



Methodologies for Optimization of Survey Design for Subsurface Radiological Contaminants

Technical Bases for the
Development of Guidance

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Proposed Methods

Use geostatistics (kriging) and prior information (Bayes) to make better use of the data

- Determine release criteria
- Create map of probabilities of exceeding release criteria based on an historical site assessment
- Use Bayesian Ellipgrid for initial survey design
- Develop criteria for secondary sampling
- Choose a variogram
- Apply Markov-Bayes
- Conduct more sampling if needed (repeat as necessary)
- Analyze final survey results using release criteria

Introduction

- ◆ Surveying contaminants in subsurface soils and how it contrasts with MARSSIM-type surface approaches
- ◆ Approaches to address survey design (including NUREG/CR-7021) and statistical methods for evaluating contaminants in the subsurface

Key Reference: NUREG-1757, Vol.2

- ◆ NUREG-1757, Vol. 2, Revision 2, “Characterization, Survey, and Determination of Radiological Criteria,” addresses remaining subsurface contamination in the vadose zone following decommissioning
- ◆ Radiation Survey and Site Investigation (RSSI) process as it relates to the subsurface
 - Presents a framework focused on development of a conceptual site model (contamination concern map (CCM))
 - CCM describes the extent, location, and significance of residual radioactivity relative to the decision criteria and provides hypothetical examples of intrusion into buried fill or excavation of a contaminated layer below the surface

Guidance on Surveys for Subsurface Radiological Contaminants

Draft White Paper

(ADAMS Accession No. ML22088A219)

- ◆ Under Development



Key Reference: NUREG/CR-7021

- ◆ Essential guidance for subsurface characterization principles
- ◆ NUREG/CR-7021, “A Subsurface Decision Model for Supporting Environmental Compliance”
 - Describes NRC-sponsored Spatial Analysis and Decision Assistance (SADA) software
 - Geospatial modeling and decision framework for conducting a subsurface compliance survey and analysis for sites that have been remediated for radioactive contamination
 - Proposes a method to extend the MARSSIM guidance into the subsurface, organizing survey methods into a highly flexible sampling, modeling, and decision analysis approach that emphasizes the quality of the decisionmaking throughout the investigation

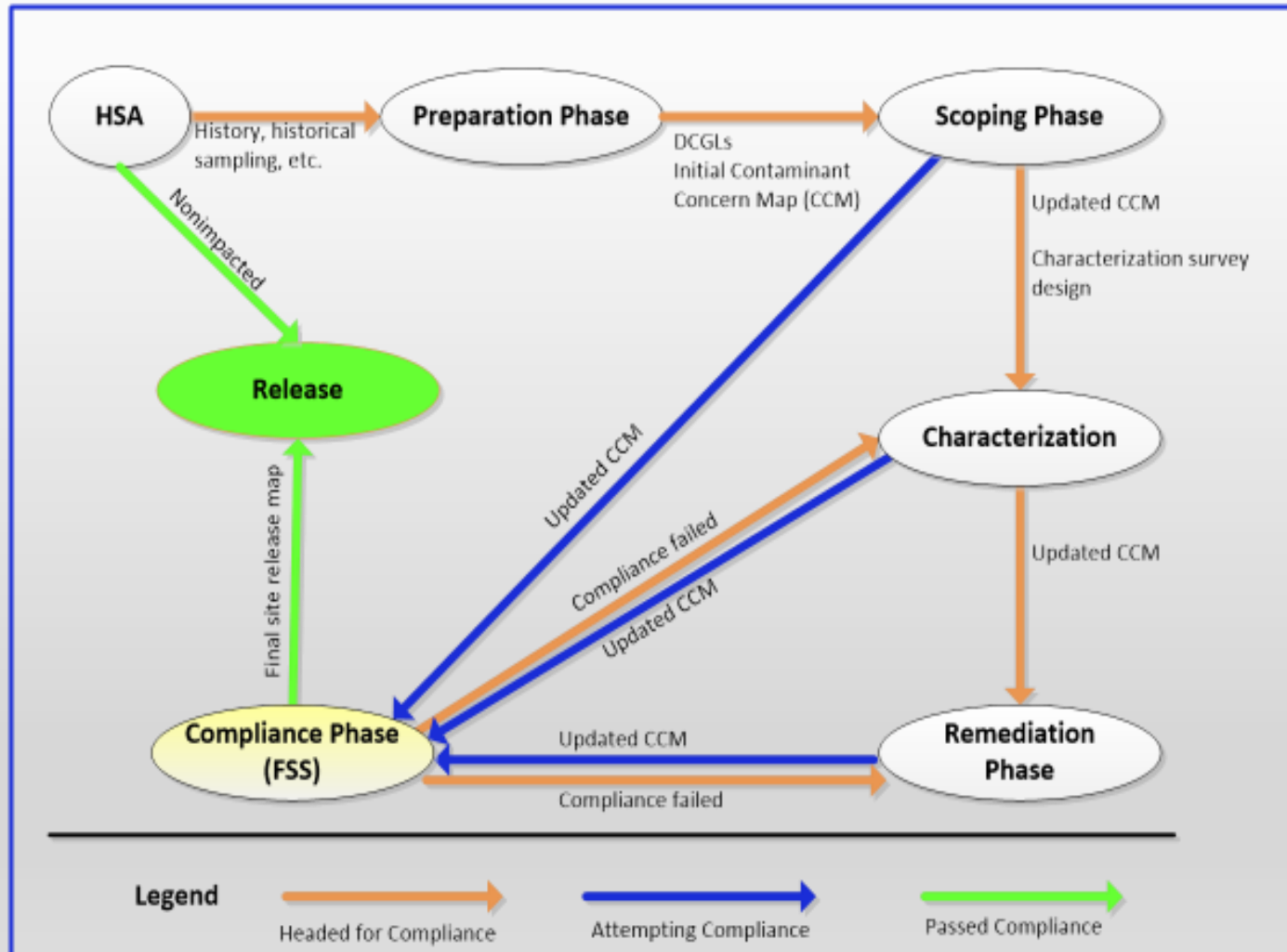
Key Reference: EPRI Report

- ◆ “Guidance for Using Geostatistics to Develop Site Final Status Survey Program for Plant Decommissioning” (2016)
 - Evaluated 17 two- and three-dimensional software packages
 - Of those evaluated, SADA is recommended because of its use in CCMs, sampling optimization, and remediation cost-benefit analysis
 - Visual Sample Plan (VSP) is also a good candidate, but it is a two-dimensional package

Stages of the Subsurface Decision Framework

- ◆ Methods and considerations for performing various types of subsurface radiological surveys
 - Historical site assessments (HSAs) and scoping, characterization, remedial action, confirmatory, and final status surveys (FSSs)
- ◆ Performance-Based Subsurface Compliance Framework
 - Phases depict how the subsurface analysis moves from a very qualitative beginning to a more quantitative conclusion

Stages of the Subsurface Decision Framework (cont.)



Stages of the Subsurface Decision Framework (cont.)

- ◆ Major themes of the framework:
 - Use the HSA to create an initial CCM
 - The output of each major phase includes the latest CCM update
 - End result is success in the compliance phase or return to an interim phase under compliance failure
- ◆ How areas of concern, contamination of concern, and derived concentration guideline levels (DCGLs) fit into the iterative data quality objective process

Determination of Release Criteria

- ◆ Requires action levels (i.e., DCGLs)
 - How the survey unit will be used
- ◆ Uses dose modeling to determine cleanup levels or DCGLs that meet regulatory criteria
- ◆ Survey unit definitions
 - Size
 - Depth

Determination of Release Criteria (cont.)

