

INTERPRETATION OF REGIONAL GEOCHEMISTRY USING OPTIMAL INTERPOLATION PARAMETERS†

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Abstract—A collection of data analysis procedures is presented which are derived from estimation of geographic interpolation parameters. Several interpolation models are discussed along with a procedure to obtain the best model. The power parameter, p , and the search radius, c , are the standard parameters in inverse distance weighting interpolation which is appropriate for sampling patterns that are not highly irregular. The power parameter is shown to characterize the regional behavior of geochemical measurements. This characterization process can be used to associate similar types of geochemical measurements, produce optimal contour maps, derive meaningful residual maps, and highlight unusual geochemical areas by a weighted sum variable. The computer program, BESTP, (used to estimate the optimum inverse distance weighting interpolation parameters) is presented, along with an example using reconnaissance groundwater data from the Plainview Quadrangle, Texas.

Key Words: Interpolation, Contouring, Mapping, Residual maps, Weighted sum, Anomaly identification, Geochemistry, IDW, BESTP.

INTRODUCTION

Interpolation methods often are used prior to contouring data because most contouring procedures require values on a regularly-spaced grid. Most interpolation procedures require specification of several parameters and it is known that the appearance of resulting contours can change drastically, depending on the choice of parameters. Because contour maps are often an important aspect of data analysis, it is reasonable to consider procedures which allow the choice of optimal contouring parameters. The computer program BESTP enables determination of optimal power parameter in the inverse distance weighting (IDW) interpolation model.

By-products of the optimal interpolation procedure are equally important for the interpretation of regional geochemistry. It is possible to compute confidence intervals for the power parameter and estimate the variance associated with the estimation process. Geochemical measurements can be grouped to characterize the regional geochemistry. Various different estimation models can be compared such as IDW, trend surface analysis (TSA), and Kriging. Finally, standard residual maps and detailed analysis methods such as weighted sum maps (Garrett, Kane, and Zeigler, 1980) can be improved.

The next section considers various estimation models relevant to interpolation, and the following section gives parameter estimation procedures with associated confidence intervals. Then, the estimation procedure is applied to regional geochemical data and a data evaluation process is given which is a natural consequence of the modeling and estimation in the previous sections. The final section discusses the computer program, BESTP, used for estimation.

INTERPOLATION MODELS

The traditional approaches to contouring can be divided into global and local fit algorithms. The usual global algorithm is trend surface analysis (TSA), where only the location of a point is used to determine its predicted value. Various modifications fit surfaces in local regions of the point being estimated. Local fit algorithms select a subset of the points surrounding the point being estimated and use the measured values for estimation. To formalize the preceding concepts, consider n sample locations from a geochemical population which are identified by an observation $z(x_i, y_i)$ which may be abbreviated by z_i corresponding to the location (x_i, y_i) for $i = 1, \dots, n$ where x_i is the decimal degree longitude, y_i is the decimal degree latitude, and z the measured quantity. Consider a location (x, y) for which a predicted z -value, \hat{z} , is desired. For example, (x, y) could be a grid node in an automatic contouring algorithm and \hat{z} the estimated value to be used in contouring. The value of z is assumed to take the form

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$$z(x, y) = f(z_1, \dots, z_n | \beta) + \epsilon \quad (1)$$

where f is a function specified by the algorithm, and β is a vector of unknown parameters. The random error ϵ is assumed to have 0 mean and variance σ^2 which is a standard assumption for nonlinear estimation (Draper and Smith, 1981).

A question that arises in the use of equation (1) is whether z should be expressed in its observed units (untransformed scale) or another scale will increase the prediction accuracy. Expression of z in a logarithmic scale may sometimes be appropriate since geochemical variables often are distributed lognormally. However, the combined lognormal distribution of variables does not consider any spacial dependence of the observations. The model in log scale is

$$\log z(x, y) = f(\log z_1, \dots, \log z_n | \beta) + \epsilon. \quad (2)$$

Note that equation (2) results in biased estimates of $z(x, y)$. Alternatively, since estimation often is considered applicable to the original scale, it is desirable to use a back-transformation model,

$$z(x, y) = \exp\{f(\log z_1, \dots, \log z_n | \beta)\} + \epsilon. \quad (3)$$

Models in the form of equations (1) or (3) are preferable to equation (2) since estimation is in the original scale of measurement and unbiased estimates are obtained for $z(x, y)$.

The form of equation (1) for TSA is a polynomial function in x and y ,

$$z = \beta_0 + \beta_1 x + \beta_2 y + \beta_3 xy + \beta_4 x^2 + \dots + \epsilon. \quad (4)$$

The major objection to TSA is that in equation (4), there is no local influence of the z_i 's for points close to (x, y) ; every point z is hypothesized to be only a function of regional trend. This assumption is expected rarely to be true for geochemical data.

There are numerous local fit approaches, a frequent formulation is

$$z(x, y) = \sum_{i=1}^n a_i z_i + \epsilon \quad (5)$$

where $a_i = w_i / \sum_{j=1}^n w_j$ and

$$w_i = \begin{cases} 0 & \text{if } r_i > c \\ r_i^{-p} & \text{if } r_i \leq c \end{cases} \quad (6)$$

with r_i the distance from a point (x, y) to (x_i, y_i) in statute miles, $r_i = 90.96[\cos(y \cdot 180/\pi)(x - x_i)^2 + (y - y_i)^2]^{1/2}$. The log transformation procedure replaces z and z_i in equation (5) by $\log z$ and $\log z_i$, where the back-transformation estimation equation is of the form

$$\begin{aligned} z(x, y) &= \exp\left\{\sum_{i=1}^n a_i \log(z_i)\right\} + \epsilon \\ &= \prod_{i=1}^n z_i^{a_i} + \epsilon. \end{aligned} \quad (7)$$

For $p = 0$, $z(x, y)$ is estimated by either the arithmetic or geometric mean using equation (5) or (7), respectively. Variations of the functional form of equation (6) include different procedures for selecting the points having non-zero weights. Sampson (1978) implemented procedures which include choosing a specified number of nearest neighbors and recognizing a specified number of points in each quadrant or octant around z .

The search radius c in equation (6) is the assumed radius of influence of z_i on z , and the w_i 's are weights for the z_i 's, which decrease with increasing distance from z for $p > 0$. These weights are a function of the power parameter p which along with c serve as the parameter β in (1). However, there is a high degree of correlation between p and c because increases in c can be offset by increasing p . Also, increasing c increases the number of nonzero w_i in equation (5) which can add appreciably to the computational time required for estimation. Thus, it is reasonable to fix c in equation (6) and estimate p , but several values of c can be considered and compared by the criteria given in the next section.

