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Standard Guide for Selection of Simulation Approaches in Geostatistical Site Investigations¹

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INTRODUCTION

Geostatistics is a framework for data analysis, estimation, and simulation in media whose measurable attributes show erratic spatial variability yet also possess a degree of spatial continuity imparted by the natural and anthropogenic processes operating therein. The soil, rock, and contained fluids encountered in environmental or geotechnical site investigations present such features, and their sampled attributes are therefore amenable to geostatistical treatment. Geostatistical simulation approaches are used to produce maps of an attribute that honor the spatial variability of sampled values. This guide reviews criteria for selecting a simulation approach, offering direction based on a consensus of views without recommending a standard practice to follow in all cases.

1. Scope

- 1.1 This guide covers the conditions that determine the selection of a suitable simulation approach for a site investigation problem. Alternative simulation approaches considered here are conditional and nonconditional, indicator and Gaussian, single and multiple realization, point, and block.
- 1.2 This guide describes the conditions for which the use of simulation is an appropriate alternative to the use of estimation in geostatistical site investigations.
- 1.3 This guide does not discuss the basic principles of geostatistics. Introductions to geostatistics may be found in numerous texts including Refs (1-3).²
- 1.4 This guide is concerned with general simulation approaches only and does not discuss particular simulation algorithms currently in use. These are described in Refs (4-6).
- 1.5 This guide offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience and should be used in conjunction with professional judgment. Not all aspects of this guide may be applicable in all circumstances. This ASTM standard is not intended to represent or replace the standard of care by which the adequacy of

a given professional service must be judged, nor should this document be applied without consideration of a project's many unique aspects. The word "Standard" in the title of this document means only that the document has been approved through the ASTM consensus process.

2. Referenced Documents

2.1 ASTM Standards:³

D653 Terminology Relating to Soil, Rock, and Contained Fluids

D5549 Guide for The Contents of Geostatistical Site Investigation Report (Withdrawn 2002)⁴

D5922 Guide for Analysis of Spatial Variation in Geostatistical Site Investigations

D5923 Guide for Selection of Kriging Methods in Geostatistical Site Investigations

3. Terminology

- 3.1 Definitions of Terms Specific to This Standard:
- 3.1.1 *conditional simulation*, *n*—a simulation approach where realizations of the random function model are constrained by values at sampled locations.
- 3.1.2 *drift*, *n*—*in geostatistics*, a systematic spatial variation of the local mean of a variable, usually expressed as a polynomial function of location coordinates.

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² The boldface numbers in parentheses refer to a list of references at the end of the text.

³ For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

⁴ The last approved version of this historical standard is referenced on www.astm.org.

- 3.1.3 *field*, *n*—*in geostatistics*, the region of one-, two- or three-dimensional space within which a regionalized variable is defined.
- 3.1.4 *indicator variable*, *n*—a regionalized variable that can have only two possible values, zero or one.
- 3.1.5 *kriging*, *n*—an estimation method where sample weights are obtained using a linear least-squares optimization procedure based on a mathematical model of spatial variability and where the unknown variable and the available sample values may have a point or block support.
- 3.1.6 *nonconditional simulation*, *n*—a simulation approach where realizations of the random function model are unconstrained by sample data.
- 3.1.7 *nugget effect, n*—the component of spatial variance unresolved by the sample spacing and the additional variance due to measurement error.
- 3.1.8 *point, n—in geostatistics*, the location in the field at which a regionalized variable is defined. It also commonly refers to the support of sample-scale variables.
- 3.1.9 *realization*, *n*—an outcome of a spatial random function or a random variable.
- 3.1.10 *regionalized variable*, *n*—a measured quantity or a numerical attribute characterizing a spatially variable phenomenon at a location in the field.
- 3.1.11 *simulation*, *n*—*in geostatistics*, a numerical procedure for generating realizations of fields based on the random function model chosen to represent a regionalized variable.
- 3.1.12 *smoothing effect, n—in geostatistics*, the reduction in spatial variance of estimated values compared to true values.
- 3.1.13 *spatial average*, *n*—a quantity obtained by averaging a regionalized variable over a finite region of space.
- 3.1.14 *support*, *n*—*in geostatistics*, the spatial averaging region over which a regionalized variable is defined, often approximated by a point for sample-scale variables.
- 3.2 Definitions of Other Terms—For definitions of other terms used in this guide, refer to Terminology D653 and Guides D5549, D5922, and D5923. A complete glossary of geostatistical terminology is given in Ref (7).

4. Significance and Use

- 4.1 This guide is intended to encourage consistency and thoroughness in the application of geostatistical simulation to environmental, geotechnical, and hydrogeological site investigations.
- 4.2 This guide may be used to assist those performing a simulation study or as an explanation of procedures for qualified nonparticipants who may be reviewing or auditing the study.
- 4.3 This guide should be used in conjunction with Guides D5549, D5922, and D5923.
- 4.4 This guide describes conditions for which simulation or particular simulation approaches are recommended. However, these approaches are not necessarily inappropriate if the stated conditions are not encountered.

