *intrinsic* and *second-order stationarity*) and isotropy provide theoretical underpinnings for modeling the local source of variability. Intrinsic stationarity assumes that for arbitrary locations $\mathbf{s}$ and $\mathbf{s}^*$ in D,

$$
\begin{aligned}
\mathrm{E}(Y(\mathbf{s}) - Y(\mathbf{s}^*)) &= 0 \\
\mathrm{Var}(Y(\mathbf{s}) - Y(\mathbf{s}^*)) &= 2\gamma(\mathbf{s} - \mathbf{s}^*)
\end{aligned}
\tag{1}
$$

where $2\gamma(\mathbf{s} - \mathbf{s}^*)$ is the *variogram* and $\gamma(\mathbf{s} - \mathbf{s}^*)$ is the *semivariogram*. Stationarity assumes that the mean and variance of the spatial process, $Y(\mathbf{s})$, do not depend on the exact locations $\mathbf{s}$ and $\mathbf{s}^*$; the mean is assumed constant and the variability only depends on the separation vector, $\mathbf{s} - \mathbf{s}^*$ (i.e., the spatial process, $Y(\mathbf{s})$, is translation invariant). If the spatial variability for a fixed distance in all directions is the same (i.e., the spatial process has rotational invariance), then the spatial process is *isotropic* and $2\gamma(\mathbf{s} - \mathbf{s}^*) = 2\gamma(\|\mathbf{s} - \mathbf{s}^*\|) = 2\gamma(d)$ where d is the Euclidean distance between sites $\mathbf{s}$ and $\mathbf{s}^*$. A stronger form of stationarity (second-order or weak) assumes that (Matheron, 1963),

$$
\begin{aligned}
\mathrm{E}(Y(\mathbf{s})) &= \mu \\
\mathrm{Cov}(Y(\mathbf{s}), \ Y(\mathbf{s}^*)) & \\
= C(\mathbf{s} - \mathbf{s}^*) &< \infty
\end{aligned}
\tag{2}
$$

where, under isotropy, $C(\mathbf{s} - \mathbf{s}^*) = C(d) < \infty$. Smith (1996) defines a process to be *homogeneous* if it satisfies both isotropy and second-order stationarity.

Cressie (1988) demonstrates that the class of intrinsically stationary spatial processes strictly contains those of second order, i.e., C determines the variogram 2γ. However, 2γ does not determine C, since stationary increments for $Y(\mathbf{s}) - Y(\mathbf{s}^*)$ do not imply that $Y(\mathbf{s})$ is stationary. In such case, $C(0)$ need not exist, hence the variogram is theoretically unbounded. Under homogeneity, the relationship between the variogram and the correlation structure is given by $2\gamma(d) = 2(C(0) - C(d))$.

In practice, the assumption of stationarity is difficult to verify since it is put on the stochastic process, not on any realizations of process, i.e., the data. For example, the sample or data based (empirical) variogram is always bounded in practice, since it is a function of real data; however, if these data are realizations of a Brownian motion (see Cressie, 1993, p. 68), then the underlying theoretical variogram is linear, which is unbounded. Furthermore, one might potentially want to model the spatial locations in

the mean and covariance structures of (2), however, identifying which component (or both) exhibits nonstationarity is not easily determined. "One person's deterministic mean structure is another person's correlated error structure" (Cressie, 1993 p. 114).