PARAMETER ESTIMATION

The estimation of the parameters in any of the models requires an optimization function. Regional geochemical data are convenient in that n is typically large (for example, $n > 200$) and it is possible to extract a representative validation data set of size n' (for example, $n' = n/4$). The prediction data set of $n-n'$ samples then can be used to estimate the n' validation samples. A natural choice for optimization is to attempt to minimize the residuals $[z_i - \hat{z}_i(\beta)]^2$ for $i = 1, \dots, n'$ where $\hat{z}_i(\beta)$ is a function of the prediction data set. A convenient function to minimize is the normalized least-squares function

$$S(\beta) = \frac{\sum_{i=1}^{n'} [z_i - \hat{z}_i(\beta)]^2}{\sum_{i=1}^{n'} (z_i - \bar{z})^2} \quad (8)$$

where \bar{z} is the sample mean of the validation samples. It should be noted that estimation using the validation samples is similar to jack-knifing (or leaving-one-out) in statistical applications (Lauchenbruch, 1975, p. 32) where estimation is improved by not considering all n samples. For the situation where n is small ($n < 100$), the BESTP computing procedure described later could be modified to repeat the estimation process n times in a classical jack-knifing application.

In the linear regression context, the multiple correlation coefficient, R^2 , and $S(\beta)$ are simply related for $n' = n$ by $S(\beta) = 1 - R^2$ and equation (8) has intuitive appeal for the nonlinear models considered in the previous section. If $S(\beta) > 1$, then on the average it would be better to replace \hat{z}_i by \bar{z} , which would imply the estimation process generally is not useful. Also, various estimation methods can be compared using equation (8). Thus, values of $S(\beta)$ can be used to evaluate the usefulness of a particular estimation procedure and to compare various methods of estimation such as TSA, IDW, and

Kriging. Finally, estimation procedures which perform poorly on the validation samples could be expected to perform poorly in the interpolation process using all n samples.

Estimation of the IDW power parameter in equation (6) is not difficult because of two considerations. First, for most geological applications, the range of p is limited between 0 and some moderate number (for example, $p \leq 6$). It is not meaningful to consider $p < 0$ because that would imply that the estimation procedure should weight samples more heavily as their distance from the point being estimated increases. Note that at $p = 0$, the w_i 's are equal in equation (6), resulting in an estimation procedure that uses an average of all samples within c miles of the point being estimated. Second, small changes in p would not be expected generally to result in large changes in $S(p)$, and, for practicality, only integral values of p are considered often. The consequence of these two considerations is that the program BESTP is able to optimize $S(p)$ by simple evaluation of $S(p)$ for $p = 0, 0.5, 1.0, 1.25, 1.5, 1.75, 2.0, 2.25, 2.5, 2.75, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5$, and 6.0. The value of c is fixed in each program execution. It may be desirable to consider several program executions for varying c . It should be noted that local maxima of $S(p)$ or other irregular behavior cannot be eliminated, but in the applications considered $S(p)$ has been a smooth, well-behaved function.

Approximate confidence intervals can be computed using standard nonlinear least-squares theory. An approximate $100(1 - \alpha)\%$ confidence region for $S(p)$ is

$$S(\hat{p})[1 + (n' - 1)^{-1} t_{n'-1}(1 - \alpha/2)] \quad (9)$$

where $t_v(\alpha)$ is the α th percentile of a t -distribution with v degrees of freedom (Draper and Smith, 1981). It often may be of interest to determine if a region where $S(p) \leq 1$ is within the interval specified by equation (9). Also, a range of $S(p)$ in equation (9) corresponds to a range of p . Similarly, joint confidence regions could be computed for p and c .

It is possible to estimate the estimation variance from least squares theory using

$$\hat{\sigma}^2 = \frac{1}{n' - q} \sum_{i=1}^{n'} (z_i - \hat{z}_i)^2 \quad (10)$$

where q is the number of β 's estimated in equations (1), (2), or (3). The assumption in the estimation of σ^2 is that there is a common estimation variance for all n' points regardless of the distances (r_i) used in equation (6). This generally would seem unrealistic because \hat{z}_i obtained from distant points should have a greater variance than \hat{z}_i obtained from close points. However, regional geochemical studies often attempt a uniform sampling distribution. For highly irregular sampling, Kriging estimates should be considered because the estimation variance is a function of the interpoint distances at each point being estimated.

PLAINVIEW QUADRANGLE EXAMPLE

The preceding data analyses are illustrated using geochemical data from groundwaters collected in the Plainview National Topographic Map Series Quadrangle, Texas (lat. $34\text{--}35^\circ\text{N}$. and long. $100\text{--}102^\circ\text{W}$.). Two distinct geological areas were identified by previous analyses of the groundwater samples (Beauchamp and others, 1980), the Ogallala Formation and the Permian units. The data are available on magnetic tape which can be obtained from the Technical Library, Bendix Field Engineering Corp., P.O. Box 1569, Grand Junction, CO 81502. A brief discussion of the geology and sampling procedures is given in Beauchamp and others, (1980), and a detailed discussion is given elsewhere (Uranium Resource Evaluation Project, 1978).

The minimum $S(p)$ value associated with each of three IDW models is given for the Ogallala Formation in Table 1 for $c = 10$ statute miles (16 km). It is desirable to have the estimated z -values in the original scale of measurement so the untransformed equation (5) or back-transformed equation (7) models are of particular interest.

