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ENVIRONMENTAL RESTORATION PROGRAM

RESPONSE TO NMED COMMENTS ON OU 1071 RFI WORK PLAN

LANL/ER/OU 1071

LOS ALAMOS NATIONAL LABORATORY

LOS ALAMOS, NEW MEXICO

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ENVIRONMENTAL RESTORATION PROGRAM

LOS ALAMOS NATIONAL LABORATORY

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176

TABLE OF CONTENTS

1.0 Introduction 1

2.0 General Comments 2

3.0 Specific Comments 6

Attachments

1 AIP Review of Operable Unit 1071 RFI Work Plan

2 Referenced Documents

1.0 Introduction

This Document presents the response to the New Mexico Environment Department (NMED) comments on the LANL Environmental Restoration Program's Operable Unit (OU) 1071 RFI Work Plan of May, 1992. The comments were prepared by the NMED Agreement In Principle Staff and were submitted to the Department of Energy's Los Alamos Area Office in a letter dated October 30, 1992 (Attachment 1).

The comments are reproduced in their entirety and are followed by a response prepared by the OU 1071 Project Leader.

2.0 General Comments

NMED COMMENT: *Sediment sampling methodology described in the Work Plan is generally vague in that it does not state the depth at sediment samples will be taken or the specific grain size(s) that will be targeted for each site. Sediment sampling at sites (drainages) that are potentially radioactively contaminated should target silt- and clay-sized sediment because of the adsorptive properties of the finer-grained particles. The primary objective for sampling in drainages should be to assess the presence of contaminants available for transport off site via ephemeral discharge in drainages. This can only be accomplished by knowing the actual concentration available for transport. Bulk samples that contain a significant amount of coarse sediment will not provide an accurate assessment.*

RESPONSE: The work plan does not state what depth sediment samples will be taken as there is currently insufficient information to make depth determinations. Sampling depths will be determined on a case by case basis through detailed geomorphic mapping of sediment traps. This was the procedure used at SWMU 0-011(d) when it was sampled in October 1992.

NMED COMMENT: *Wording in the Work Plan suggests that phased investigations may occur in the event that "Stage I data show that contaminants are present above action levels". Unless Stage I investigations are adequate for confidently determining the vertical and horizontal extent of contamination, Phase II investigations will be required.*

RESPONSE: The term "may" is used to accommodate the possibility that Phase I investigations may, in some instances, define the extent of the contaminants.

NMED COMMENT: *The decision logic of estimating mean contaminant levels over an exposure unit has been suggested in this and several other of the Work Plans reviewed to date by the AIP staff. Our understanding is that Subpart S does not allow for the practice of contaminant "dilution" in this manner. Please explain.*

RESPONSE: Review of Subpart S shows no specific reference to this issue. Generally speaking, Subpart S refers to other guidance documents, notably to the four-volume RCRA Facility Investigation Guidance (Interim Final: EPA 530/SW-89-031, May 1989). Within that document are a number of averaging procedures, ranging from composite sampling to isopleth maps to the use of predictive models. More extensive risk-based decision making procedures are found in CERCLA guidance documents (notably the RAGS and the 1987 DQO guidance). The use of exposure units is explicit in the latter documents.

Decisions are generally based on some kind of summary of the data (a statistic), not on the raw data. Planning to make decisions in this way provides a basis for designing sampling plans before the fact and for data quality assessment after the fact.

There are many ways to make data-based environmental decisions, and there are words throughout Subpart S that support choosing an appropriate one for each problem and tailoring data collection

accordingly. In the OU 1071 work plan, we propose to make decisions based on a couple of different statistics. One is the sample maximum. This is a reasonable choice when attempting to determine if contamination is present, particularly in the absence of any historical information suggesting that a release ever occurred.

NMED COMMENT: *Most or all of the channel sediment sampling plans propose to collect samples "as close to the outfall points as possible". This methodology for characterizing the outfall areas and associated drainages does not provide enough certainty that contaminants, if present, will be found. It is not necessarily the case that contaminants are still located in sediments immediately below the outfall points. Contaminated sediments may have moved some distance down-channel, and could be buried beneath younger sediments.*

RESPONSE: Generally, sampling sediment traps near outfalls is driven by a combination of data quality objectives, geographic domain, and the OU 1071/OU 1049 boundary. Once the sediments are transported down-drainage and are outside a SWMU domain they belong to the Canyons operable unit (OU 1049), and will be addressed in that OU's RFI workplan.

NMED COMMENT: *Statements like "no contamination is expected to be found" are potentially misleading and suggest a bias toward expected results of the sampling, and could be interpreted to affect early phase investigations.*

RESPONSE: The statement "no contamination is expected to be found" is used only where archival information indicates that contaminants are probably not present. Inspection of the sampling plans for SWMUs, where contaminants are not expected, will show that they were designed without bias.

NMED COMMENT: *It is understood that the pending HWSA Permit modification will correct the SWMU list to include only those sites that are actually SWMUs by definition. It is suspected that underground storage tanks (USTs) used for petroleum products will fall out of the HWSA Permit. OU 1071 contains a number of USTs, as do other locations within the Lab boundary or in the Townsite. Investigations and Voluntary Corrective Actions (VCAs) of USTs should be done pursuant to NMED's Underground Storage Tank Bureau (USTB). Registration and closure of USTs should be under the oversight of the Prevention/Inspection Program of USTB. Confirmed or suspected releases should be reported to the Remedial Action Program of the USTB for oversight of investigation and corrective actions. Questions regarding these matters should be referred to Mr. Tony Moreland of the USTB at (505) 827-0214.*

RESPONSE: All tank removals and tank site characterizations will be conducted according to NMED regulations.

3.0 Specific Comments

NMED COMMENT: (2.2.3 p4)

This section suggests that a given sample size (N) provides a degree of confidence (P) that not more than a certain percentage of the site exceeds action levels, and that these results will lead to the conclusion that no contamination exists at that site. Please cite and provide selected passages from peer reviewed journal article(s) where this type of statistical calculation has been used for determination of appropriate sample populations for a site.

RESPONSE: The term "suggests", as used in this comment, is too weak a word for a mathematical identity. This is a consequence of the definition. Specifically, underlying this assertion is the following statistical procedure:

> Suppose that n <u>independent</u> observations are made of a variable that is known to be bounded below by zero (e.g., concentrations of a chemical in soil). Let x_{max} be the largest of these observations. Then the interval $[0,x_{max}]$ provides an interval estimate for the $(1-\gamma)^{th}$ quartile of the population, $\theta_{1-\gamma}$ (that is, an interval which may, or may not, contain the true value of that quantile.) This <u>procedure</u> for generating an interval estimate produces an interval that contains $\theta_{1-\gamma}$ $100(1-(1-\gamma)^n)\%$ of the time. Therefore x_{max} is a $100(1-(1-\gamma)^n)\%$ upper confidence bound for $\theta_{1-\gamma}$.