A convenient parameterization of the correlation structure in (2) is $C(d) = \tau^2 + \sigma^2 \rho(\boldsymbol{\varphi}, d)$ where ρ is a valid correlation function and τ^2, σ^2 and $\boldsymbol{\varphi}$ are model parameters. Note that $\boldsymbol{\varphi}$ is a vector of model parameters that control the strength of spatial correlation and/or the smoothness of the resulting prediction of the spatial process (continuity and differentiability of the random field). The class of all valid correlation functions in $\mathbb{R}^n$ may be expressed through Bochner's Theorem (see Cressie, 1993, p. 84). Ecker and Gelfand (1997, p. 351) provide several one parameter correlation functional forms, $\rho(\phi, d)$, commonly found in geostatistical analyses. Figure 1 displays their corresponding semivariograms. The exponential, Gaussian, rational quadratic (Cauchy) and spherical are monotonic correlation functions while the Bessel is a dampened sinusoidal correlation structure.
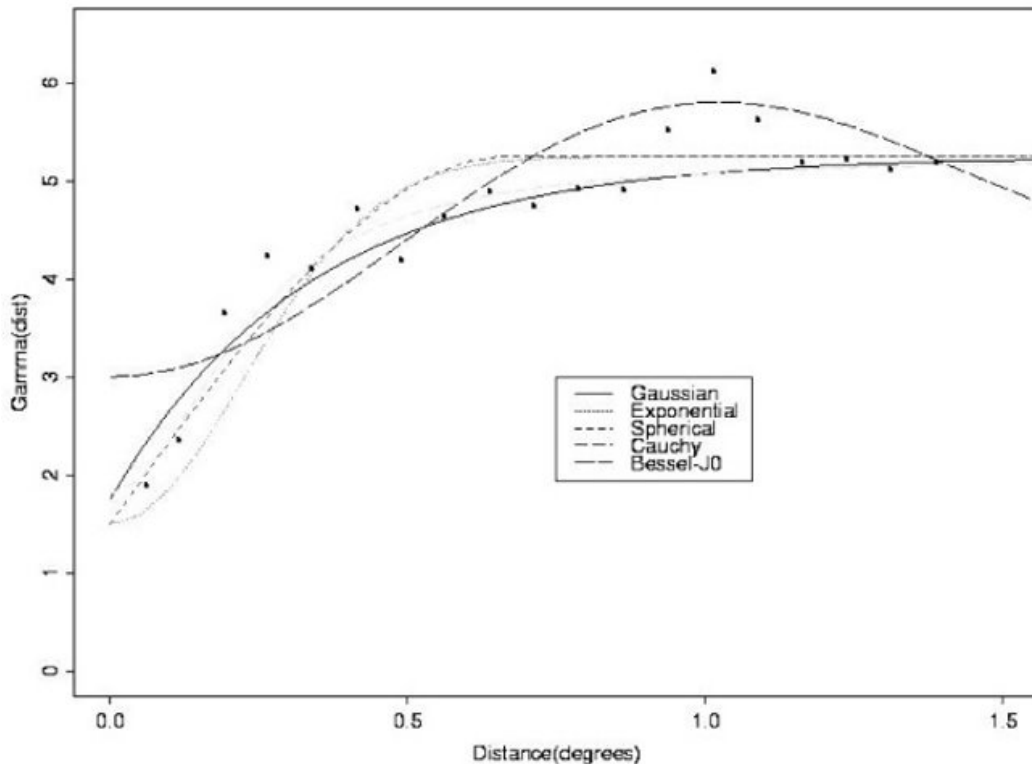

Figure 1 : Five commonly used semivariograms in geostatistical analyses.

Common two parameter monotonic correlation structures include the Matern and general exponential. The Matern correlation function (Matern, 1986) is defined for $\boldsymbol{\varphi} = (v, \varphi)'$ as

$$\rho(\boldsymbol{\varphi}, d) = \frac{1}{2^{v-1}\Gamma(v)}(\varphi d)^v K_v(\varphi d) \tag{4}$$

where $v \geq 0$, $\varphi > 0$, $\Gamma(\cdot)$ is the standard gamma function and $K_v(\cdot)$ is a modified Bessel function of the third kind of order v (Abramowitz and Stegun, 1965). The shape of the postulated variogram near the origin controls the differentiability of the random field, which dictates the smoothness of the resulting spatial prediction. For the Matern model, the parameter v controls the smoothness of the associated random field; $v \geq 0$ ensures continuous realizations and realizations are $\lozenge(v-1)$ times (mean square) differentiable where $\lozenge$ is the integer ceiling function (Handcock and Stein, 1993, p. 406). Special cases of the Matern correlation function include the exponential ($v = \frac{1}{2}$) and the Gaussian ($v \to \infty$). Fortran code that evaluates the Matern correlation function (for use with, for example, Compaq Visual Fortran Professional version 6.5 - including IMSL) is included in the appendix. The general exponential correlation function is defined for $\boldsymbol{\varphi} = (\alpha, \varphi)'$

$$\rho(\boldsymbol{\varphi}, d) = \exp(-\varphi d^\alpha) \tag{5}$$

where $0 < \alpha \leq 2$ and $\varphi > 0$. Special cases of the general exponential correlation structure include the exponential ($\alpha = 1$) and the Gaussian ($\alpha = 2$). Though (5) may be computationally easier to work with than (4), less appealing sample function behavior results. For $\alpha < 2$, continuous, but nondifferentiable realizations are obtained and when $\alpha = 2$, analytic realizations are observed. So, excluding $\alpha = 2$, the general exponential correlation structure places no mass on differentiable realizations, which induces fairly rough prediction over the region.