Table 1. Comparison of three methods of inverse-distance weighting estimation in the Ogallala Formation

Variable ^(a)	Untransformed Scale					Back-Transformed Scale					Transformed Scale				
	Overall Mean	Overall S.D.	Minimum S(p)	95% Confidence Interval for p	Suggested p-Value	Estimation Standard Deviation	Minimum S(p)	95% Confidence Interval for p	Suggested p-Value	Estimation Standard Deviation	Minimum S(p)	95% Confidence Interval for p	Suggested p-Value	Estimation Standard Deviation	
L_i	104	52	0.46	(1.5, 3.0)	2	29.3	0.49	(1.75, 4.0)	3	30.2	0.52	(1.0, 3.0)	2	0.33	
$y^{(b)}$	20	16	0.83	(1.0, 1.75)	1	9.62	0.71	(1.25, 2.75)	2	8.91	0.73	(1.0, 3.0)	2	0.48	
Total Alkalinity	256	44	0.72	(0.0, 0.5)	0	31.6	0.69	(0.1, 1.0)	0	31.2	0.66	(0.1, 1.0)	0	0.14	
Mg	31	13	0.77	(1.0, 2.0)	1	7.43	0.96	(1.25, 3.0)	2	8.30	1.22	(0, 1.5)	1	0.30	
As	4.5	2.3	0.81	(1.25, 3.5)	2	2.08	0.88	(1.5, 6.0)	3	2.17	0.85	(0.5, 2.0)	1	0.45	
Specific Conductance	797	247	0.90	(0.5, 2.25)	1	190.	0.88	(1.0, 2.25)	1	188.	0.76	(1.0, 2.5)	2	0.20	
$B^{(b)}$	206	165	1.10	(0, 1.0)	0	94.2	0.95	(0, 1.25)	1	88.2	0.84	(0, 1.25)	1	0.39	
$SO_4^{(b)}$	33	87	0.99	(1.0, 3.5)	2	37.9	0.99	(0, 4.0)	2	38.1	0.78	(1.0, 2.75)	2	0.61	
$Ba^{(b)}$	95	66	1.11	(0.5, 2.0)	1	48.1	1.02	(1.5, 2.0)	1	46.1	1.0	(0.5, 1.75)	1	0.42	
$Na^{(b)}$	9	7	1.27	(0, 2.0)	1	4.40	1.02	(1.5, 2.25)	1	3.93	1.06	(0.5, 2.5)	1	0.43	
$Na^{(b)}$	45	36	1.19	(0, 0.5)	0	26.0	1.09	(0, 1.0)	0	24.8	1.08	(0, 1.25)	0	0.53	
U	6.9	4.3	1.16	(0, 1.0)	0	3.97	1.20	(0, 1.5)	0	4.03	1.29	(0, 1.25)	0	0.53	
Ca	46	30	1.19	(1.0, 2.5)	2	11.0	1.30	(1.0, 3.5)	2	11.5	1.42	(0, 1.25)	1	0.26	

(a) Units in ppb except for total alkalinity, Mg, SO_4 , Na, and Ca in ppm, and specific conductance in $\mu\text{hos}/\text{cm}$.

(b) Back-transformed scale is preferable to untransformed scale for estimation.

Vanadium, boron, barium, molybdenum, and sodium have appreciably lower $S(\hat{p})$ -values in the back-transformation model. It should be noted that the back-transformation model uses the log concentrations for estimation. If this model is appropriate, the implication is that local highs should not be emphasized for estimation. It is interesting to note that many of the 13 variables exhibit an apparent lognormal distribution when all n samples are considered collectively. However, there appears to be no correspondence between an element having a lognormal distribution and the selection of the best interpolation model for the element.

The confidence intervals for the p -values are generally wide and selection of integral values of \hat{p} seems justified. Additional insight in any resulting contour map is gained by comparison of the overall standard deviation (using n samples) with the estimation standard deviation (using n' samples, column 7). Ideally, the estimation standard deviation would be considerably smaller if the inter-

polation process used in contouring produced a meaningful grid. However, for uranium the overall standard deviation of 4.3 is only slightly greater than the estimation standard deviation of 3.97. Combined with a minimum $S(\hat{p})$ value of 1.16, the contour map for uranium could not be expected to be representative of the observed data. Arsenic exhibits a similarly small reduction in the standard deviation, but a smaller scale of total variation produces a reasonable $S(\hat{p})$ of 0.81. Conversely, lithium shows a marked reduction in the standard deviation and the lowest $S(\hat{p})$ -value of 0.46. The contour map could be expected to be representative of the lithium data.

It is instructive to plot $S(p)$ vs p for a fixed c from the output of BESTP. Figure 1 illustrates that $S(p)$ is a smooth function and has a single minimum for the examples considered. For some elements, such as sodium, boron, total alkalinity, and calcium, the selection of an appropriate p -value is important and only a narrow

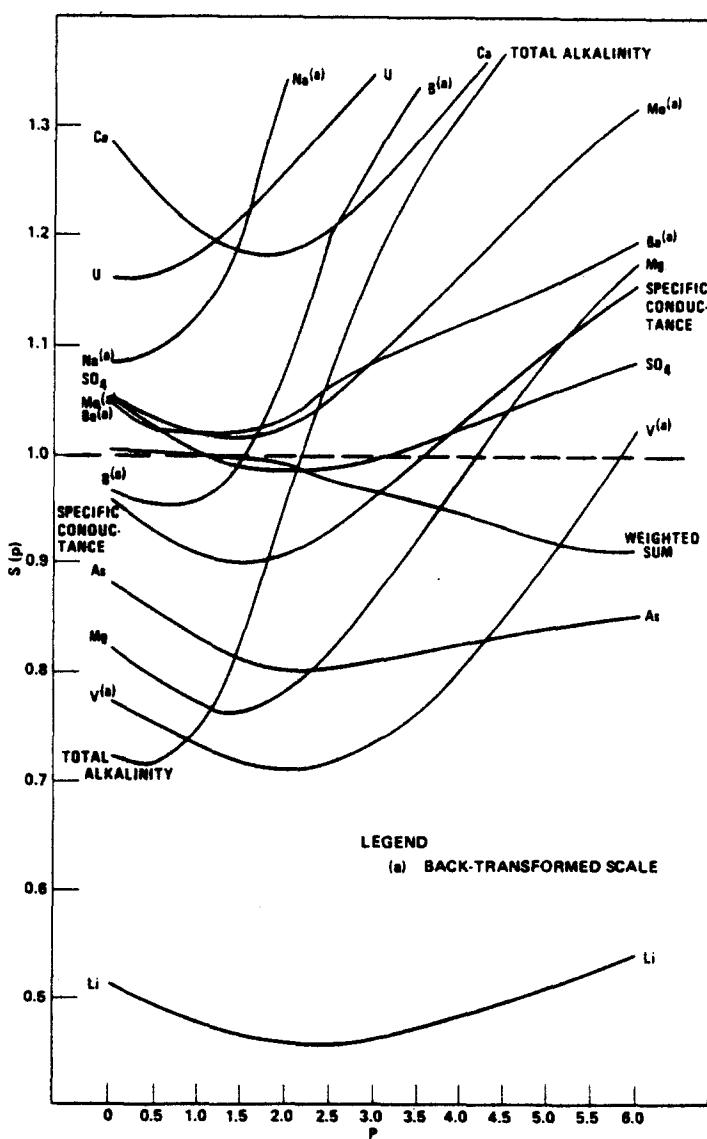


Fig. 1. $S(p)$ vs p for Ogallala Formation

range of \hat{p} is appropriate. For example, arbitrary choice of a p -value of 3 rather than 0.5 for total alkalinity could result in a poor geochemical map. Other elements such as lithium seem insensitive to changing p .