There is only one statistical assumption underlying this procedure, and that is the assumptions that the observations are statistically independent. No assumptions about the nature of the distribution of soil concentrations in the population of interest (that is, the site) are required. Given that assumption, the remainder is an immediate

consequence of the definitions. The main part of the proof goes:

$$Pr\{x_{max} \geq \theta_{1-\gamma}\} = 1 - Pr\{x_{max} < \theta_{1-\gamma}\}$$

$$= 1 - \prod_{i=1}^{n} Pr\{x_i < \theta_{1-\gamma}\}$$

$$= 1 - (1-\gamma)^n$$

where the first equality is a defining property of probability, the second follows from the independence of the observations, and the third from the definition of $\theta_{1-\gamma}$.

The assumption of independence is of course essential. We recommend a stratified sampling plan, or sampling on a regular grid, in order to achieve spatial separation of the samples and minimize the correlation among them (as well as to achieve a representative sampling of the site). In particular, a pair of field duplicates counts as only one sample as far as computing **n** goes.

Modification of this scheme to accommodate correlation among the observations is the subject of a peer-reviewed article:

> R.J. Barnes (1988), "Bounding the Required Sample Size for Geologic Site Characterization", *Mathematical Geology* 20(5), pp. 477-490.

The entire article is attached. The correlation actually has to be quite large before the confidence in the above procedure is seriously

affected.

A very similar procedure is discussed at length in a 1989 EPA guidance document,

> U.S.E.P.A. (1989), "Methods for Evaluating the Attainment of Cleanup Standards. Volume 1: Soils and Solid Media", EPA 230/02-89-042 (NTIS #PB 89-234-959), prepared by Westat Research, Inc., Rockville, MD and published in February 1989. (A copy is attached.)

Chapter 2 provides an introduction to statistical risk-based decision making, which is the approach that the LANL ER Program has elected to follow.

Chapter 7, "Determining whether a proportion or percentile of the site is less than a cleanup standard", deals with procedures analogous to the procedure under discussion here. However, in all of the tests proposed in Chapter 7, it is assumed that "false positives" are to be controlled, as well as "false negatives". The OU 1071 procedure makes no attempt to control false positives; in effect we are willing to let the statistical power of the test be zero, or to take $\beta = 1$ in the notation of Chapter 7. This allows us to use somewhat smaller sample sizes than are shown in Tables Z-3 through A-10.

Note that, by controlling false positives (or even by admitting the concept of a false positive), this document implies that EPA is willing to accept a decision not to continue site cleanup even when part of a site is known to be above the cleanup standard.

The work plan does not state "that these results will lead to the conclusion that no contamination exists at that site". The statistical conclusion will be that contamination does not affect more than a fraction β of the site. The proposed decision in this case will be No Further Action, on the grounds that contamination affects less than a fraction β of the site, and is not of sufficient concern to warrant further expenditures. No matter how much sampling we do, we will never be able to conclude, statistically, that "no contamination exists at the site". 100% confidence is not achievable statistically, only nonstatistically through process or physical knowledge (we know concentrations are not less than zero) or through a census (observe everything, without measurement error).

In practice, other analyses may be performed once the data are available, such as the calculation of the probability that the SAL is exceeded using a Tchebychev bound,

$$Pr\{X \geq SAL\} \leq \frac{E(g(X))}{g(SAL)}$$

where g is any function that is nonnegative and nondecreasing on the nonnegative real numbers. (Common choices are $g(t) = t_2$ and $g(t) = e_{st}$ for some $s > 0$.) This is particularly effective if the detection level used is well below the SAL. Of course E(g(X)) will have to be estimated from the data, and a 95% upper confidence bound on this estimate should be used in the above equation. These are post-sampling data assessment procedures, however, and not very useful for designing a sampling plan.

NMED COMMENT: (5.1.1 p1) *There is not enough information provided in the Work Plan regarding final dates of the handling of RCRA wastes to determine if the Western Steam Plan qualifies as a SWMU. If it was in service until Spring 1990, and maintained the same practice since operations began, then it is not a SWMU, but a non-HWSA RCRA unit.*

RESPONSE: There is no information to document whether operations at the Western Steam plant remained unchanged throughout its history. The plant was last used in the mid-1980s.

NMED COMMENT: (5.1.6.2.1 p1) *The text in the key in figure 5-3 is misleading and should explain that sampling points shown below the outfalls and in pavement drainage areas represent generalized sampling areas and also do not represent the actual number of samples to be taken. At that depth will the samples be taken? Will the samples represent composites of shallow cores?*

RESPONSE: The text in the sampling plan states that the number and locations of sampling points will be determined in the field. While the legend of Figure 5-3 does not specifically state this, the supporting text provides adequate clarification.

See response to the first general comment for depth at which sediment samples will be taken.

NMED COMMENT: (f5-4) *The table does not provide a key explaining what the asterisk (*) represents.*

RESPONSE: The asterisk (*) key was inadvertently omitted from this figure. It means the same as all other similar figures, i.e. 50% of the samples will be analyzed. A corrected Figure 5-4 will be included in the Work Plan Modification

NMED COMMENT: (5.2.2.1 p3) *Samples take at SWMU 0-033 should also be analyzed for volatile organic compounds, since the full range of potential contaminants is unknown.*

RESPONSE: Volatile organic compounds should have been included on SWMU 0-033. The plan has been altered to include them. A corrected Figure 5-9 will be included in the Work Plan modification.

NMED COMMENT: (5.2.5.1 p2) *Wording in this paragraph suggests that field screening for organic vapor constitutes Level III/IV data. Field screening is not Level III/IV data.*

RESPONSE: The paragraph cites the use of Level II/III data, not III/IV data.

NMED COMMENT: (5.2.6.3.2 p2) *It is unclear whether samples taken from the bottom of cores that penetrate to the fill/tuff interface will actually be sampling fill or tuff. It is recommended that, at a minimum, the tuff be sampled in these cases. This concern applies to several of the proposed sampling plans in the Work Plan.*

RESPONSE: Samples at the fill-tuff interface will include both fill and tuff. This

applies to all coring in this workplan.

NMED COMMENTS: (5.4.4 p2) *The Work Plan does not provide enough information regarding the practice of using mean concentrations for contaminants over exposure units. The procedure does not appear to be acceptable.*

RESPONSE: See response to the third general comment.

NMED COMMENT: (5.5.1 p5) *Cleanup levels were determined by the DOE's LAAO for decontamination at SWMU 0-017. It is stated that cleanup that occurred in 1977 achieved those levels. What were the actual levels that were used?*

RESPONSE: Clean up levels were 25 pCi/g.

NMED COMMENT: (5.5.4 p1) *How is it proposed to decontaminate-in-place the contaminated pipe?*

RESPONSE: If it is necessary to decontaminate the pipe in place, the method/procedure to do this will be developed based on the situation, using LANL's prior experience with similar operations.

NMED COMMENT: (5.5.4 p2) *There should be verification sampling at actual locations that were found to be contaminated in the previous investigation.*

RESPONSE: There is insufficient documentation of the pipe-removal operation to locate remediated areas, precluding performing verification sampling.

NMED COMMENT: (5.5.6.3.2 p1) *This sampling plan suggests that if field screening does not indicate the presence of contamination, only a single sample will be taken, and that it will be collected from the upper-most tuff interval. It is recommended that at least two samples be taken from each core (one in the upper-most tuff interval and one in the finest-grained portion of the fill material) in the event that field screening does not detect the presence of contamination.*

RESPONSE: Since radionuclides are the major contaminants of concern, a thorough field screening will provide a reliable method for detecting the presence of radionuclides above background levels.