Adopting the Matern correlation structure in preference to the general exponential because of increased differentiability is a mechanistic decision. While Stein (1987) shows that the shape of the variogram near the origin (the derivative of the variogram approaching the origin) can be consistently estimated, the strong correlation between v and φ for the Matern model would require an enormous amount of data near the variogram origin, i.e., at close spatial resolution, to discern the true underlying smoothness of the spatial process. As an illustration, Figure 2 provides a fairly smooth, twice differentiable Matern model ($v = 2.5$) which is nearly indiscernible, in particular near the variogram origin, from a non-differentiable general exponential model.

Under homogeneity, the theoretical variogram is bounded and the *sill* of the variogram is $\lim d \to \infty \; 2\gamma(d) = 2(\tau^2 + \sigma^2)$ which represents the theoretical variance of the spatial process. Some monotonically increasing variogram forms, such as the spherical, achieve their sill exactly i.e. for finite d, while others (exponential, Gaussian and Cauchy or rational quadratic) reach their sills asymptotically. For monotonic variograms that reach their sill exactly, the *range* is defined to be the distance at which the variogram reaches its sill or equivalently the distance at which $\rho(\boldsymbol{\varphi}, d)$ becomes

zero. Hence, responses at sites separated by distances greater than the range are spatially uncorrelated. For asymptotically silled variograms, two points will only be spatially uncorrelated in the limit as $d \to \infty$. In such case, one identifies the *effective range*, a concept that is not uniquely defined. Two possible definitions are noted; one facilitates interpretation in the variogram space of the process and the other in the correlation space. The first (McBratney and Webster, 1986, p. 623) defines the effective range, r_C, as the distance where the variogram reaches $2(\tau^2 + 0.95\sigma^2)$. Thus, the effective range r_C is achieved when the spatial correlation of the process diminishes to 5%. Mathematically, r_C solves $\rho(\varphi, d = r_C) = 0.05$. A second definition (Cressie, 1993, pp. 67-68) of the effective range, r_V, is the distance at which the variogram reaches 95% of its sill. Then, r_V solves $\rho(\varphi, d = r_V) = 0.05\left(\dfrac{\tau^2 + \sigma^2}{\sigma^2}\right)$.

Note that r_V would not exist if $\left(\dfrac{\tau^2 + \sigma^2}{\sigma^2}\right) > 20$, but this would be unlikely in practice.

For the one parameter, asymptotically silled variograms given in Figure 1, the relationship between the scalar correlation parameter ϕ and the effective ranges r_C and r_V are presented in Table 1. It is obvious that $r_V \leq r_C$ with equality if $\tau^2 = 0$. Many authors adopt r_C and parameterize ϕ to be the effective range r_C. Henceforth, the term range shall refer to either the effective range or the exact range. For the dampened sinusoidal Bessel variogram and other non monotonic variograms, the range is not defined. The *nugget* of the variogram is $\lim d \to 0 \ \ 2\gamma(d) = 2\tau^2$ which need not be zero due to measurement error and/or a microscale effect resulting from extrapolation of the variogram from the minimum sampled distance, $\min \ d$, to the origin.
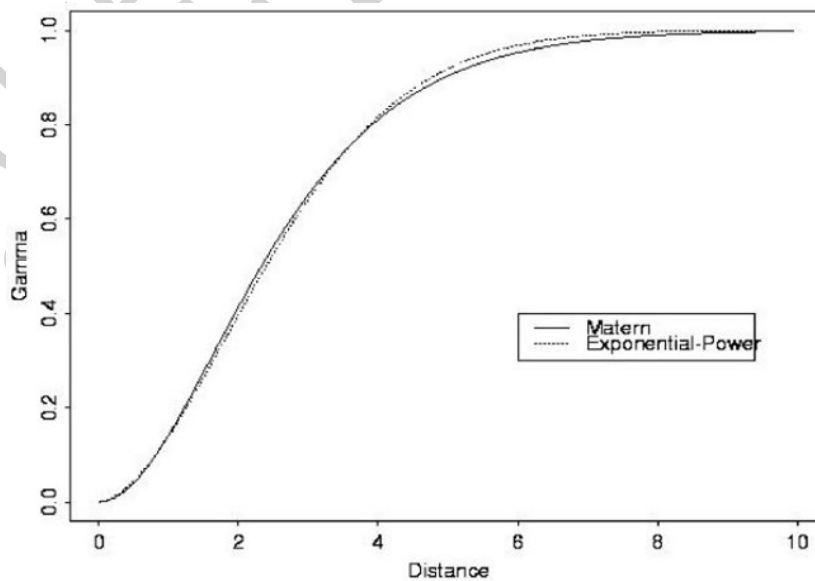

Figure 2: Illustrative comparison of Matern and general exponential variograms.