It is possible to group the variables by either of two methods in an attempt to characterize the regional geochemistry. The first grouping method simply forms groups of variables based on the minimum $S(p)$ -values based on the appropriate untransformed or back-transformed models. Table 2 gives a grouping of variables derived from the Table 1 $S(\hat{p})$ -values. This grouping method associates variables that have similar predictability based on the surrounding samples. For example, vanadium, total alkalinity, magnesium, and arsenic have similar predictability as shown in Table 2.

Another possible consideration in grouping variables is to associate variables having similar shaped curves in Figure 1. The shape of an individual curve characterizes the relationship of distant samples to a point being estimated. The large p -values give decreasing weight to samples as their distance increases from the point being estimated. For example, the lithium small p -values (for example, $0 \leq p \leq 2$) have $S(p)$ -values close to the optimum which suggests that distant samples are related to a point being estimated. Similarly, samples close to a point being estimated are related to the point since large values of p produce comparable $S(p)$ -values. Conversely, uranium, sodium, total alkalinity, and boron are estimated best by an average of the points within c miles of the point being estimated. Additional groups are given in Table 2.

As the optimum value for p decreases, the value for $S(p)$ increases in Figure 1 with the exception of total alkalinity and calcium. This implies that better interpolation estimates are possible for elements where close samples are weighted heavily. A geologic explanation of this observation is that elements such as lithium, which are soluble in Ogallala Formation waters, vary regionally with relatively little local relief and are estimated best by concentrations at adjacent sampling locations. Conversely, elements such as uranium are soluble under a restricted range of conditions in the Ogallala Formation which results in more local variability. Consequently, low p -values produce the best estimates due to a smoothing effect produced by weighting distant samples more heavily. A general conclusion is that the more soluble elements with uniform distribution and little local

relief will be estimated best by adjacent samples with a corresponding low value of $S(p)$.

The value of $S(\hat{p})$ also can be used to estimate the relative quality of a contour map prepared by IDW interpolation. The geologist utilizing a contour map can assess the emphasis to be placed on the location of particular contour lines with knowledge of the $S(\hat{p})$ -value. For example, a contour map of uranium would not represent the observed data well in the Ogallala Formation. However, the geologist may place more emphasis on the location of contours of pathfinder elements for uranium such as vanadium and arsenic which have appreciably lower $S(\hat{p})$ -values in the Ogallala Formation (Table 1).

The $S(\beta)$ -value also can be used to compare totally different methods of estimating \hat{z} . Myers, and others, (1983) compared IDW, Kriging, and TSA on the Ogallala Formation validation samples. The TSA procedure gave large $S(\beta)$ -values in the untransformed scale and is not reported. The results reported in Table 3 provide a useful synthesis of numerous data analyses and are discussed in Myers, and others (1980, 1983).

Several types of residual plots derived from the best IDW estimation model provide additional insight into the regional geochemistry. Figure 2 gives histogram and normal probability plots of the normalized IDW residuals for the uranium ($\hat{p} = 0$) and lithium ($\hat{p} = 2$) from the untransformed scale models. Each of the n samples was estimated by the IDW model with $c = 10$ miles and $p = \hat{p}$ in equation (6), and the residual was calculated. The estimation standard deviation from Table 1 was used to normalize the residuals. The uranium histogram indicates an unusually large number of samples having positive residuals (observed > predicted). Notice that the normalization by σ is reasonable because the interval (-2, 2) contains most of the residuals. The lithium histogram indicates a separate population of large residuals. For both variables, the linearity of the main portion of the probability plots implies that the normal distribution of the residuals is appropriate. Characterizing the geographic distribution of the residuals may be of interest because a contiguous group of unusual residuals indicates a departure from the overall regional model. A group of 7 large uranium residuals (> 1.0 standard deviation) is shown on the summary map in Figure 3.

The optimization procedure can be applied successfully to a combination of variables. Kane (1977), Butz

Table 2. Grouping of variables in the Ogallala Formation

Variables Grouped by Predictability [minimum $S(p)$]	Variable Groups by Influence of Surrounding Samples [shape of $S(p)$ curve]
Li	U, Na, Total Alkalinity, B
V, Total Alkalinity, Mg, As	Specific Conductance, Ba, Mg Mo, Ca, V
Specific Conductance, B SO ₄ , Mo, Ba	SO ₄ , As, Li
Na, U, Ca	

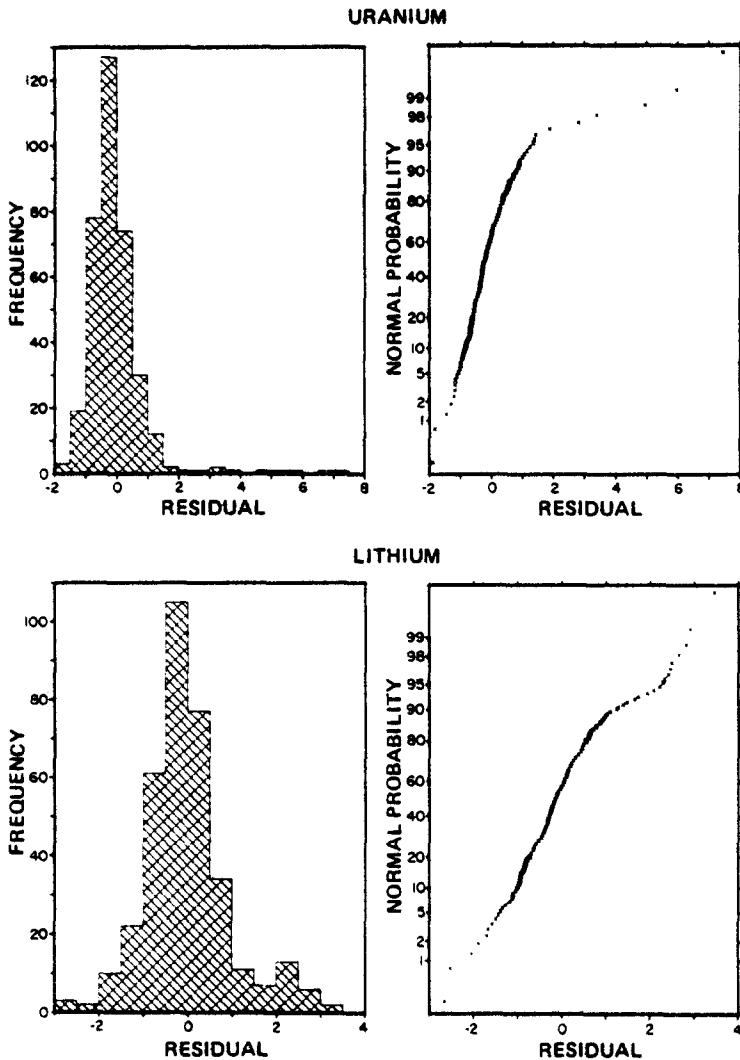


Fig. 2. Histogram and probability plots of normalized residuals from optimum inverse distance weighting models for uranium and lithium.