NMED COMMENT: (5.6.6.2.1 p1) *Sampling at only two of the sludge-drying beds does not constitute an adequate Phage I, Stage I investigation. Results from the Stage I sampling plan would not be considered adequate data for potential consideration for NFA for this SWMU.*

RESPONSE: The sampling plan is designed to take cores in the oldest sludge drying beds at the Pueblo and Bayo Canyon waste water treatment plants. These cores will reflect the entire site history rather than only part of the site history that would be reflected in cores from the younger beds. Additionally, cores are being taken from the sludge dump/fill areas, which also contain material from the earliest operations at these sites. The likelihood for contamination is greatest in the sludge fill at the Pueblo plant and sludge dump area at the Bayo plant where sludge from the drying beds was disposed. The history of the sludge drying beds at the former Central Wastewater treatment plant is not so well known. Therefore cores

will be taken at each of the four beds. The sampling plan will be modified so that a core will be taken at all four sludge drying beds in SWMU 0-019.

NMED COMMENT: (5.6.6.2.1 p1) *The figures (e.g. 5-24) should show exact, or closer approximations, of sampling points that will correspond to numbers of proposed sampling points in the text.*

RESPONSE: The screening and analysis Table for SWMU Group 0-2 (Figure 5-26) has been corrected to reflect the increase in the number of cores to be collected at SWMU 0-019 and to accurately reflect the sampling plan description. A corrected figure will be included in the Work Plan Modification.

NMED COMMENT: (5.8.4 p2) *There is no reason to believe that contaminants will be uniformly distributed, given the presence of run-off channels and certain variability in infiltration rates and amounts across the irrigated fields. Sampling should be comprehensive and especially target drainages and other low-lying areas. Stage I investigations at SWMU Aggregate 0-3 are not adequate for determining that no contamination exists and that results from the investigation could warrant NFA nomination.*

RESPONSE: The 2 ft contour interval topographic map of the golf course will be field checked and refined by a surface process geologist. That map will be then used to select sampling locations which will be preferentially sited in drainages.

NMED COMMENT: (5.8.6.2.1 p2) *Again, it appears that none of the core locations are proposed for drainages and low-lying areas on the golf course or athletic field. Are samples at the "tuff contact" collected above or below the contact?*

RESPONSE: (See preceding response). Samples at the soil-tuff contact will include both soil and tuff.

NMED COMMENT: (5.13.6.2.1 p1) *Soil gas and radiological surveys are not useful for guiding sampling locations for metals and semi-volatiles. A judgmentally-based set of sampling locations should be chosen in order to address the possibility of metals and semi-volatile contamination.*

RESPONSE: As the site history of these SWMUs is unknown, it is not unreasonable to assume that metals and semi-volatiles, if present, are distributed as are the other contaminants. Thus analysis of soil gas and/or radioactive hot spots should also show metals and/or semi-volatiles if they are present. However, to allow for the possibility that contaminants may be segregated a minimum of two cores will be judgmentally sited at each SWMU.

NMED COMMENT: (5.14.2.1 p3) *Neither Laboratory surveillance documents nor general Laboratory surveys for organics are adequate for use in determining that no releases have occurred from any specific SWMU.*

RESPONSE: Agree. The sampling plan does not make that statement. It simply states that the existing documents and surveys do not show

releases, which is different from stating that they have never occurred.

NMED COMMENT: (5.14.6.2.2 p3) *Since no adequate documentation exists as to which hazardous materials were used at this SWMU group, analyses should also target the full suite of volatile organic compounds.*

RESPONSE: Subsurface samples will be field screened for volatile organic compounds. The sediment trap samples are surface soil samples and will not be field screened for VOCs, as any VOCs would have evaporated.

NMED COMMENT: (5.15.6.3.1 p1) *Some core samples should be taken on the mesa top for verification, independent of where surface sampling and radiological screening indicate surface contamination.*

RESPONSE: If no hot spots are found, cores will be located based on best professional judgment.

Attachment 1

AIP Review of Operable Unit 1071 RFI Work Plan

State of New Mexico
ENVIRONMENT DEPARTMENT
Harold Runnels Building
1190 St. Francis Drive, P.O. Box 26110
Santa Fe, New Mexico 87502
(505) 827-2850

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October 30, 1992

Mr. Jerry Bellows, Manager
Department of Energy
Los Alamos Area Office
528 35th Street
Los Alamos, NM 87544

RE: AIP Review of Operable Unit
1071 RFI Work Plan

My Agreement In Principle (**AIP**) staff have reviewed the RCRA Facility Investigation (**RFI**) Work Plan for Operable Unit (**OU**) 1071. General and specific comments on the Work Plan are enclosed. Please address your response to these comments to this office. If you have any questions regarding technical aspects of the memo, please contact Danny Katzman of my staff at 827-4313 or 665-7127.

Sincerely,

Kathleen M. Sisneros

Kathleen M. Sisneros, Director
Water and Waste Management Division

KMS:dk

Enclosure

cc: Neil Weber, Chief, DOE Oversight
Barbara Driscoll, EPA Region 6
File, LANL, Red '92

cc w/o enclosure:
Benito J. Garcia, Chief, HRMB
Bruce Swanton, Program Manager, DOE Oversight/LANL
Ed Horst, Manager, RCRA Enforcement
Barbara Hodistchek, Program Manager, RCRA Permits

a: wp/1071kat

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M E M O R A N D U M

To: Kathleen M. Sisneros, Director
Water and Waste Management Division

Through: Benito J. Garcia, Chief
Hazardous and Radioactive Materials Bureau
Bruce Swanton, Manager
DOE Oversight Program

From: Danny Katzman
HRMB/DOE Oversight Program

Subject: Comments on the Operable Unit 1071 RFI Work Plan

Date: October 30, 1992

The Hazardous and Radioactive Materials Bureau (**HRMB**) Agreement in Principle (**AIP**) personnel have completed their review of the Operable Unit (**OU**) 1071 RCRA Facility Investigation (**RFI**) Work Plan. This memo contains HRMB's questions and concerns regarding the Work Plan. We are requesting through your office that DOE/LANL respond to our comments in writing rather than including their response in the one prepared for EPA. Part of the HRMB's mission under the AIP is to insure that environmental restoration efforts are conducted in compliance with state regulations. This goal would be compromised if DOE/LANL were to merge its response to our comments with those directed to EPA Region 6.

General Comments

Sediment sampling methodology described in the Work Plan is generally vague in that it does not state the depth at sediment samples will be taken or the specific grain size(s) that will be targeted for each site. Sediment sampling at sites (drainages) that are potentially radioactively contaminated should target silt- and clay-sized sediment because of the adsorptive properties of the finer-grained particles. The primary objective for sampling in drainages should be to assess the presence of contaminants available for transport offsite via ephemeral discharge in drainages. This can only be accomplished by knowing the actual concentration available for transport. Bulk samples that

contain a significant amount of coarse sediment will not provide an accurate assessment.