- ◆ ***How many and where should samples be taken?***
 - How deep should cores be?
 - Should cores be layered?
 - If the cores are layered, should they be composited?
- ◆ After remediation, a final status survey confirms that residual radioactivity on site meets the License Termination Rule radiological criteria
- ◆ What function (i.e., statistic) of the sample data will be used in the decision rule?

Derived Concentration Guideline Levels

- ◆ MARSSIM surface survey units (sizes, shapes or classifications) may not align with subsurface survey units
- ◆ Multiple DCGLs for multiple depths or environmental media could be employed, resulting in a more complex final status survey
- ◆ A layered approach may be used for excavations
 - That is, multiple subsurface layers or strata are considered individually and then the cumulative risk from the multiple layers or strata is assessed

Statistical Methods and Tests

- ◆ Because subsurface sampling is costly, survey design should include some measure of the value added to the decisionmaking process for each additional location sampled
 - Number of samples based on a metric that changes as sample size increases
 - A measure like the statistical power in MARSSIM is desirable, also to evaluate the adequacy of the final status survey

Statistical Methods and Tests (cont.)

- ◆ Most promising methods for designing efficient subsurface surveys
 - Bayesian Ellipgrid (geometrical)
 - Markov-Bayes (geostatistical)
 - Both implemented in SADA
- ◆ Historical site assessment can provide the prior information needed to use the Bayesian tools and thus needs to be as complete and accurate as possible
- ◆ No single software package provides all the tools that would be desirable for subsurface sampling design and analysis

Statistical Methods and Tests (cont.)

- ◆ VSP and SADA appear to have the set of features that may be most useful for RSSIs:
 - VSP is supported, maintained, and updated periodically with new features; SADA is available to download but not currently supported, maintained, or updated
 - SADA contains many features not normally used for NRC decommissioning problems and could be simplified to be more specific to decommissioning
 - Both SADA and VSP have options to use only the MARSSIM parts of the code, but this would exclude geostatistical operations; SADA does not implement MARSSIM Scenario B

Statistical Methods and Tests (cont.)

- ◆ Whatever software (or combination) is chosen, it would be important to have detailed written instructions and examples to demonstrate how it would be used in subsurface applications
- ◆ It may not be fruitful to spend a great amount of effort in calculating and fitting variograms

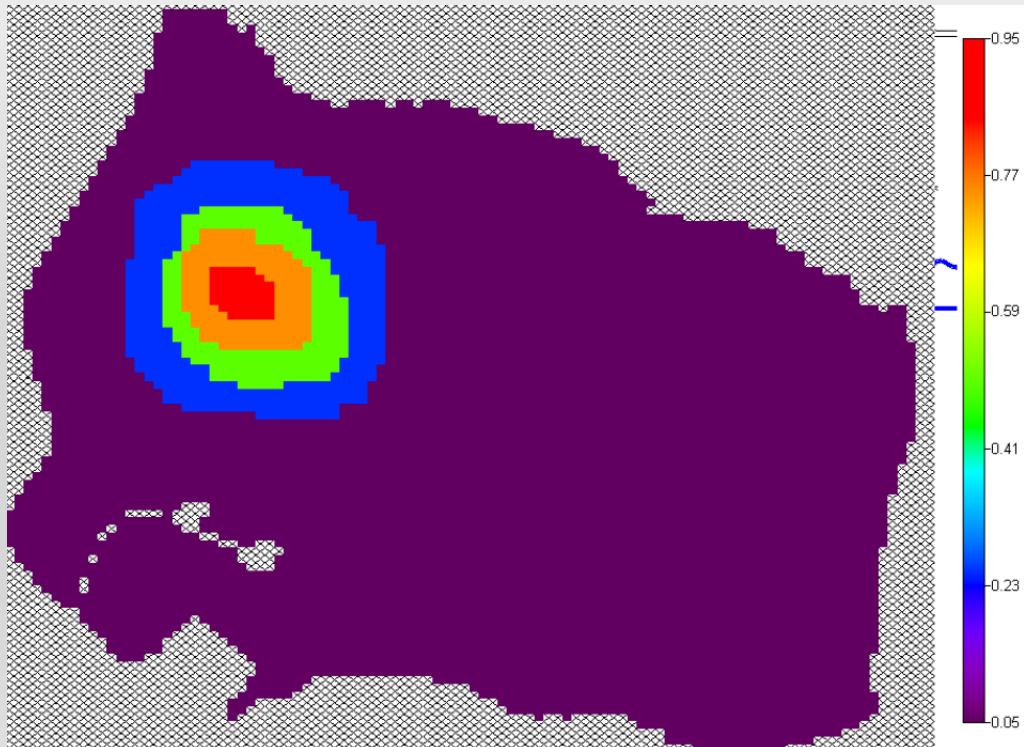
Sample Planning and Analysis Tools

- ◆ Spatial Analysis and Decision Assistance
 - SADAV5HelpFile.chm
 - SADA Version 5 User's Guide
- ◆ Visual Sample Plan
 - VSP Version 7.0 User's Guide
- ◆ Both codes can estimate the number of samples needed, but some starting point is required

Conceptual Site Model

◆ Initial CCM


- Map of probabilities of exceeding release criteria based on an historical site assessment
- Probabilistic user models (SADA User's Guide, p. 409)



Ellipgrid

VSP User's Guide, Section 3.2.5, Locating a Hot Spot

One Acre Field



Locating a Hot Spot

Locating a Hot Spot | Grid | Hot Spot | Costs

Specify Parameter to Calculate

I want to solve for:

- the grid spacing / # of samples / total cost required to detect a hot spot of a specified size.
- probability of detecting a hot spot of a specified size with a fixed number of samples.
- the size of hot spot that can be detected with a fixed number of samples.

Input Parameters

I want to specify how many samples to take in terms of:

- the grid spacing (see Grid page)
- the total number of samples*: samples will be required.
- the total cost (see Costs page). \$ will be required for sampling costs.

I want to have at least a % chance of detecting the specified hot spot.

In order to have a 95% probability of locating a circular hot spot with a radius of 15.00 feet using point samples arranged in a triangular grid pattern, you need a maximum spacing of 28.98 feet between samples (see diagram on grid page). This would require approximately 60 samples and a budget of \$30,000.00. (The actual sample configuration on the map uses 54 samples and a budget of \$27,000.00.)

* Based on a total sampling area of 43560.00 feet².