(1977), and Garrett, Kane, and Zeigler, (1980) described the use of a weighted sum variable where the weights are derived from standardizing the measured variables and applying a subjective importance to the individual variables. One such model is

$$\begin{aligned} \text{WS} = & 1.6(\log U - 1.8) \\ & + 1.3(\log Li - 4.5) \\ & + 1.7(\log As - 1.4) \\ & + 1.1(\log V - 2.7) \\ & + 1.5(\log Mo - 2.0) \\ & + 2.1(\log Mg - 3.4). \end{aligned}$$

The WS variable was input in BESTP and the resulting curve for $S(p)$ appears in Figure 1. The optimum $\hat{p} = 5$ was used to contour the WS variable. Larger values of p are to be expected for the WS variable because the weighted sum computation produces smoothed data and distant samples should be good predictors. The anomalous areas are given in Figure 3. Areas A and B

were identified by Amaral (1979) as having potential for uranium mineralization. One high-level WS contour corresponds with Area B. A second contour corresponds with the anomalous uranium residuals and Area IIIC identified by Beauchamp, and others (1980).

BESTP PROGRAM DESCRIPTION

The purpose of the program is to calculate $S(p)$ and the mean square residual (MSR) where

$$\text{MSR}(p) = \frac{1}{n' - 1} \sum_{i=1}^{n'} [z_i - \hat{z}_i(p)]^2.$$

A random selection of the input data to form a validation data set of size $n' \leq n$ would not ensure necessarily that samples were selected uniformly from all sampling areas. Therefore, the following method of selection is used: (1) a cell grid is established for the map area using the input parameters, (2) one sample is selected randomly from each nonempty grid cell, (3) a random subset is selected if the number of nonempty grid cells is greater than n' ,

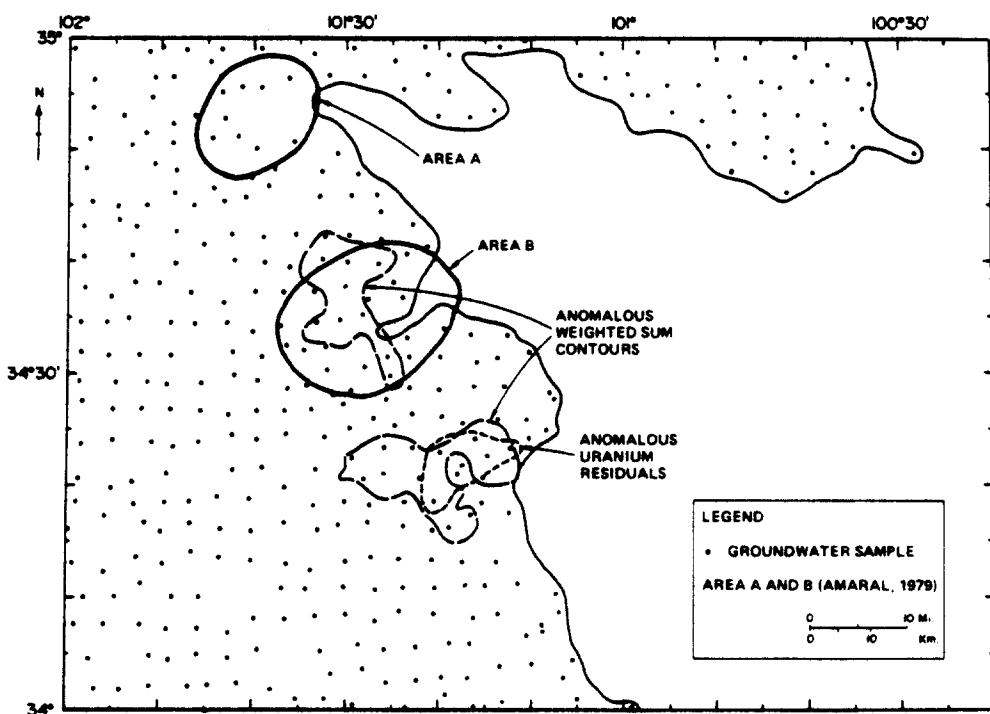


Fig. 3. Summary map for inverse distance weighting analyses.

Table 3. Comparison of estimation procedures using $S(\beta)$ values

Variable	Untransformed Scale		Back-transformed Scale		Log Transformed Scale		
	IDW	Kriging	IDW	Kriging	IDW	Kriging	TSA
Li	0.46	0.43	0.49	1.09	0.52	0.88	0.62
V	0.83	--(a)	0.71	0.93	0.73	0.82	0.99
Total Alkalinity	0.72	1.32	0.69	1.24	0.66	1.04	0.58
Mg	0.77	3.96	0.96	5.35	1.22	2.12	1.20
As	0.81	0.84	0.88	0.96	0.85	1.00	1.00
Specific Conductance	0.90	1.59	0.88	1.40	0.76	0.93	0.78
B	1.10	1.56	0.95	2.33	0.84	1.26	0.89
SO ₄	0.99	--	0.99	1.26	0.78	0.81	0.84
Ba	1.11	--	1.02	1.15	1.00	1.29	1.06
Mo	1.27	20.1	1.02	--	1.06	--	0.91
Na	1.19	2.91	1.09	5.98	1.08	1.56	0.99
U	1.16	2.03	1.20	1.59	1.29	1.81	1.36
Ca	1.19	4.24	1.30	5.98	1.42	2.17	1.14

(a) Analysis not performed.

and (4) a second randomly selected sample is obtained from the nonempty grid cells if an insufficient number of samples is obtained in step 2. The grid size should be selected so that there are approximately n' nonempty cells. A random ordering of input data with regard to sampling location will ensure a random selection of grids and samples within a grid. Once the validation set is formed, each validation sample is estimated by equation (5) for varying values of p and the results are summarized. A listing of the program appears in Appendix 1.