Wording in the Work Plan suggests that phased investigations **may** occur in the event that "Stage I data show that contaminants are present above action levels". Unless Stage I investigations are adequate for confidently determining the vertical and horizontal extent of contamination, Phase II investigations will be required.

The decision logic of estimating mean contaminant levels over an exposure unit has been suggested in this and several other of the Work Plans reviewed to date by the AIP staff. Our understanding is that Subpart S does not allow for the practice of contaminant "dilution" in this manner. Please explain.

Most or all of the channel sediment sampling plans propose to collect samples "as close to the outfall points as possible". This methodology for characterizing the outfall areas and associated drainages does not provide enough certainty that contaminants, if present, will be found. It is not necessarily the case that contaminants are still located in sediments immediately below the outfall points. Contaminated sediments may have moved some distance down-channel, and could be buried beneath younger sediments.

Statements like "no contamination is expected to be found" are potentially misleading and suggest a bias toward expected results of the sampling, and could be interpreted to affect early phase investigations.

It is understood that the pending HWSA Permit modification will correct the SWMU list to include only those sites that are actually SWMUs by definition. It is suspected that underground storage tanks (**USTs**) used for petroleum products will fall out of the HWSA Permit. OU 1071 contains a number of USTs, as do other locations within the Lab boundary or in the Townsite. Investigations and Voluntary Corrective Actions (**VCAs**) of USTs should be done pursuant to NMED's Underground Storage Tank Bureau (**USTB**). Registration and closure of USTs should be under the oversight of the Prevention/Inspection Program of the USTB. Confirmed or suspected releases should be reported to the Remedial Action Program of the USTB for oversight of investigation and corrective actions. Questions regarding these matters should be referred to Mr. Tony Moreland of the USTB at (505) 827-0214.

Specific Comments

2.2.3 p4 This section suggests that a given sample size (N) provides a degree of confidence (P) that not more than a certain percentage of the site exceeds action levels, and that these results will lead to the conclusion that no contamination exists at that site. Please cite and provides selected passages from peer reviewed journal article(s) where this type of statistical calculation has been used for determination of appropriate sample populations for a site.

5.1.1 p1 There is not enough information provided in the Work Plan regarding final dates of the handling of RCRA wastes to determine if the Western Steam Plant qualifies as a SWMU. If it was in service until Spring 1990, and maintained the same practice since operations began, then it is not a SWMU, but a non-HSWA RCRA unit.

5.1.6.2.1 p1
The text in the key in figure 5-3 is misleading and should explain that sampling points shown below the outfalls and in pavement drainage areas represent generalized sampling areas and also do not represent the actual number of samples to be taken. At what depth will the samples be taken? Will the samples represent composites of shallow cores?

f5-4 The table does not provide a key explaining what the asterisk (*) represents.

5.2.2.1 p3
Samples taken at SWMU 0-033 should also be analyzed for volatile organic compounds, since the full range of potential contaminants is unknown.

5.2.5.1 p2
Wording in this paragraph suggests that field screening for organic vapor constitutes Level III/IV data. Field screening is not Level III/IV data.

5.2.6.3.2 p2
It is unclear whether samples taken from the bottom of cores that penetrate to the fill/tuff interface will actually be sampling fill or tuff. It is recommended that, at a minimum, the **tuff** be

sampled in these cases. This concern applies to several of the proposed sampling plans in the Work Plan.

5.4.4 p2 The Work Plan does not provide enough information regarding the practice of using mean concentrations for contaminants over exposure units. The procedure does not appear to be acceptable.

5.5.1 p5 Cleanup levels were determined by the DOE's LAAO for decontamination at SWMU 0-017. It is stated that cleanup that occurred in 1977 achieved those levels. What were the actual levels that were used?

5.5.4 p1 How is it proposed to decontaminate-in-place the contaminated pipe?

5.5.4 p2 There should be verification sampling at actual locations that were found to be contaminated in the previous investigation.

5.5.6.3.2 p1
This sampling plan suggests that if field screening does not indicate the presence of contamination, only a single sample will be taken, and that it will be collected from the upper-most tuff interval. It is recommended that at least two samples be taken from each core (one in the uppermost tuff interval and one in the finest-grained portion of the fill material) in the event that field screening does not detect the presence of contamination.

5.6.6.2.1 p1
Sampling at only two of the sludge-drying beds does not constitute an adequate Phase I, Stage I investigation. Results from the Stage I sampling plan would not be considered adequate data for potential consideration for NFA for this SWMU.

5.6.6.2.1 p1
The figures (e.g. 5-24) should show exact, or closer approximations, of sampling points that will correspond to numbers of proposed sampling points in the text.

5.8.4 p2 There is no reason to believe that contaminants will be uniformly distributed, given the presence

of run-off channels and certain variability in infiltration rates and amounts across the irrigated fields. Sampling should be comprehensive and especially target drainages and other low-lying areas. Stage I investigations at SWMU Aggregate 0-E are not adequate for determining that no contamination exists and that results from the investigation could warrant NFA nomination.

5.8.6.2.1 p2

Again, it appears that none of the core locations are proposed for drainages and low-lying areas on the golf course or athletic field.
Are samples at the "tuff contact" collected above or below the contact?

5.13.6.2.1 p1

Soil gas and radiological surveys are not useful for guiding sampling locations for metals and semi-volatiles. A judgmentally-based set of sampling locations should be chosen in order to address the possibility of metals and semi-volatile contamination.

5.14.2.1 p3

Neither Laboratory surveillance documents nor general Laboratory surveys for organics are adequate for use in determining that no releases have occurred from any specific SWMU.

5.14.6.2.2 p3

Since no adequate documentation exists as to which hazardous materials were used at this SWMU group, analyses should also target the full suite of volatile organic compounds.

5.15.6.3.1 P1

Some core samples should be taken on the mesa top for verification, independent of where surface sampling and radiological screening indicate surface contamination.

Attachment 2

Referenced Documents

Mathematical Geology

The official journal of the International Association for Mathematical Geology

Formerly *Journal of the International Association for Mathematical Geology*

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Bounding the Required Sample Size for Geologic Site Characterization[1]

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The proposed objective of limited sample geologic site characterization is to minimize the chance of unknown and unexpected extremes. This problem proves to be extremely difficult when the data are spatially correlated. A generalization of the classical one-sided nonparametric tolerance interval, based upon the statistical concept of associated random variables, establishes a rigorous, almost distribution-free, tool for computing the minimum required sample size for site characterization. An upper bound on the required number of samples follows from a heuristic measure for the quantity of information in a spatially dependent sample; the measure presented is the equivalent number of uncorrelated samples and is calculated using an estimated variogram. An empirical check of the upper and lower bounds, using more than 2 million simulations and seven real data sets produces a heuristic rule for quantifying the required number of samples.

KEY WORDS: sample design, site characterization, associated random field, nonparametric tolerance interval.

INTRODUCTION

This paper starts from the premise that estimating a spatial average is not the usual objective of geologic site characterization. Rather, it is often more important to collect samples that accurately represent the underlying distribution for the variable of interest; particularly, samples that reflect extreme values of the distribution.