Close Cancel Apply Help

Locating a Hot Spot

Locating a Hot Spot | Grid | Hot Spot | Costs

Sample Type

Point Samples

Grid Cell Samples

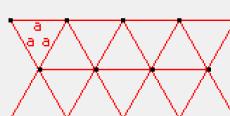
Size of Grid Cell: Feet

Grid Type

Square

Triangular

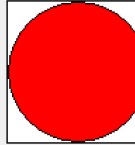
Rectangular



Length of grid side: Feet (a)

Locating a Hot Spot

Locating a Hot Spot | Grid | Hot Spot | Costs



Area of Hot Spot: Feet²

Radius: Feet

Radius:

Ellipse Shape (0.2 - 1.0):

Circle (A shape of 1.0 is a circle)

Angle of Orientation to Grid

Degrees:

Random

Ellipgrid Using Prior Belief

At Least Some
High
Percentage of
the Sampling
Area Is
Acceptable?
VSP User's
Guide,
Section 3.2.6

Presence / Absence Sampling

Presence / Absence | Sample Placement | Costs | Data Analysis | Analytes

None of the grid cells in my sample can be unacceptable

I want to account for prior belief in my design

I want to include judgment samples in my design

My decision area contains a total of 2497 grid cells. Pick Judgment Grid Cells

I will sample 30 grid cells based on my own judgment.

Before any sampling takes place, I expect there is a High (90%) (90.000 %) probability that a judgmentally selected grid cell is acceptable.

I believe that a judgmentally selected grid cell is 3 times more likely to be unacceptable than a randomly selected grid cell.

I want 99.000 % confidence that at least 99.000 % of the decision area is acceptable.

Number of grid cells that must be randomly selected and examined: 300

If all 30 judgmentally selected grid cells and all 300 randomly selected grid cells are acceptable, then I am 99% confident that at least 99% of the decision area is acceptable.

If any of the judgment or random samples are unacceptable, then the confidence statement above no longer applies and I must assume that at least some portion of the decision area is unacceptable.

Calculate number of samples Calculate % confidence based on number of samples

Bayesian Ellipgrid

SADA User's Guide, Chapter 41, pages 539–543

F = The object is found DF = The object is not found

E = The object exists DE = The object does not exist

So $P(F) = P(F|E) \times P(E) + P(F|DE) \times P(DE)$ and $P(F|DE) = 0$

What is the probability its missed when it's really there—i.e., $P(DF|E)$?

$$P(F|E) + P(DF|E) = 1$$

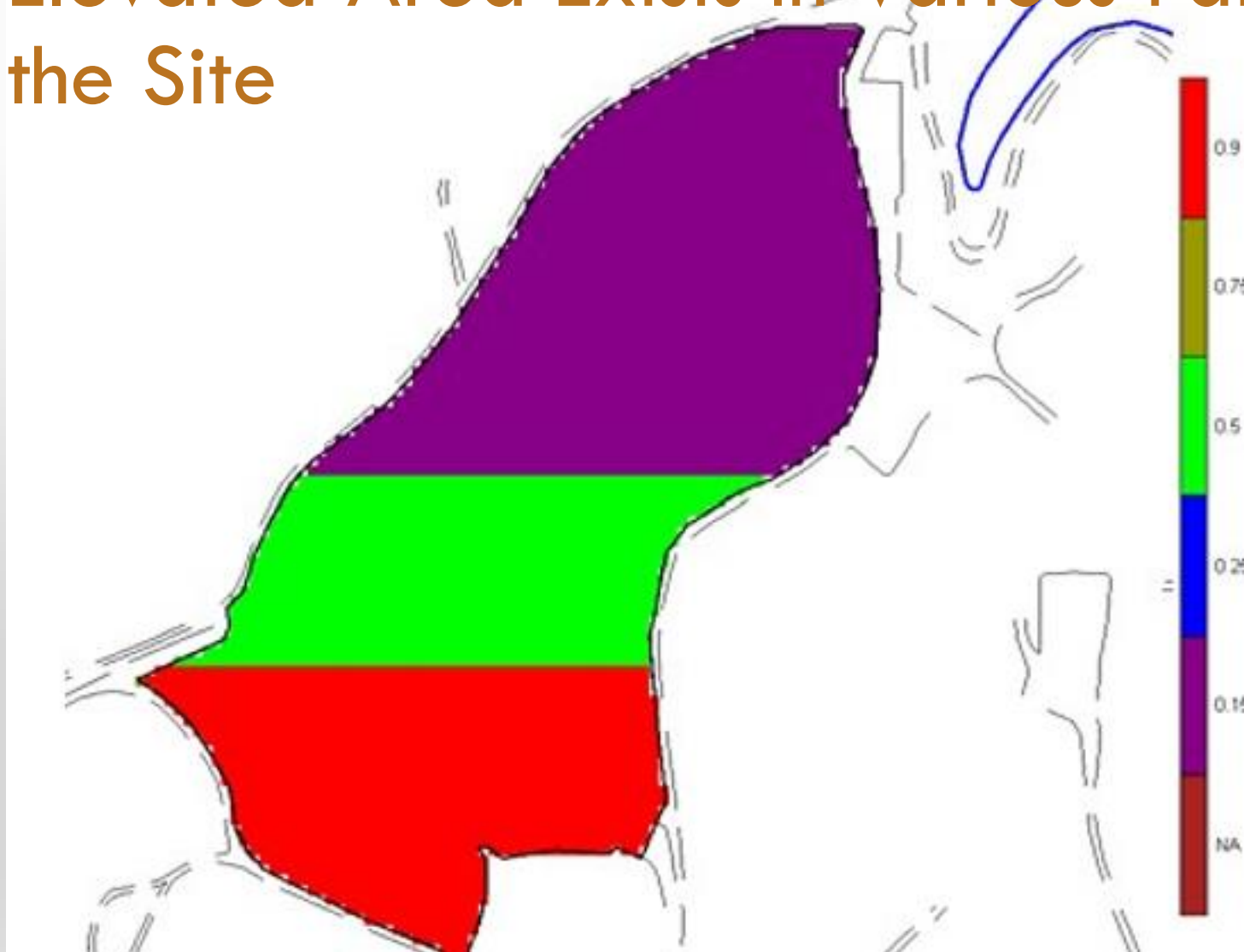
$$P(F|E) = 1 - P(DF|E)$$

Using these in the equation above:

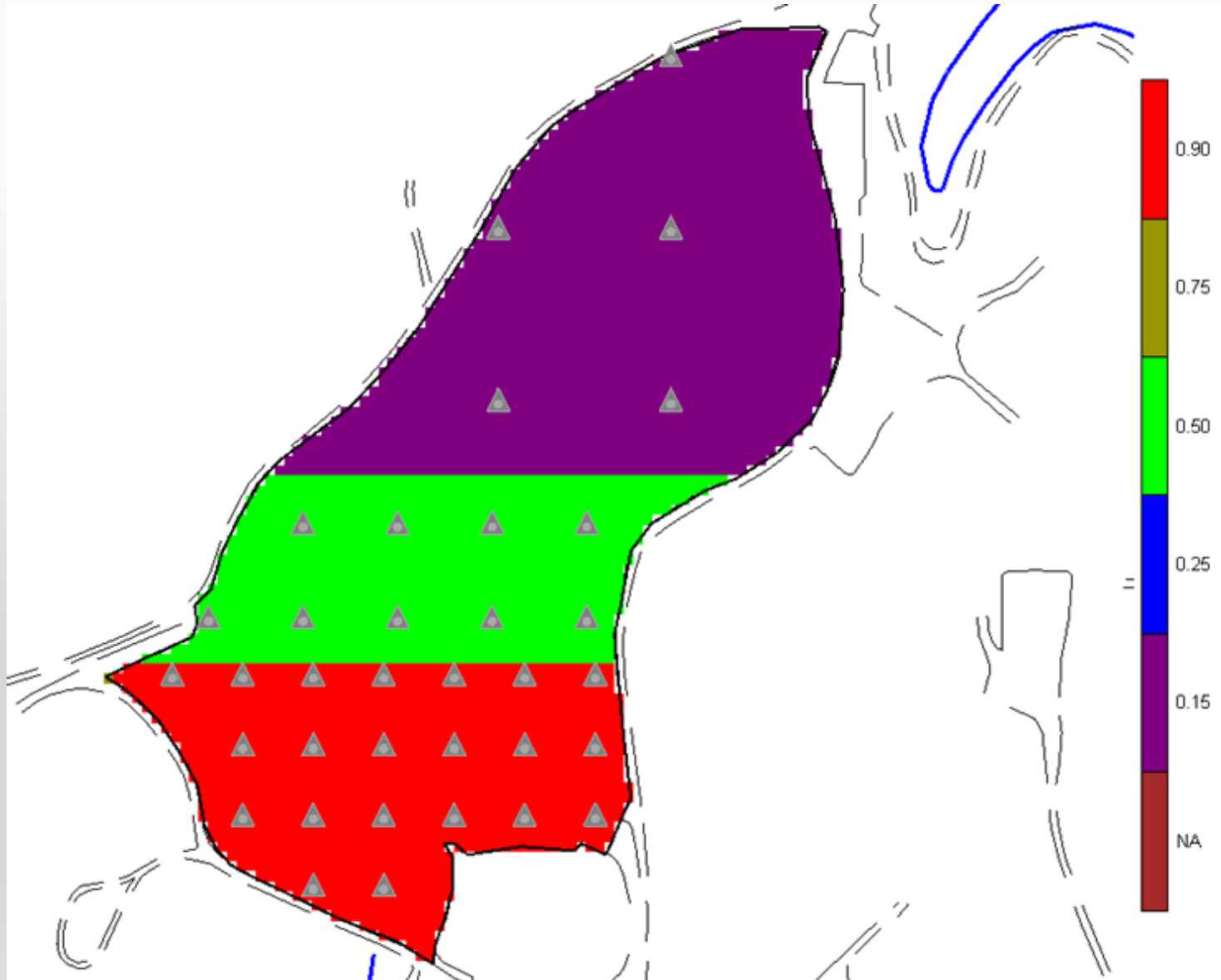
$$P(F) = [1 - P(DF|E)] \times P(E)$$

$P(E)$ obtained from the user probability map

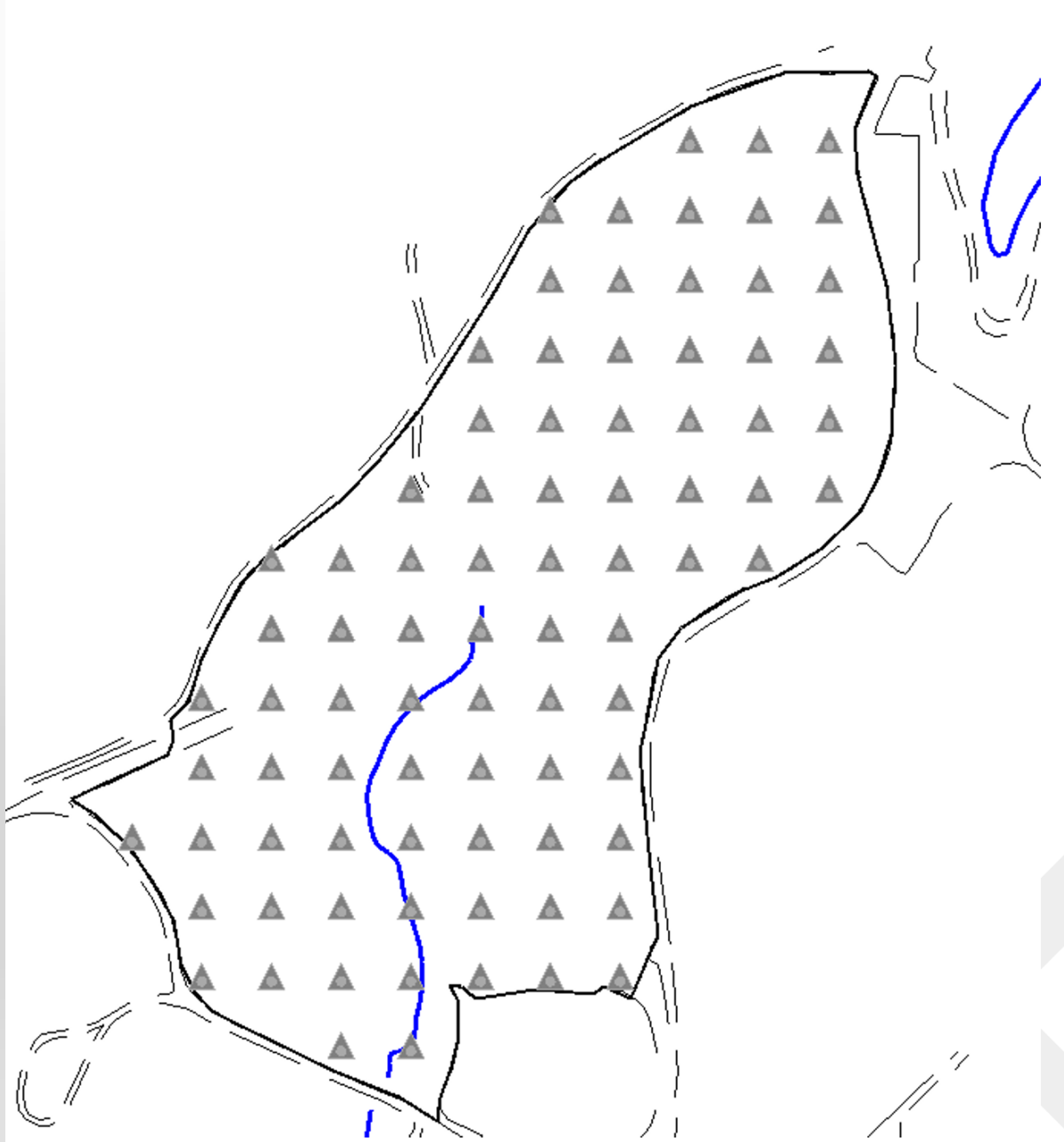
Bayesian Ellipgrid: Likelihood that an Elevated Area Exists in Various Parts of the Site



Initial Survey Design: 37 Samples



Without Prior Probabilities: 87 Samples



Secondary Sampling

- ◆ After taking the initial samples, a secondary sampling plan can be constructed
 - SADA User's Guide, Chapter 38; VSP User's Guide, Chapter 3 and Section 5.1
- ◆ Both VSP and SADA have several ways to do this, depending on the statistic to be used in the release criterion and the certainty needed in its value to achieve the desired data quality objectives for decision making

Markov-Bayes

SADA User's Guide, pages 335–338

- ◆ In Markov Model 1 (MM1), only one direct variogram needs to be modeled and the other variograms and cross variograms are derived from it. MM1 states that the variogram is proportional to the variogram of the primary variable.
- ◆ Markov-Bayes is a special application of the Markov model for probability mapping using both hard and soft (prior probabilities) indicators.
- ◆ Markov Bayes uses the assumption that additional (soft) information can be taken into account for the assessment of prior distributions at selected locations. Rather than ordinary cokriging, indicator cokriging is used. Hard data are first converted to 0s or 1s, depending on whether they exceed a specified criterion. The cokriging method is then applied to these 0s and 1s, along with the user-defined prior probability map. This results in an updated probability map that contains the influences of both the hard and soft data.