5. Selection of Simulation Approaches

- 5.1 Simulation Versus Estimation—A common objective of geostatistical site investigations is to produce a two- or three-dimensional spatial representation of a regionalized variable field from a set of measured values at different locations. Such spatial representations are referred to here as maps. Estimation approaches, including all forms of kriging, yield maps that exhibit a smoothing effect, whereas simulation approaches yield maps that preserve the spatial variability of the regionalized variable.
- 5.1.1 If mapped values of the regionalized variable are required to provide an estimate of actual values at unsampled points, then an estimation approach such as kriging is appropriate.
- 5.1.2 If mapped values of the regionalized variable are to preserve the spatial variability of values at unsampled points, then simulation rather than estimation should be used.

Note 1—Preservation of in-situ spatial variability is important if mapped values of the regionalized variable are to be entered in a numerical model of a dynamic process, and therefore, simulation should generally be used. For example, mapped values of transmissivity to be entered in a numerical model of groundwater flow should be generated by simulation (8). However, if the numerical process model is insensitive to spatial variations of the regionalized variable, then an estimation approach may also be used.

- 5.2 Conditional Versus Nonconditional Simulation—Geostatistical simulation methods are able to produce maps of a regionalized variable that honor values observed at sampled points, a selected univariate distribution model, and a selected model of spatial variation. The univariate distribution model may be that of the observed sample values or a model that is deemed more appropriate. The model of spatial variation may be that of observed sample values or a model of spatial variation that is deemed more appropriate.
- 5.2.1 If the simulated field need honor only a univariate distribution model and a spatial variability model, then a nonconditional simulation approach is sufficient.
- 5.2.2 If the simulated field is to honor values of the regionalized variable observed at sampled points in addition to histogram and spatial variability models, then a conditional simulation approach should be used.
- 5.2.3 If the regionalized variable exhibits a drift or other feature that is not explicitly considered in the geostatistical model, then conditional simulation may be used to impart some of this feature in the simulated field.
- 5.2.4 If part of the nugget effect exhibited by the sampled regionalized variable is due to sampling error and the simulation is to reproduce in-situ spatial variability, then a conditional simulation approach may be used if it ensures that the differences between observed and simulated values of the regionalized variable at sampled points are consistent with the sampling precision.
- 5.3 Gaussian Versus Indicator Simulation—Gaussian and indicator geostatistical simulation approaches each have their own particular characteristics rendering them more suitable for some applications than others. Simulation algorithms based on Gaussian (normal) variables produce realizations in which there is a maximum scatter of extreme high and low values.

Simulation algorithms based on indicator variables, on the other hand, are intended to produce realizations that honor the spatial variability of extreme values.

- 5.3.1 If the simulated regionalized variable is binary or categorical, then an indicator-based simulation approach should be used.
- 5.3.2 If the simulated regionalized variable is continuous and the spatial variability of extreme values must be reproduced, then this variable may be coded into a sequence of indicator variables that should be simulated using an indicator-based approach.
- 5.3.3 If the simulated regionalized variable is continuous and the spatial variability of extreme values is unimportant, then a Gaussian-based simulation approach should be used.
- 5.3.4 If the simulated regionalized variable is continuous but may be grouped into two or more distinct populations, then an indicator-based approach may be used to simulate group boundaries and a Gaussian-based approach may be used to simulate the regionalized variable within each group.
- 5.3.5 If available sample data are limited and a Gaussian model cannot be refuted, then a Gaussian-based simulation approach is the conventional default.
- 5.4 Single Versus Multiple Realizations—Geostatistical simulation approaches may be used to generate one or more possible maps of a regionalized variable that honor specified probability distribution and spatial variation models and, if desired, data values at sampled points.

- 5.4.1 If uncertainty in mapped values of the regionalized variable is the focus of a sensitivity analysis, then multiple realizations should be simulated.
- 5.4.2 If the simulated field is part of a Monte-Carlo sensitivity analysis, then a simulation approach capable of generating equally probable realizations is required.
- 5.5 Point Versus Block Simulation—Geostatistical simulation approaches may be used to generate maps of regionalized variables with either point or block support. These simulation approaches must ensure that the spatial variability of simulated values is consistent with the spatial averaging or change-of-support process.
- 5.5.1 If the simulated regionalized variable has a point support or the same support as the sampled variable, then a point simulation approach should be used.
- 5.5.2 If the simulated regionalized variable has a block support discretized by a finite number of points, then point simulation followed by spatial averaging over the discretized blocks is an approach that can be used provided the spatial averaging process is known.
- 5.5.3 If the simulated regionalized variable has a block support and the spatial averaging process is arithmetic, then a direct block simulation approach may be used.

6. Keywords

6.1 estimation; geostatistics; kriging; simulation

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