Consider the following example. Although the average fracture density will ultimately be useful in the geotechnical design of a high-level nuclear waste repository, the initial geological site characterization must focus on locating and quantifying the most fractured zones. For it is these highly fractured areas that will most significantly affect the evaluation of the site. In this situation, the sampling objective is to assess the upper tail of the distribution, not to better estimate a mean. Other equivalent examples occur during economic feasibility

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analysis of a greatly variable gold ore deposit, and the assessment of a potentially contaminated hazardous waste site.

If the variable of interest does not exhibit spatial correlation, the common tools of mathematical statistics (e.g., tolerance intervals) could be used to answer many of most pressing questions. How many samples have to be collected to achieve a prescribed level of certainty? With the samples already collected, how certain can the conclusions be? How can different competing sampling objectives best be balanced? However, spatial correlation is more often the rule than the exception.

This paper presents and attempts to motivate a computationally simple heuristic that incorporates the spatial correlation of geologic data by converting the actual number of samples N to an equivalent number of uncorrelated samples N'.

BACKGROUND

Optimal sample network design is a well-studied problem. The published theoretical and applied works span 50 yr, encompass many disciplines, and include more than 40 technical papers in the last decade alone. However, to date, the published research in this field has focused on the goal of improved estimation of a mean. In some cases, the problem is estimation of punctual values and in other cases the problem is estimation of areal or volumetric spatial averages. The ensuing objective function for network design has always been one of three possibilities:

- minimize an estimation variance using a specified number of samples
- minimize the number of samples required to achieve a specified level of the estimation variance, or
- minimize a cost function that combines the estimation variance and the cost of samples

and Rodríguez-Iturbe (1985) give a lucid discussion of these different cases.

In contrast, the goal of geologic site characterization is expressed here as the construction of an appropriate model for the problem at hand (develop a suitable working hypothesis). The initial objective of sample design must be to collect enough information to build this original appropriate model. After building this model, the sampling objective becomes to minimize the chance of surprises, i.e., to minimize the probability of the existence of unknown features requiring a radical modification to the model.

An ore genesis model would be an example of the models constructed during geologic site characterization: "This deposit is of hydrothermal origin, includes only one intrusive event, and was structurally controlled." Alternatively, the modeling might involve the selection of suitable engineering design tools: "An isotropic boundary element computer code may be used to analyze/design this underground opening." A surprise in the first example might be the existence of an unknown fault zone through the deposit; in the second example, an unmeasured and unexpectedly large variation in the orientation of principal field stresses could constitute a surprise.

TOLERANCE INTERVALS

Roughly speaking, an important characteristic of a set of geologic samples is that they adequately represent a long distributional tail, if such a tail exists. A finite set of geologic samples will not capture the greatest value over the field of interest, serendipity notwithstanding (Galambos, 1979, p. 156–173; Adler, 1981, p. 159–167). A statistician's demand that the collected samples statistically cover the underlying distribution is a wiser position.

Nonparametric tolerance intervals (e.g., David, 1981, p. 18–19) offer a simple, robust tool for assessing the probable sample set coverage. The issues addressed by tolerance intervals are typified by the following question:

> Given that N samples are collected in a well-defined manner, what is the probability (P) that the corresponding maximum sample value is greater than or equal to the β percentile of the underlying distribution?

(Tolerance intervals are much more general than indicated here; however, for the sake of presentation clarity, this discussion will focus on the large-value extremes.)

For independent, identically distributed random variables, the relevant computational formula is astonishingly simple (Mood et al., 1974, p. 252)

$$\Pr(\text{maximum of } N \text{ samples} \geq \beta \text{ percentile}) = 1 - \beta^N \qquad (1)$$

Given the acceptable probability of coverage P, Eq. (1) can be solved for a lower bound on the necessary sample size

$$N_{\text{low}} = \log(1 - P)/\log(\beta) \qquad (2)$$

This formula is independent of the underlying distribution shape, distribution mean, and distribution variance. Intervariable correlations, however, can not be ignored.

The classic development of nonparametric tolerance intervals begins with an assumption of independent, identically distributed random variables. This is unrealistic for the geologic environment—in general, geologic site characterization data are not independent.

The exact calculation for the probability of coverage by a spatially correlated sample set requires the evaluation of a multivariate probability integral. Even in the simplest case (multivariate normal), such evaluations are computationally intractable (Johnson and Kotz, 1976, p. 43); further, direct computations always demand an explicit distributional assumption. Bounding the probability, using as few assumptions as possible, offers a more pragmatic alternative.

The pertinent formula, Eq. (1), has two parameters: β and N. An intuitively appealing revision to this formula incorporates the spatial correlation by converting N to an equivalent number of uncorrelated samples N_{eq}. Thus, the revised formula reads

$$\Pr(\text{maximum of } N \text{ correlated samples} \geq \beta \text{ percentile}) = 1 - \beta^{N_{eq}} \quad (3)$$

Continuing, the parallel for Eq. (2) yields the design requirement

$$N_{eq} \geq N_{low} = \log(1 - P)/\log(\beta) \quad (4)$$

Equation (4) provides the basis for bounding the required number of samples for site characterization. The difficulty is, of course, in calculating N_{eq}.

UPPER BOUNDS ON N_{eq}

Under a mild assumption (discussed below) the probability of acceptable coverage is bounded above

$$\Pr(\text{maximum of } N \text{ correlated samples} \geq \beta \text{ percentile}) \leq 1 - \beta^{N} \quad (5)$$

thus, the equivalent number of uncorrelated samples is bounded above by

$$N_{eq} \leq N \quad (6)$$

A sufficient condition for Eq. (5) is that samples be drawn from associated random variables (Esary et al., 1967, Theorem 5.1). The set of random variables $X_1, \ldots, X_n$ are said to be associated if

$$\mathrm{Cov}\left[f(X_1, \ldots, X_n), g(X_1, \ldots, X_n)\right] \geq 0$$

for all nondecreasing functions f and g for which the covariance exists (Esary et al., 1967). A weaker sufficient condition for Eq. (5) requires that the random variables be "positively orthant dependent" (generalizing Lehmann, 1966)

$$\Pr(X_1 \geq x_1, \ldots, X_n \geq x_n) \geq \Pr(X_1 \geq x_1) * \cdots * \Pr(X_n \geq x_n)$$

Positive orthant dependence is implied by association (Rüschendorf, 1981), and it is implied also by a number of other, often weaker, conditions (e.g., Karlin and Rinott, 1980; Block and Ting, 1981; Alan and Saxena, 1981; Shaked, 1982).

Pitt (1982) shows that multivariate normal random variables are associated if and only if their intervariable correlations are nonnegative. Esary et al. (1967, p. 1467) prove that any set of nondecreasing functions of associated random variables are associated. Thus, Eqs. (5) and (6) rigorously hold for any set of random variables that can be transformed to multinormality using nondecreasing functions where the resulting intervariable correlations are nonnegative. (Note: the allowed transformations are far more general than a simple normal

score transformation). This is a sufficient condition, not a necessary condition. A more complete characterization of the necessary conditions for association (positive orthant dependence) is at the forefront of current statistical research (e.g., Shaked and Tong, 1985; Eaton, 1987).