The BESTP program was written in FORTRAN for an IBM system. Implementation on other machines only need consider the use of A4 formats in BESTP. The program consists of a main routine and two subroutines. The main routine reads the program input and prints summary statistics for the validation data set. Subroutine PICK selects the test samples from the data set. Subroutine TRYP calculates the estimate of each test sample for varying values of p . Each sample is assumed to have a latitude and longitude in decimal degrees followed by values of the variables to be analyzed. The user can use optionally a log transformation on the concentration data.

The program is dimensioned to process a maximum of 1000 samples with 25 different variables. An upper limit of 1000 for the number grid cells also is used. Array DATA contains the input data and would need to be redimensioned for larger problems, along with arrays X and Y. The array IPICK should be dimensioned to the maximum of the number of grid cells or the number of validation samples. Arrays C₀DE, XM, XSD, UR, R, UXM, and UXSD will need to be increased to analyze

more than 25 variables in a program execution. The input consists of 5 card types followed by the data:

Card 1, columns 1-80 (TITLE, 20A4).

An alphanumeric title for the data.

Card 2, columns 1-5 (NTRY, 15).

The number of samples to be used in the data set (NTRY = -1 implies all input data will be used).

Card 2, columns 6-10 (NV, 15).

The number of variables for each sample (excluding latitude and longitude).

Card 3, columns 11-15 (ITRAN, 15).

An option to use raw data (ITRAN = 0) or the logarithms of the data (ITRAN = 1).

Card 3, columns 16-20, (IPRINT, 15).

An option to print (IPRINT = 1) validation data samples and the individual sample estimation results; IPRINT = 0 excludes this output.

Card 3, columns 11-20 (GRIDX, F10.0).

The longitude grid interval size in decimal degrees.

Card 3, columns 21-30 (GRIDY, F10.0).

The latitude grid interval size in decimal degrees.

Card 4, columns 1-4, 5-8, etc. (C₀DE(I), I = 1, ..., NV, 20A4).

The alphanumeric code names for the variables.

Card 5, columns 1-80 (FMT, 20A4).

The format used to input the data; the first two values for each sample should be longitude and latitude, followed by NV variables.

Card 6, etc., columns 1-80 (DATA, FMT).

The input data set read according to FMT.

The selected input options are printed by the program in the first output section. If requested (IPRINT = 1), the values and estimates of each sample are listed as shown in Figure 4. Summary statistics for the validation, total, and prediction data sets are given as shown in Figure 5 to enable the user to determine how well the validation

EXAMPLE DATA FROM WHITEHORSE AND CLOUD CHIEF GROUPS, PLAINVIEW QUADRANGLE

VALIDATION DATA SET:

VARIABLE	OBS	AVERAGE	P= .5	P=1	P=1.25	P=1.5	P=1.75	P=2	P=2.25	P=2.5	P=2.75	P=3	P=3.5	P=4	P=4.5	P=5	P=5.5	P=6	
LOCATION:	100.010	34.920																	
LI	40.00	59.00	55.86	52.88	51.48	50.17	48.94	47.81	46.77	45.83	44.98	44.22	42.94	41.95	41.20	40.62	40.20	39.88	
MG	88.70	115.95	113.83	111.80	110.86	109.96	109.13	108.37	107.66	107.02	106.45	105.93	105.07	104.40	103.89	103.50	103.21	103.00	
SON	151.00	1217.50	102127.36	102127.90	102127.50	102127.91	102127.58	102127.67	102128.33	102128.31	102128.39	102128.96	102130.81	102130.93	102131.13	102131.20	102131.27	102131.30	
NA	129.50	108.10	107.24	106.42	106.03	105.67	105.33	105.02	104.74	104.48	104.24	104.03	103.68	103.41	103.20	103.05	102.93	102.84	
U	4.59	11.08	11.36	11.62	11.75	11.87	11.98	12.08	12.17	12.25	12.33	12.40	12.51	12.60	12.66	12.72	12.75	12.78	
CA	610.90	468.90	481.74	493.97	499.69	505.07	510.10	514.74	518.99	522.85	526.33	529.48	534.66	538.71	541.81	544.15	545.90	547.20	
LOCATION:	100.280	34.070																	
LI	23.00	40.25	39.54	39.05	38.89	38.77	38.70	38.66	38.65	38.66	38.68	38.70	38.76	38.81	38.85	38.89	38.92	38.94	
MG	12.90	53.37	47.54	41.91	39.35	37.05	35.06	33.40	32.05	30.98	30.17	29.55	28.75	28.33	28.11	28.00	27.94	27.92	
SON	875.00	392.88	349.78	303.25	280.98	260.65	242.95	228.26	216.59	207.72	201.25	196.75	191.93	190.47	190.58	191.32	192.21	193.04	
NA	46.10	41.65	41.39	41.39	41.50	41.67	41.89	42.13	42.39	42.65	42.89	43.12	43.51	43.82	44.05	44.23	44.35	44.45	
U	1.19	4.89	4.18	3.52	3.23	2.97	2.76	2.59	2.45	2.34	2.27	2.21	2.14	2.11	2.10	2.10	2.09	2.09	
CA	78.20	216.36	187.67	160.45	148.31	137.61	128.52	121.11	115.27	110.84	107.57	105.23	102.52	101.38	101.03	101.02	101.15	101.31	
LOCATION:	100.260	34.140																	
LI	43.00	37.29	36.35	35.19	34.62	34.09	33.63	33.26	32.96	32.78	32.58	32.48	32.40	32.41	32.47	32.55	32.62	32.69	
MG	76.90	42.91	45.30	48.23	49.82	51.43	53.01	54.54	55.97	57.30	58.51	59.81	61.50	63.01	64.21	65.17	65.92	66.52	
SON	65.00	367.29	361.60	361.29	363.40	366.91	371.59	377.17	383.33	389.86	396.35	402.79	414.87	425.46	434.42	441.84	447.87	452.73	
NA	45.80	40.10	39.12	37.95	37.34	36.77	36.23	35.76	35.34	34.98	34.69	34.44	34.06	33.81	33.64	33.52	33.44	33.38	
U	7.40	3.76	4.32	5.08	5.50	5.94	6.36	6.75	7.12	7.45	7.75	8.01	8.45	8.78	9.03	9.22	9.37	9.49	
CA	216.00	166.79	161.28	157.38	156.21	155.68	155.73	156.28	157.22	158.45	159.88	161.41	164.54	167.49	170.09	172.30	174.13	175.62	
LOCATION:	100.270	34.472																	
LI	37.00	57.00	56.02	54.56	53.73	52.89	52.06	51.27	50.54	49.88	49.30	48.78	47.96	47.36	46.94	46.64	46.44	46.30	
MG	76.90	130.50	128.23	124.94	123.10	121.24	119.41	117.68	116.09	114.64	113.36	112.24	110.44	109.14	108.23	107.59	107.14	106.84	
SON	864.00	1702.33	1684.33	1621.57	1615.34	1614.98	1614.63	1614.31	1614.02	1601.376	1641.354	111334.641303.881282.021266.781256.291249.131244.25							
NA	319.00	172.83	199.62	225.20	236.76	247.23	256.50	264.55	271.43	277.23	282.06	286.05	291.99	295.92	298.49	300.17	301.27	301.99	
U	6.57	18.12	18.72	19.23	19.44	19.62	19.77	19.89	19.98	20.06	20.12	20.16	20.22	20.26	20.26	20.27	20.28	20.28	
CA	216.10	520.37	493.80	467.12	454.65	443.14	432.74	423.53	415.54	408.68	402.88	398.01	390.62	385.60	382.24	379.99	378.50	377.51	
LOCATION:	100.340	34.038																	
LI	25.00	43.27	43.42	43.76	44.01	44.31	44.67	45.08	45.53	46.03	46.57	47.15	48.38	49.67	50.97	52.22	53.39	54.46	
MG	14.10	65.45	65.87	66.84	67.57	68.46	69.54	70.78	72.20	73.77	75.50	77.36	81.39	85.70	90.09	94.40	98.50	102.29	
SON	817.00	682.18	654.55	626.67	613.01	599.74	587.02	574.99	563.79	553.54	544.31	536.18	523.31	514.87	510.43	509.32	510.77	514.01	
NA	63.00	59.07	58.30	57.52	57.13	56.75	56.38	56.02	55.68	55.36	55.06	54.78	54.29	53.90	53.59	53.36	53.18	53.06	
U	1.88	6.05	6.06	6.13	6.20	6.28	6.39	6.52	6.67	6.84	7.03	7.23	7.48	8.16	8.65	9.14	9.60	10.02	
CA	72.90	270.35	275.76	283.36	288.09	293.49	299.56	306.30	313.70	321.70	330.27	339.32	358.55	378.66	398.88	418.52	437.05	454.11	