Correlation Structure	$\rho(\boldsymbol{\varphi},d)$	r_C	r_V
Exponential	$\exp(-\phi d)$	$\frac{3}{\phi}$	$\dfrac{3-\log\left(\frac{\tau^2+\sigma^2}{\sigma^2}\right)}{\phi}$
Gaussian	$\exp(-\phi d^2)$	$\sqrt{\frac{3}{\phi}}$	$\sqrt{\dfrac{3-\log\left(\frac{\tau^2+\sigma^2}{\sigma^2}\right)}{\phi}}$
Cauchy	$\frac{1}{1+\phi d^2}$	$\sqrt{\frac{19}{\phi}}$	$\sqrt{\dfrac{19\sigma^2-\tau^2}{\phi(\tau^2+\sigma^2)}}$

Table 1: Range definitions for monotone asymptotic correlation functions

Fitting semivariogram models under the distribution-free methodology can be viewed as a curve fitting exercise. For each of the $\frac{N(N-1)}{2}$ pairs of observed locations s_i and s_j in D, a collective plot of each Euclidean distance, d_{ij}, versus $\frac{1}{2}\left(Y(s_i)-Y(s_j)\right)^2$, a point estimate of the variability for the pair, is the *semivariogram cloud*. The Matheron (1963) estimator of the semivariogram,

$$\gamma_k^*(d_{ij}) =$$
$$\frac{1}{2N_{B_k}} \sum_{(i,j):d_{ij}\in B_k} \left(Y(s_i)-Y(s_j)\right)^2 \tag{3}$$

smoothes the semivariogram cloud by aggregating distances into K sets $B_1,B_2,...,B_K$ where $B_k=d_{ij}:b_{k-1}\le d_{ij}<b_k$ for constants b_{k-1} and b_k, $k=1,...,K$ with $b_0=0$. The constants b_k are typically chosen to be $k\cdot\eta$ where η is the *lag* or width of each distance bin B_k. A plot of γ_k^* versus the midpoint of the interval (b_{k-1},b_k) or the average distance of all $d_{ij}\in B_k$ for $k=1,...,K$ is called the Matheron *empirical semivariogram*. Figure 1 displays the five aforementioned correlation functions overlaid on the Matheron empirical semivariogram for a dataset of scallop catches. Other variogram estimators exist (see Genton, 1998, pp. 328-330; Ecker and Gelfand, 1997, p. 361), however, use of the Matheron estimator is ubiquitous.

Since a correlation matrix must be positive definite (the associated variogram must be conditionally non-negative definite), only certain functions are allowable to model variograms. Hence, a valid theoretical variogram model (such as those from Figure 1) is typically fitted to the Matheron semivariogram by techniques (Cressie, 1993, section

2.6) such as least squares, generalized least squares or fitting by inspection. The standard variogram fitting algorithm of Cressie (1985) uses a weighted least squares procedure. However, it fails to account for the correlation of the empirical variogram values at two distinct lags, since the same $Y(s_i)$ would typically appear multiple times both within the same variogram lag and across several different lags. Genton (1998) has proposed an algorithm that closely approximates the correlation structure of the variogram at two distinct lags. In addition, by using the variogram cloud, Müller (1999) employs the exact variogram correlation structure to develop an iterative fitting algorithm.

The distribution-free approach to variogram fitting is widely used. Its principal advantage over parametric or likelihood-based methods, including a fully Bayesian approach, is that for variogram parameter estimation and subsequent spatial prediction, one only needs intrinsic stationarity, not some distributional assumption for $Y(s)$. Not assuming a distribution for $Y(s)$ is appealing; however, it does introduce some limitations. First, parameter estimation is not invariant to the lag choice η or equivalently to the choice of sets B_k (see Curriero and Lele, 1999). Thus, it is possible to arrive at quite different parameter estimates for the same model using different lag values. To mitigate the lag invariance criticism, Webster and Oliver (1992) suggest gathering over 150 samples. For an isotropic spatial process, McBratney and Webster (1986, p. 630) claim that if the lag is small then the smoothing or regularization of the variogram "is small enough to be ignored". Many ad hoc rules exist in the distribution-free methodology (see Lamorey and Jacobson, 1995, pp. 331-332). For example, Journel and Huijbregts (1978) suggest only using sets B_k where N_{B_k} is greater than 30 and discarding sets B_k where $b_k > \dfrac{\max\ (d_{ij})}{2}$ because the variogram tends to be erratic for higher lags.

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