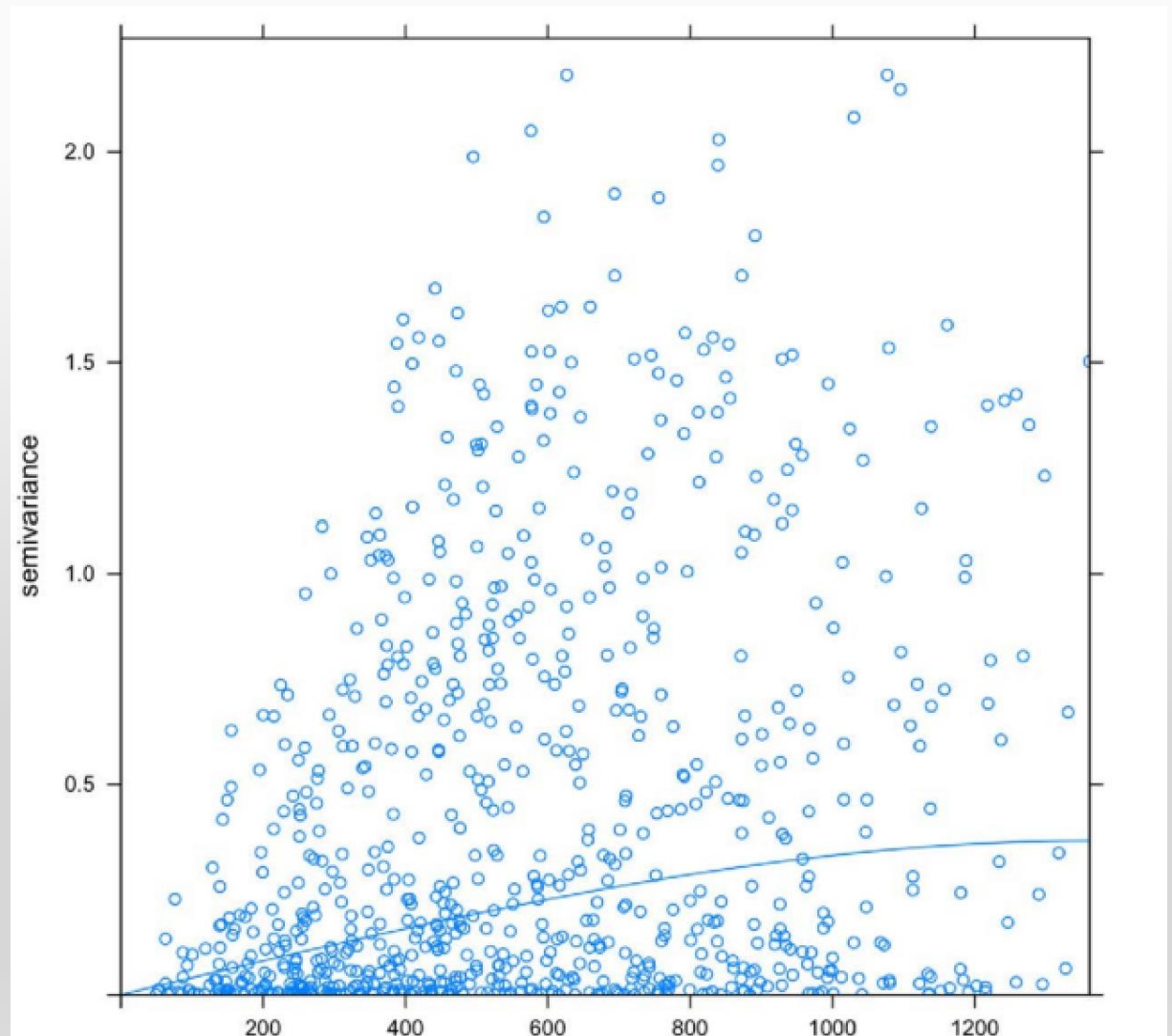
Variogram Cloud

A variogram cloud is a scatterplot of the set of pairs $(h, \gamma(h))$ where:

$$h = ((x_i - x_j)^2 + (y_i - y_j)^2)^{1/2}$$

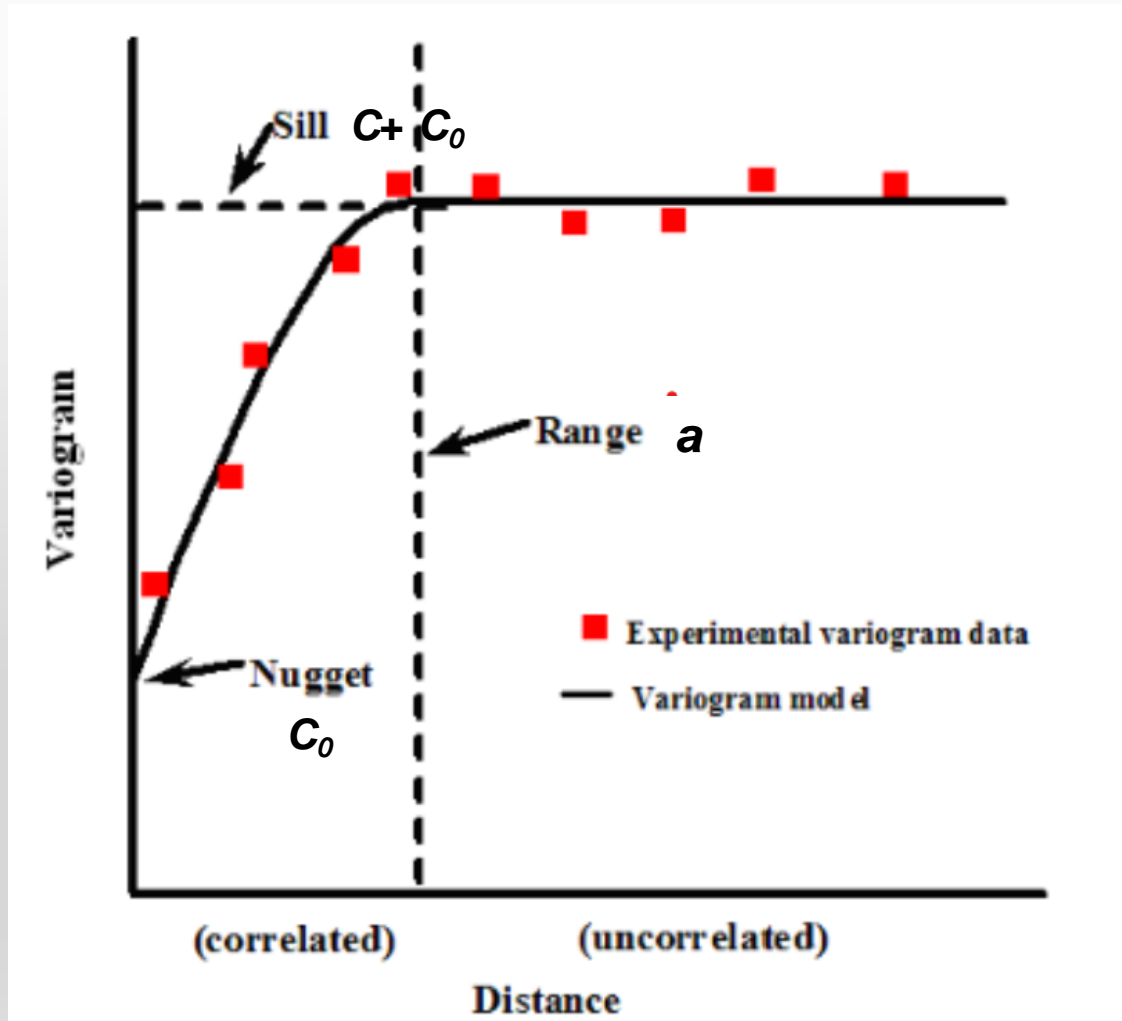
$$\gamma(h) = 0.5 (z_i - z_j)^2$$

and $i \neq j$



Choosing a Variogram

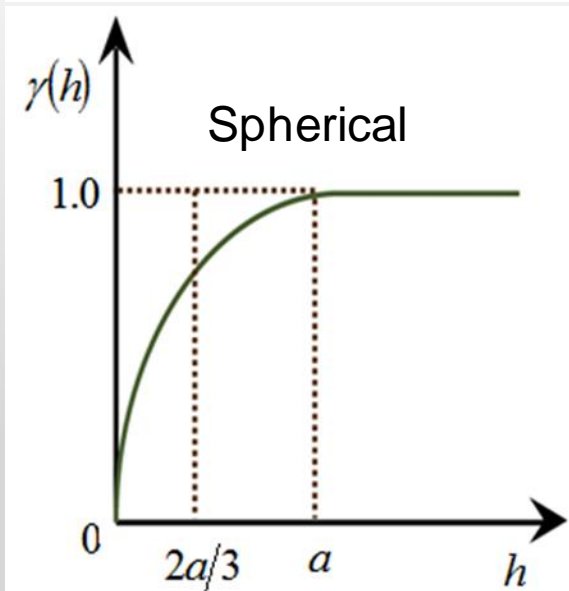
Parameters for a valid variogram are estimated from an empirical variogram



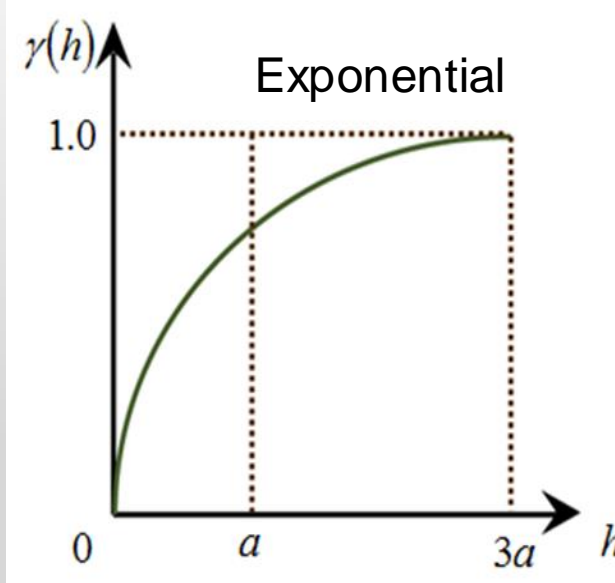
Spherical and Exponential Variograms

Compared with the spherical model, the exponential model has a linear growth in a short distance and then climbs with a very high slope. Finally, it reaches the sill value smoothly with a lower slope.

$$\gamma(h) = \begin{cases} 0, & h=0 \\ C_0 + C\left(\frac{3h}{2a} - \frac{1}{2}\frac{h^3}{a^3}\right), & 0 < h \leq a \\ C_0 + C, & h > a \end{cases}$$



$$\gamma(h) = c * \left[1 - \exp\left(-\frac{(3h)^2}{a^2}\right) \right]$$



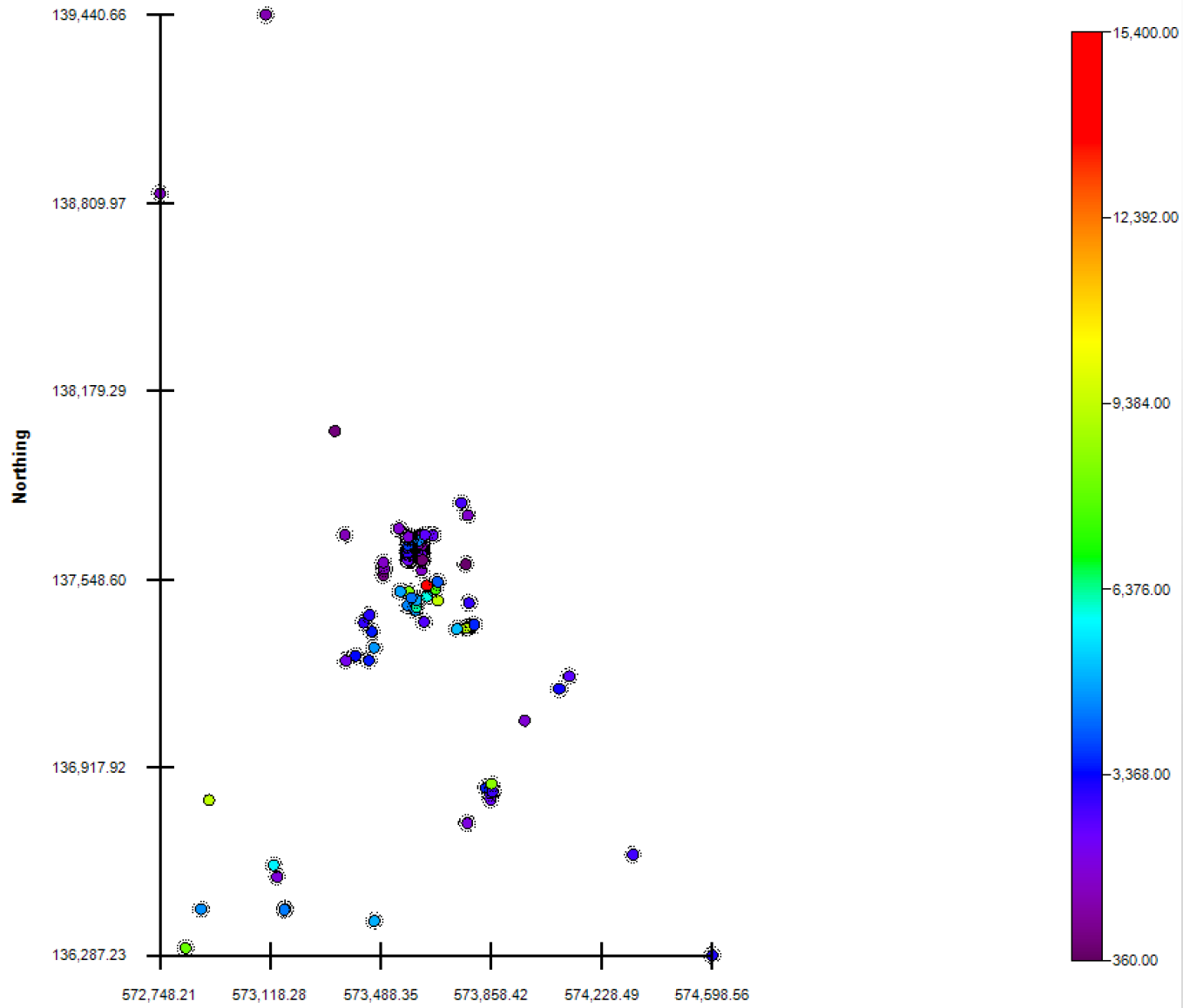
where C_0 is the nugget constant, $C + C_0$ is the sill, C is the structure variance, and a is the effective range. The slope rate at the point of origin is $3C/2a$, and the intersection between the sill value and x-axis is $2a/3$.