Fig. 4. Example output of observed and predicted values of validation samples.

EXAMPLE DATA FROM WHITEHORSE AND CLOUD CHIEF GROUPS, PLAINVIEW QUADRANGLE

SUMMARY STATISTICS

VARIABLE	VALIDATION DATA SET (N= 50)		TOTAL DATA SET			PREDICTION DATA SET		
	MEAN	S.D.	MEAN	S.D.	N	MEAN	S.D.	N-N _T
Li	87.58	77.50	78.97	59.84	274	77.05	55.16	224
Mg	132.1	105.8	134.9	86.44	274	135.5	81.75	224
SO ₄	1343.	675.0	1457.	628.0	274	1483.	615.8	224
Na	167.6	224.7	155.5	231.8	274	152.8	233.8	224
U	12.21	11.89	11.19	11.88	274	10.97	11.89	224
Ca	433.3	197.5	481.4	172.9	274	492.1	165.5	224

NOTE: N MAY NOT BE THE SAME FOR ALL VARIABLES DUE TO MISSING DATA.

Fig. 5. Example output of summary statistics for validation, total, and prediction data sets.

EXAMPLE DATA FROM WHITEHORSE AND CLOUD CHIEF GROUPS, PLAINVIEW QUADRANGLE

TABLE OF S(P)

VARIABLE	AVERAGE	P= .5	P=1	P=1.25	P= 1.5	P=1.75	P= 2	P=2.25	P= 2.5	P=2.75	P= 3	P= 3.5	P= 4	P= 4.5	P= 5	P= 5.5	P= 6
Li	0.880*	0.886	0.900	0.909	0.918	0.926	0.932	0.937	0.941	0.944	0.947	0.951	0.955	0.960	0.964	0.968	0.973
Mg	0.784	0.780*	0.781	0.785	0.792	0.800	0.810	0.821	0.834	0.848	0.853	0.893	0.923	0.950	0.976	0.999	1.020
SO ₄	0.843*	0.853	0.871	0.883	0.898	0.914	0.933	0.952	0.972	0.992	1.013	1.053	1.090	1.122	1.150	1.175	1.195
Na	0.965	0.924	0.922*	0.930	0.939	0.946	0.950	0.951	0.951	0.950	0.949	0.947	0.947	0.949	0.951	0.954	0.958
U	1.207	1.204*	1.215	1.225	1.238	1.252	1.267	1.283	1.300	1.317	1.335	1.372	1.413	1.456	1.502	1.550	1.598
Ca	0.834	0.793	0.758	0.743	0.730	0.720	0.711	0.705	0.700	0.698	0.696*	0.698	0.703	0.712	0.723	0.734	0.746

ASTERISK DENOTES MINIMUM S(P) VALUE.

50 VALIDATION SAMPLES WERE USED FOR THE ABOVE TABLE.

Figure 6. Example output of S(p) values.

samples represent the total data set. The S(p) values then are output in tabular form as shown in Figure 6 for all values of p for each variable. An asterisk indicates the minimum S(p) for a variable. Tables giving MSR(p) for estimation of σ^2 in (10) and the comparison to MSR(2) also are output. If logarithms of the data are requested, the same tables are output for both the transformed and back-transformed models. Data for the Permian age Whitehorse and Cloud Chief Group used in the previous example appear in Appendix 2. The data are listed in the order longitude, latitude, Li, Mg, SO₄, Na, U, and Ca.