Within geostatistics, the assumptions behind normal and lognormal kriging (Rendu, 1979), and multi-Gaussian kriging (Verly, 1983) lead directly to Eq. (6), as long as the sample-to-sample correlations are nonnegative; however, such distributional assumptions are not required. The experiments, described below, support the confident application of the upper bound given by Eq. (6) if the underlying variogram has a sill and is monotonically increasing (e.g., the spherical, exponential, or Gaussian models).

LOWER BOUNDS ON N_{eq}

For independent, identically distributed random variables, the underlying population mean is estimated most commonly by the arithmetic average of sample values: Sum all values and divide by N. The estimation variance σ^2_{avg} for the arithmetic average of N samples is given by the well-published formula

$$\sigma^2_{avg} = \sigma^2_{pop}/N$$

where σ^2_{pop} is the population variance. Turning this equation around yields the following formula for N

$$N = \sigma^2_{pop}/\sigma^2_{avg} \quad (7)$$

In the case of correlated random variables, the underlying population mean can be estimated by ordinary kriging (Matheron, 1971, p. 125, 126); the resulting estimation variance is called the global kriging variance. This offers a simple, intuitively appealing method for quantifying the effective number of uncorrelated samples N_{eff} (even if global kriging is not used). In a parody of Eq. (7), define N_{eff} as

$$N_{eff} \equiv \sigma^2_{pop}/\sigma^2_k \quad (8)$$

where σ^2_k is the kriging variance from estimation of the underlying population mean using all available samples. As derived in Appendix A, Eq. (8) algebraically reduces to the simple formula

$$N_{eff} = \mathbf{1}'\boldsymbol{C}^{-1}\mathbf{1} \quad (9)$$

where $\boldsymbol{C}$ is the sample-to-sample correlation matrix and $\mathbf{1}$ is a vector of ones. In words, N_{eff} equals the sum of all terms in the inverse of the sample-to-sample correlation matrix. The specific computational details for efficiently evaluating Eq. (9) are presented in Appendix B.

N_{eff} [Eq. (9)] is a heuristic estimate for N_{eq} of Eq. (4). Although not rigorously derived, N_{eff} possesses a number of proper attributes. For example, if the samples are mutually independent, C^{-1} is an identity matrix and N_{eff} equals N. Conversely, as sample-to-sample correlations increase, N_{eff} will decrease asymptotically to 1. Thus, at both extremes of the degree in correlation, N_{eff} equals N_{eq}.

Because N_{eff} is a heuristic, its use must be numerically tested. The numerical check, discussed in detail below, incorporates 2.4 million geostatistical simulations and seven real world data sets. The results are clear: N_{eff} underestimates the equivalent number of uncorrelated samples. That is, the heuristic N_{eff} produces a lower bound for N_{eq}

$$N_{eff} \leq N_{eq} \tag{10}$$

EMPIRICAL ESTIMATE OF N_{eq}

Equation (6) gives an upper bound for N_{eq}, Eq. (10) gives a lower bound; unfortunately, the distance between these bounds can be large. For geological sampling design, an ignorant estimate of N_{eq} could be built by taking the point halfway between the two bounds; however, a better approach is available.

Using the computer as a laboratory, the following numerical experiment was carried out.

Step (1) Randomly locate N hypothetical sample points within a predefined area. Use a uniform distribution for each coordinate; this is known as a planar Poisson process (Karlin and Taylor, 1981, p. 398–404).

Step (2) Using a predetermined variogram function, compute N_{eff} [Eq. (9)] for the sample location geometry. The variogram is defined by the multivariate distribution function used in Step (3).

Step (3) Using a predetermined multivariate distribution function consistent with the variogram used in Step (2), geostatistically simulate values for each of the N locations. Determine and save the largest of the N simulated values.

For the same sample locations, variogram, and distribution, repeat Step (3) 10,000 times, generating a long list of "largest out of N" values.

Step (4) Using the quasimaximum likelihood method (Appendix C), estimate the true N_{eq} for the simulated setup from the list of "largest out of N" values.

This experiment was replicated 240 times using values of N ranging from 5 to 70, a spherical variogram with ranges varying from 0.1 to 10 times the length of the sampled area, variogram nugget effects varying from 0 to 100% of the

sill, and multivariate normal, multivariate lognormal (Johnson and Kotz, 1976), and multivariate χ^2 (Adler, 1981) distributions.

Using the techniques of graphical and numerical exploratory data analysis (e.g., Tukey, 1977), an empirical relationship between N_{eff} and N_{eq} was found

$$N_{eq} \approx N_{eff} * \exp(1 - N_{eff}/N) \tag{11}$$

Although such a purely phenomenological result lacks rigor and lacks foundational understanding, it does satisfy four important criteria for being a useful geological tool. (1) It is a simple, computationally tractable formula. (2) It conforms to the required values at the extremes. (3) It fits the controlled experimental data remarkably well (Fig. 1). (4) No better relationship is known.

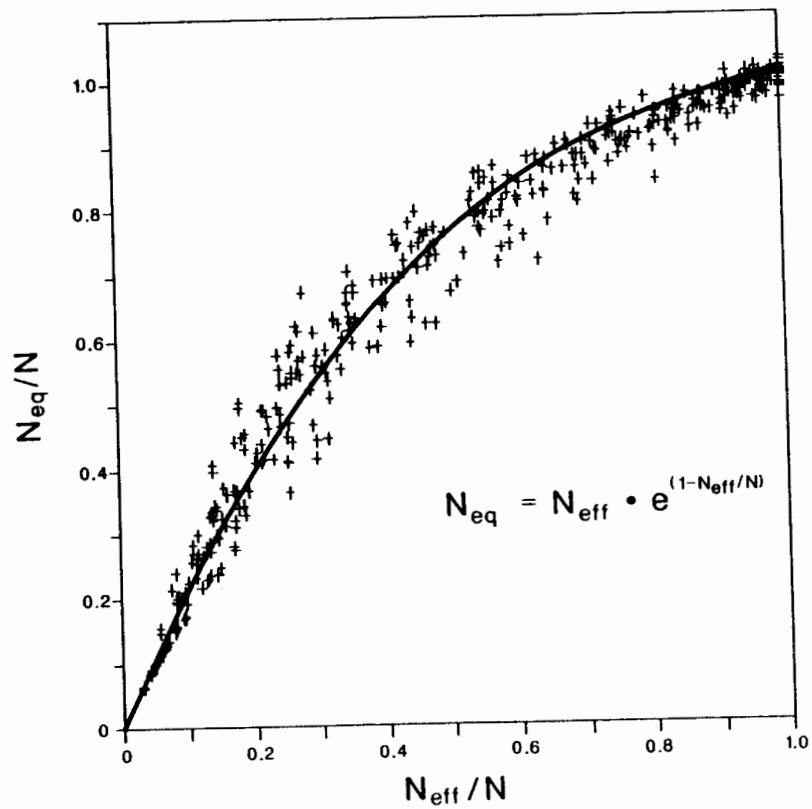

Fig. 1. N_{eq} as a function of N_{eff} using 2.4 million simulations.

A CRITICAL EXPERIMENT

Equation (9) presents a formula for calculating N_{eff} given the variogram and sample locations, Eq. (11) maps N_{eff} into N_{eq}, and Eq. (3) makes a strong probability statement using N_{eq}. Thus, a model is available for estimating N_{eq} using the sample location geometry and the estimated variogram. This model was subjected to the following critical experiment in an effort to refute its application with real data.