Source: Spatial Statistical Analyst 10.0 OnlineHelp (SuperGeo Technologies 2017)
https://www.supergeotek.com/Spatial_Statistical_ENG_HTML/index.html?spherical_mode.htm

Estimating Variograms

- ◆ Both VSP and SADA provide methods to estimate variograms from recommended default settings
- ◆ It is difficult to evaluate the recommended values since the assumptions and methods used for these values are not fully transparent

Arsenic Samples



Choose Data

First Variable

Second Variable

Data Transforms

Explore Experimental Semi-variography

Previous Results

Use Direction

Name	Major	Minor
Caption	Default	Default
Lag Number	20	20
Lag Distance	61.67833333...	61.67833...
Lag Tol	61.67833333...	61.67833...
Angle	0	0
Tol	90	90
Band	3153.429999...	3153.429...
Dip	0	0
ZTol	90	90
ZBand	4.87035	4.87035

Model Semi-variography Values

Model

Major Range	570.4340020...
Minor Range	570.4340020...
Angle	0
Contribution	6911052.631...
Z Angle	0
Z Range	4.87035
Rotation	0

Nugget

SADA5

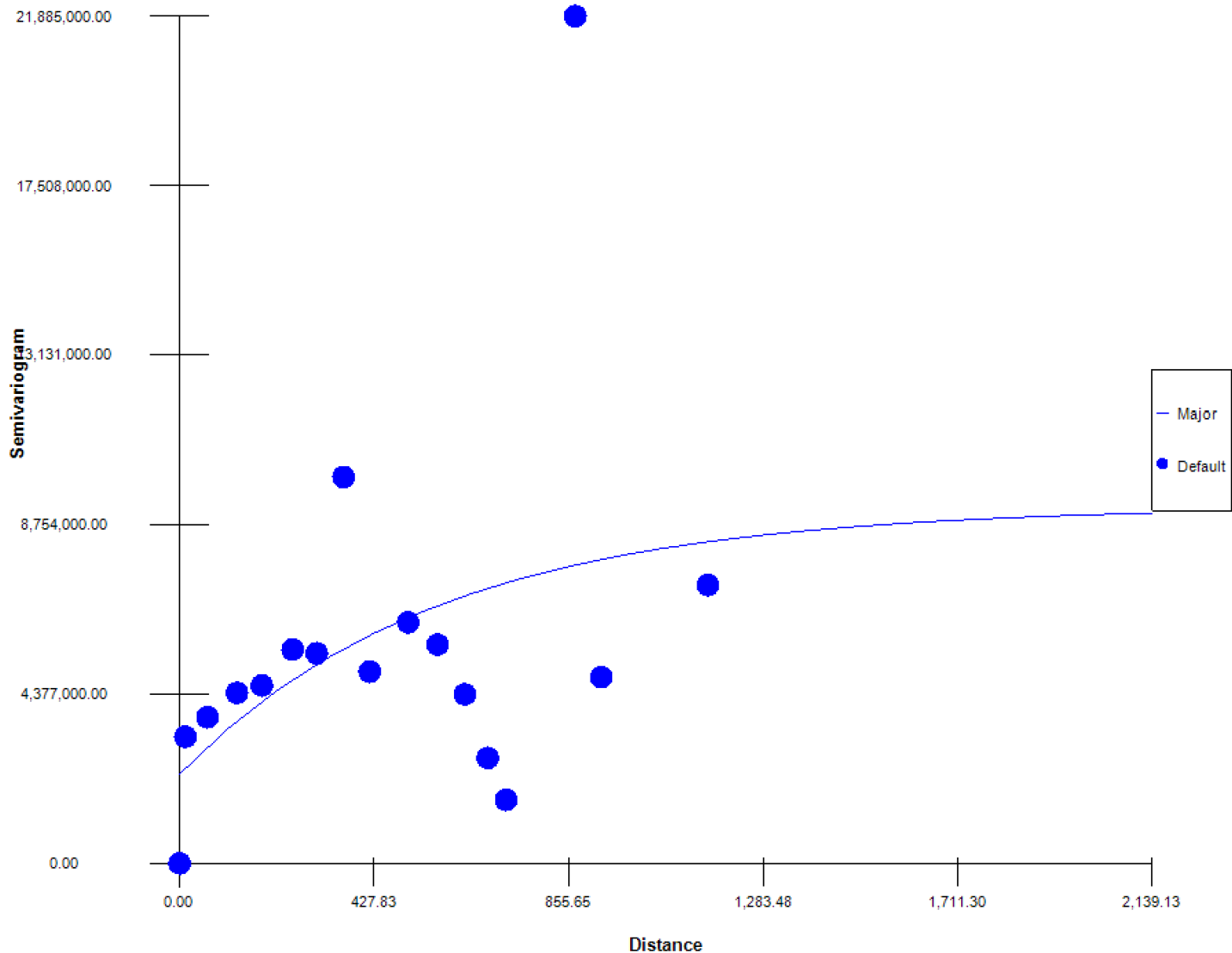


SADA will now calculate some rough default parameters to begin your semi-variogram exploration with. Both the major and minor directions will be filled with a omni-directional parameters that cover about 2/3rds the site. These parameters should not be blindly used, but should be further refined by the user in searching for any correlation structure that may exist. Would you like to continue?