Step (1) Select a data set of interest, a percentile of interest (β), and a subset size N (less than 10% of the original data set).

(The data set must be large enough to enable accurate estimation of the variogram and the true β percentile of the underlying distribution.)

Step (2) Randomly select a subset of size N from the original data set.

Step (3) Using the "known" variogram, Eq. (9), Eq. (11), and Eq. (3) calculate and save p_i for the current subset; where

$$p_i = 1 - \beta^{N_{eq}}$$

(The p_is are heuristic assessments of the probability that the largest of the N samples is greater than the β percentile of the distribution.)

Step (4) Determine the largest value included in the selected subset and compare it to the "known" β percentile. Let T_i equal 1 if the largest value is greater than the β percentile and 0 otherwise.

Using the original data set, repeat Step (2) through Step (4) M times, counting the number of cases where the largest subset value is greater than the β percentile.

If the N_{eq} concepts presented are appropriate for the data set under investigation, the individual T_is are Bernoulli random variables with parameters p_i (Mood et al., 1974, p. 87–90). Thus, the total number of times that the largest subset value is greater than the β percentile will approximately follow a binomial distribution. Using the normal approximation to the binomial distribution, the sum of the T_is will be approximately normal with the mean and variance given by

$$\mu = \sum_{i=1}^{M} p_i$$

$$\sigma^2 = \sum_{i=1}^{M} p_i(1 - p_i)$$

Thus, a standard statistical hypothesis test can be performed as a reasonable check on the N_{eq} concepts. Note, however, that this check is not a rigorous hypothesis test because it ignores the potential correlations between the T_is.

Table 1. Empirical Validation of the N_{eq} Concept (β = 95th percentile)

Case[a]	S[b]	N[c]	Actual count	Expected count	Computed[d] Z score
A	250	25	546	547	−0.08
B	203	20	467	474	−0.46
C	248	24	514	535	−1.42
D	305	30	605	600	+0.34
E	154	15	415	401	+0.96
F	186	18	465	444	+1.30
G	109	10	267	286	−1.34

Note: [a] A, Thickness of a geologically simple coal seam; B, Depth to an identified rock strata; C, Percent sulfur of a western U.S. coal deposit; D, Gold assay grades on a bench of a surface mine; E, Soil subgrade strength values R; F, Soil contamination values; G, Permeability of an identified aquifer.
[b] S = Original data set size.
[c] N = Selected proper subset size.
[d] Z score = (actual − expected)/(standard deviation).

The experiment discussed above was carried out on seven different data sets using a β of 95% and an M of 1000. The results (Table 1) demonstrate in all cases that the N_{eq} concepts prove satisfactory; that is, they appear to comprise a useful tool.

ONE APPLICATION FOR THE TOOL

The following five-step approach captures the essential concepts in a simple two-phase sampling strategy.

Step (1) Considering the risk economics of the question at hand, select an appropriate percentile β and probability of coverage P.

Step (2) Using Eq. (6) and Eq. (4), calculate the lower bound on the number of samples required, N_{low}.

Step (3) Using all available information, locate and collect N_{low} samples. This will be called Phase I sampling.

Step (4) Using the N_{low} samples collected during Phase I, estimate the variogram for the site.

Step (5) Solicit Phase II candidate sampling plans in an ordinary manner but, using the estimated variogram Eq. (9) and Eq. (11), select only from the plans which satisfy Eq. (4).

The important point in this approach is the use of the lower bound given by Eq. (6) and Eq. (4) to determine the number of Phase I samples. This lower bound is independent of the underlying variogram. Only after Phase I samples have

been collected and the variogram estimated is the more sophisticated N_{eq} concept applied to the problem.

LIMITATIONS AND ASSUMPTIONS

Two significant limitations must be emphasized. First, derivation of Eq. (9) (Appendix A) assumes that the population to be characterized has a large geographic extent relative to the range of the variogram. This assumption does not, however, require that the actual collected samples be distributed across the entire geographic population. Specifically, the correlation between any single sample and the population as a whole must be effectively zero. Practically speaking, this requires that the geographic extent of the population to be characterized be greater than three or four variogram ranges.

Although this first shortcoming may be eliminated by redefining N_{eff} to incorporate the kriging variance associated with estimation of a proper subset of the geographic population (e.g., a block) rather than the entire population, this has not yet been investigated.

Second, calculation of N_{eff} is explicitly based on the variogram. Thus, if the variogram is ill-defined (poorly or improperly estimated), N_{eff} is ill-defined. In such situations, sensitivity analysis must be carried out to determine the significance of the uncertainty in the variogram parameters as it should be in any geostatistical application.

CONCLUSIONS

In initial geologic site characterization, assessing extreme values is usually a serious concern, not estimating a spatial average. That is, the objective of site characterization is to minimize the chance of surprises; this can be quantified by the probability of unknown and unexpected extremes. In such situations, nonparametric tolerance intervals are an appropriate tool.

For a given level and probability of distributional coverage, a lower bound on the required number of samples can be calculated using the concepts of associated random variables when considering spatially correlated data. This lower bound can be computed before a variogram is estimated and even before any samples are taken.

Given the appropriate variogram, a site characterization sampling design can be summarized by a heuristic equivalent number of uncorrelated samples, N_{eq}. Using N_{eq}, the standard formulas for nonparametric tolerance intervals offer a powerful set of tools for site characterization sampling design.

A critical experiment was carried out on seven real cases. Despite the fact that these seven cases support the proposed heuristic model, they do not "validate" the approach; rather, they merely fail to invalidate. The model must be applied to many more data sets, by many different scientists and engineers, and only if the evidence supports the model may it then be considered validated.

APPENDIX A: DERIVATION OF N_{eff}

In general, the ordinary kriging system (e.g., Rendu, 1978, p. 61) can be written in partitioned matrix form as

$$\begin{bmatrix} \mathbf{A} & \mathbf{1} \\ \mathbf{1}' & 0 \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{1} \end{bmatrix} \tag{A1}$$

where $\mathbf{A}$ is the sample-to-sample covariance matrix, $\mathbf{1}$ is a vector of all ones, $\mathbf{1}'$ is its transpose, $\mathbf{b}$ is the vector of covariances between the samples and the object to be estimated, $\mathbf{w}$ is the vector of kriging weights, and λ is the Lagrange multiplier associated with the unbiasedness constraint. Similarly, the general formula for the estimation variance of kriging can be written in partitioned matrix form as

$$\sigma_k^2 = \sigma_v^2 - [\mathbf{b}' \quad \mathbf{1}] \begin{bmatrix} \mathbf{w} \\ \lambda \end{bmatrix} \tag{A2}$$

where σ_k^2 is the kriging variance (estimation variance) and σ_v^2 is the dispersion variance of the object to be estimated.

When computing the estimation variance for the underlying population mean, $\mathbf{b}$ and σ_v^2 are equal to zero (Matheron, 1971, p. 125–126). Taking advantage of this simplification, solving Eq. (A1) for the vector of kriging weights, and substituting the resulting solution into Eq. (A2) produces

$$\sigma_k^2 = -[\mathbf{0}' \quad \mathbf{1}] \begin{bmatrix} \mathbf{A} & \mathbf{1} \\ \mathbf{1}' & 0 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ \mathbf{1} \end{bmatrix} \tag{A3}$$

Expanding Eq. (A3), the kriging variance is seen to be the negative of the lower right-hand term of the kriging matrix inverse. Employing Proposition 32 of Dhrymes (1978, p. 38–39) on Eq. (A3), the kriging variance is given by

$$\sigma_k^2 = 1/(\mathbf{1}' \quad \mathbf{A}^{-1} \quad \mathbf{1}) \tag{A4}$$

In words, Eq. (A4) states that the estimation variance from kriging the underlying population mean equals the reciprocal of the sum of all terms in the inverse of the sample-to-sample covariance matrix.

Substituting Eq. (A4) into Eq. (8), the effective number of independent samples is given by

$$N_{eff} = \sigma_{pop}^2(\mathbf{1}' \quad \mathbf{A}^{-1} \quad \mathbf{1}) \tag{A5}$$

Factoring the reciprocal of the population variance out of the covariance matrix inverse cancels the scalar term σ_{pop}^2 and provides the desired result

$$N_{\text{eff}} = \mathbf{1}' \ \mathbf{C}^{-1} \ \mathbf{1} \tag{A6}$$

Thus, N_{eff} equals the sum of all terms in the inverse of the sample-to-sample correlation matrix.

APPENDIX B: COMPUTING N_{eff}

Equation (9) states that N_{eff} equals the sum of all terms in the inverse of the sample-to-sample correlation matrix. In principle, a computer program could set up the entire sample-to-sample correlation matrix, compute the matrix inverse, and then add up all of the terms. This is, however, far more computational work than is actually necessary.

Because **C** is a correlation matrix, it is symmetric and (if all of the geologic samples are unique) positive-definite (Graybill, 1983, Theorem 8.7.2, p. 214). It follows that **C** is amenable to Cholesky decomposition (Golub and Van Loan, 1983, Theorem 5.2-3, p. 88)

$$\mathbf{C} = \mathbf{L} \ \mathbf{L}' \tag{B1}$$

where L is a lower triangular matrix with positive-diagonal entries. Applying the rules of matrix inversion to Eq. (B1)

$$\mathbf{C}^{-1} = (\mathbf{L}^{-1})' \ (\mathbf{L}^{-1}) \tag{B2}$$

follows directly. Substituting Eq. (B2) into Eq. (9) yields

$$N_{\text{eff}} = \mathbf{1}' \ (\mathbf{L}^{-1})' \ (\mathbf{L}^{-1}) \ \mathbf{1} \tag{B3}$$

Letting vector **z** be defined by $\mathbf{z} = \mathbf{L}^{-1} \ \mathbf{1}$

$$\mathbf{Lz} = \mathbf{1} \quad \text{and} \tag{B4}$$

$$N_{\text{eff}} = \mathbf{z}' \ \mathbf{z} \tag{B5}$$

The resulting algorithm for efficiency computing N_{eff} has four steps:

Step (1) Set up the sample-to-sample correlation matrix **C**; because **C** is symmetric, setting up the lower triangular portion is sufficient.

Step (2) Carry out the Cholesky decomposition of $\mathbf{C} = \mathbf{L} \ \mathbf{L}'$ (e.g., Golub and Van Loan, 1983, Algorithms 5.2-1, p. 89). In the pathological case where two or more of the geologic samples are perfectly correlated, a subset selection process would be required before the Cholesky decomposition (e.g., Golub and Van Loan, 1983, Sec. 12.2, p. 414–419).

Step (3) Using a forward elimination algorithm, solve Eq. (B4) for **z** (e.g., Golub and Van Loan, 1983, Algorithm 4.1-1, p. 53).

Step (4) Calculate N_{eff} using Eq. (B5).

APPENDIX C: M.L.E. FOR N_{eq}

Consider the following thought experiment. N independent, identically distributed random values are generated from known distribution $F_X(x)$: $\{x_1, \ldots, x_N\}$. The actual count N is unknown; only the largest generated value is available. If this procedure is repeated M times, how can the unknown parameter N be estimated?

The maximum likelihood method of estimation is particularly attractive in this situation. Letting the largest value of the ith repetition be y_i, the parametric distribution function for the random variable Y_i is

$$F_Y(y_i; N) = F_X(y_i)^N$$

If the parametric density function exists for Y_i, it is given by

$$f_Y(y_i; N) = NF_X(y_i)^{(N-1)} f_X(y_i)$$

From this, the log-likelihood function for the y_i is

$$M \log [N] + (N-1) \sum_{i=1}^{M} \log [F_X(y_i)] + \sum_{i=1}^{M} \log [f_X(y_i)]$$

Setting the derivative of the log-likelihood function with respect to N equal to zero and solving for N yields the maximum likelihood estimator of N

$$N_{\text{MLE}} = -M \Big/ \sum_{i=1}^{M} \log [F_X(y_i)]$$

This maximum likelihood estimator exhibits the appealing properties of statistical consistency and asymptotic efficiency (Mood et al., 1974, p. 358–362). In particular, the asymptotic variance of the estimator is N^2/M.

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The Geometric Signature: Quantifying Landslide-Terrain Types from Digital Elevation Models[1]

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Topography of various types and scales can be fingerprinted by computer analysis of altitude matrices (digital elevation models, or DEMs). The critical analytic tool is the geometric signature, a set of measures that describes topographic form well enough to distinguish among geomorphically disparate landscapes. Different surficial processes create topography with diagnostic forms that are recognizable in the field. The geometric signature abstracts those forms from contour maps or their DEMs and expresses them numerically. This multivariate characterization enables once-intractable problems to be addressed. The measures that constitute a geometric signature express different but complementary attributes of topographic form. Most parameters used here are statistical estimates of central tendency and dispersion for five major categories of terrain geometry; altitude, altitude variance spectrum, slope between slope reversals, and slope and its curvature at fixed slope lengths. As an experimental application of geometric signatures, two mapped terrain types associated with different processes of shallow landsliding in Marin County, California, were distinguished consistently by a 17-variable description of topography from 21 × 21 DEMs (30-m grid spacing). The small matrix is a statistical window that can be used to scan large DEMs by computer, thus potentially automating the mapping of contrasting terrain types. The two types in Marin County host either (1) slow slides: earth flows and slump-earth flows, or (2) rapid flows: debris avalanches and debris flows. The signature approach should adapt to terrain taxonomy and mapping in other areas, where conditions differ from those in Central California.

KEY WORDS: geomorphology, hazard analysis, terrain classification, topography.

INTRODUCTION

The quantification of landform analysis from digital elevations is a developing emphasis in geomorphology. It has evolved from the long-recognized need to characterize topography in terms more exact than "flat," "rolling," or "hilly" (Wolfanger, 1941; Wood and Snell, 1960). Much of the current impetus to treat landform numerically derives from mapping-intensive programs for the assessment and mitigation of natural hazards, such as landslides (U.S. Geological Survey, 1982; Carrara, 1984).

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