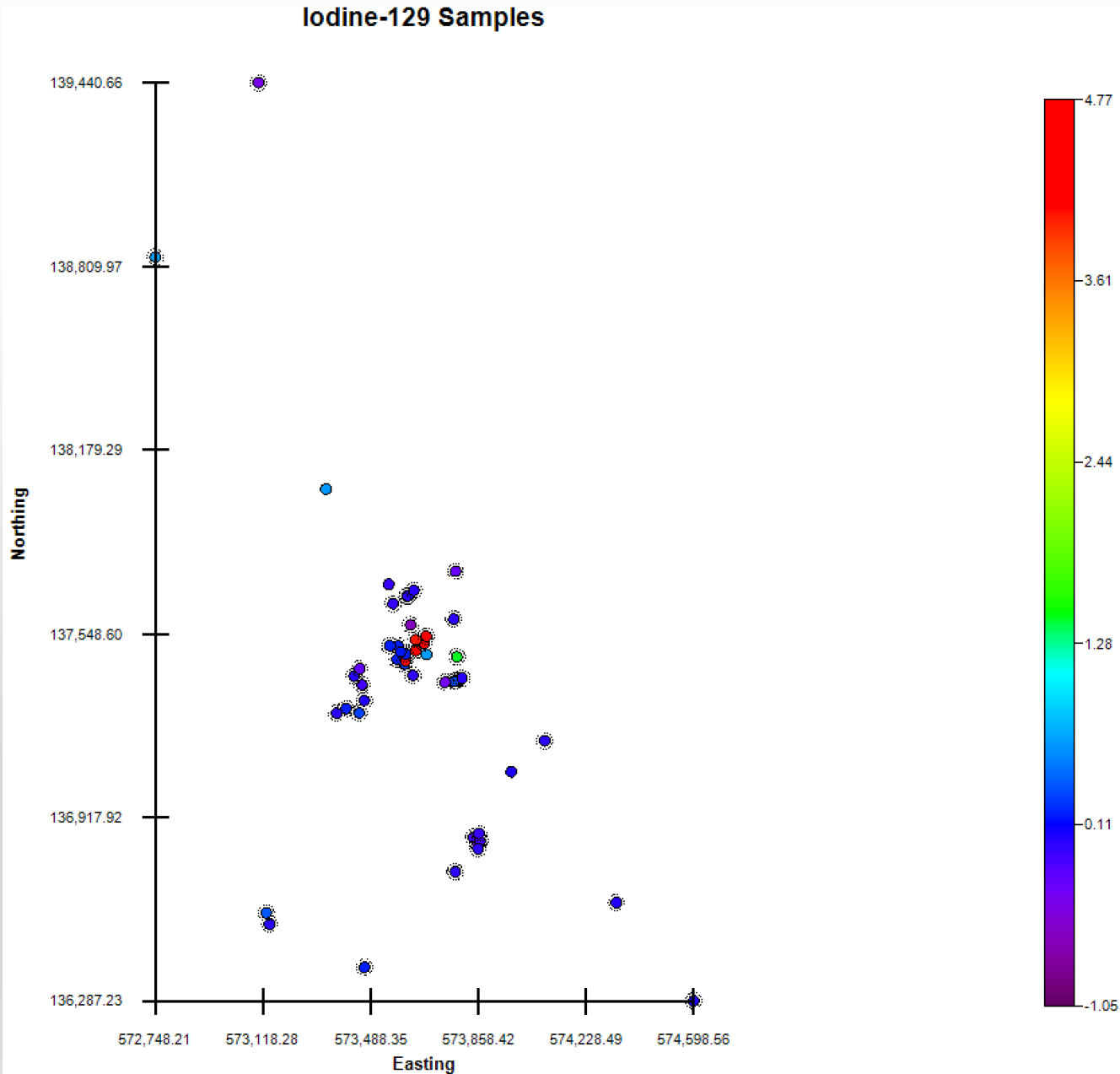
Yes

No

Arsenic Correlation Model



Iodine-129 Samples



Choose Data

First Variable

Second Variable

Data Transforms

Explore Experimental Semi-variography

Previous Results

Use Direction

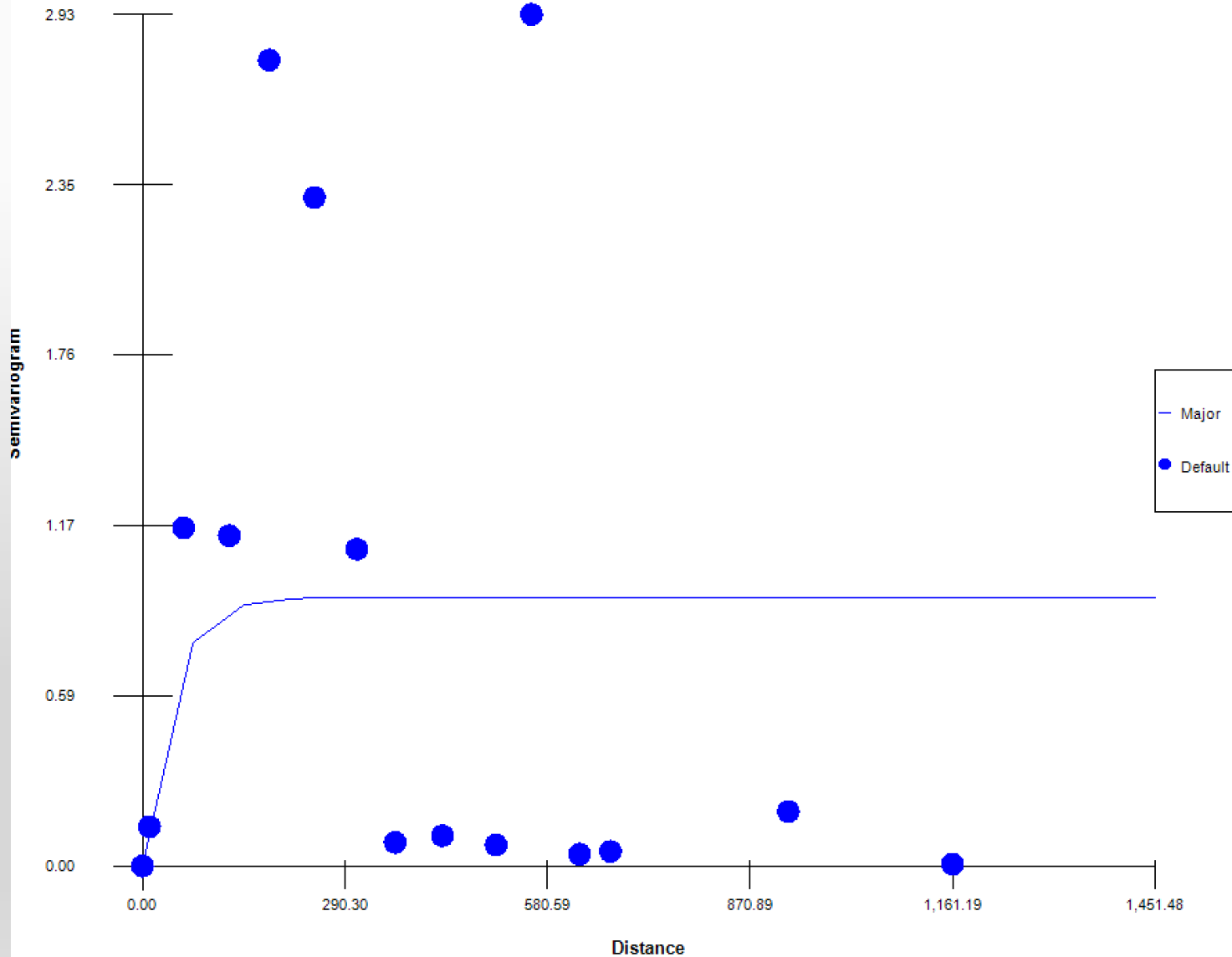
Name	Major	Minor
Caption	Default	Default
Lag Number	20	20
Lag Distance	61.67833333...	61.67833...
Lag Tol	61.67833333...	61.67833...
Angle	0	0
Tol	90	90
Band	3153.429999...	3153.429...
Dip	0	0
ZTol	90	90
ZBand	4.87035	4.87035

Model Semi-variography Values

Model

Major Range	40.83814322...
Minor Range	40.83814322...
Angle	0
Contribution	0.925751801...
Z Angle	0
Z Range	4.87035
Rotation	0

Iodine-129 Correlation Model



Discussion Questions

- ◆ What are methods to determine the hot spot size of concern?
- ◆ Is the use of the Bayesian Ellipgrid appropriate for MARSSIM users and use scenarios?
- ◆ What should be the criteria for secondary sampling?
- ◆ Is the use of Markov-Bayes appropriate for MARSSIM users and use scenarios?

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