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APPENDIX I

Program lasting

EXAMPLE DATA FROM WHITEHORSE AND CLOUD CHIEF GROUPS, PLAINVIEW QUADRANGLE

50	6	0	1					
10.	.075			.075				
LI	MG	SO4	NA	U	CA			
(8F10.3)								
100.660	34.410	67.000	185.300	1916.000	48.000	92.210	524.000	
100.630	34.360	76.000	152.200	1821.000	69.700	13.780	546.900	
100.580	34.366	61.000	130.000	1859.000	48.400	15.670	515.800	
100.570	34.330	67.000	137.700	1902.000	59.500	10.940	557.200	
100.460	34.317	61.000	129.000	1781.000	100.000	11.070	557.400	
100.480	34.357	46.000	145.000	1814.000	99.700	13.850	596.300	
100.540	34.363	54.000	134.200	1773.000	53.800	4.380	599.200	
100.410	34.410	45.000	120.000	1787.000	75.500	10.480	573.000	
100.490	34.413	57.000	138.100	1859.000	69.900	17.300	572.400	
100.430	34.467	60.000	117.900	1887.000	165.100	18.200	543.800	
100.440	34.390	49.000	36.000	1454.000	16.900	6.110	594.800	
100.420	34.317	43.000	112.300	1644.000	98.800	4.340	535.200	
100.420	34.348	36.000	127.200	2006.000	302.400	4.990	520.700	
101.240	34.672	220.000	105.500	1615.000	530.700	18.480	478.800	
101.020	34.541	33.000	46.700	824.000	24.200	4.920	354.400	
100.960	34.719	56.000	94.200	1502.000	20.800	5.180	498.900	
100.990	34.697	123.000	198.800	2044.000	77.100	4.140	506.000	
100.960	34.655	32.000	50.800	765.000	13.300	2.330	266.300	
100.990	34.665	34.000	66.600	1524.000	11.200	3.460	563.400	
100.950	34.491	155.000	167.300	1961.000	986.000	9.780	565.500	
100.980	34.486	137.000	108.500	1719.000	145.200	19.850	541.000	
100.950	34.470	70.000	124.300	1719.000	84.100	7.300	528.000	
101.170	34.559	113.000	81.400	57.000	119.700	75.770	542.200	
100.960	34.547	224.000	520.400	2700.000	217.300	0.850	429.000	
101.150	34.589	164.000	341.900	2728.000	253.200	18.810	560.600	
101.130	34.561	222.000	497.100	2382.000	196.100	17.410	600.800	
101.090	34.586	57.000	91.000	1647.000	72.300	8.850	674.900	
101.080	34.561	167.000	317.700	2382.000	224.700	15.440	555.900	
100.860	34.505	87.000	202.100	2004.000	35.400	12.130	623.300	
100.870	34.467	118.000	136.900	1981.000	122.000	6.720	646.700	
100.840	34.418	133.000	171.200	1919.000	71.200	7.900	642.100	
100.800	34.372	110.000	221.400	2098.000	57.100	1.660	604.500	
100.820	34.402	33.000	51.500	1413.000	3.300	6.930	350.700	
100.770	34.332	59.000	148.100	1775.000	28.100	7.230	705.200	
100.740	34.359	134.000	211.100	2042.000	78.300	4.630	624.300	
100.590	34.505	51.000	141.100	1726.000	34.900	5.870	718.000	
100.680	34.328	101.000	163.200	1774.000	50.900	5.850	634.500	
100.690	34.365	118.000	196.700	1935.000	109.400	12.210	613.000	
100.640	34.325	55.000	167.000	1765.000	103.600	40.060	555.800	
100.710	34.321	83.000	151.200	1864.000	48.400	6.740	517.400	
100.790	34.428	126.000	196.100	2047.000	90.400	3.980	498.700	
100.870	34.436	200.000	193.100	2264.000	366.100	28.030	509.100	
100.710	34.459	75.000	141.300	1698.000	16.800	13.570	581.100	
100.760	34.400	147.000	284.300	2352.000	111.200	5.310	509.100	
100.680	34.483	68.000	131.000	1448.000	57.900	3.000	514.800	
100.620	34.452	107.000	170.600	1907.000	145.100	7.010	577.200	
100.600	34.409	77.000	183.500	1677.000	82.900	7.310	495.200	
100.730	34.440	67.000	141.500	1620.000	40.200	9.820	507.900	
100.060	34.902	79.000	97.100	1361.000	111.400	7.810	552.700	
100.090	34.825	20.000	15.000	75.000	76.100	1.780	69.500	
100.160	34.812	67.000	70.800	1057.000	278.500	6.270	457.000	
100.160	34.772	59.000	74.000	191.000	146.100	5.480	128.300	
100.100	34.757	77.000	78.500	1319.000	75.400	4.730	625.300	
100.020	34.885	39.000	102.400	1325.000	102.600	12.860	550.800	
100.010	34.920	40.000	88.700	1514.000	129.500	4.590	610.900	
100.040	34.857	79.000	129.500	1110.000	113.600	9.300	387.000	
100.420	34.841	41.000	56.800	329.000	24.200	8.080	156.300	
100.410	34.768	63.000	132.500	1730.000	79.300	19.840	541.100	
100.440	34.798	43.000	69.500	364.000	24.800	9.190	164.300	
100.460	34.766	36.000	74.100	1048.000	37.200	8.420	365.900	
100.540	34.457	56.000	126.000	1711.000	47.500	9.780	515.000	
100.560	34.384	47.000	137.000	1705.000	69.500	8.960	549.900	
100.490	34.457	67.000	126.600	1812.000	218.800	21.820	553.900	
100.110	34.789	67.000	67.300	618.000	108.100	5.100	251.600	
100.510	34.913	53.000	121.100	706.000	13.400	4.700	265.900	
100.530	34.822	35.000	55.900	580.000	22.100	2.890	198.500	
100.500	34.865	83.000	125.500	1590.000	28.100	25.870	510.500	
100.020	34.774	92.000	91.200	1476.000	112.900	10.320	508.000	
100.190	34.775	20.000	14.600	89.000	94.200	2.170	42.600	
100.610	34.469	96.000	129.200	1535.000	103.500	10.130	490.200	
100.630	34.514	80.000	160.700	1519.000	95.200	22.730	603.300	
100.700	34.402	81.000	145.900	1489.000	52.400	11.440	529.600	
100.640	34.186	67.000	337.600	2575.000	180.500	33.240	453.700	
100.540	34.149	29.000	85.800	1341.000	74.900	10.580	481.800	
100.530	34.103	40.000	96.500	1399.000	23.700	14.570	464.700	
100.540	34.081	59.000	96.300	1473.000	16.600	21.470	483.100	
100.570	34.074	46.000	106.000	1361.000	23.200	34.890	594.200	

100.810	34.228	53.000	38.900	471.000	114.400	9.170	227.200
100.810	34.267	63.000	97.400	1404.000	33.300	2.210	567.700
100.790	34.258	373.000	273.200	2486.000	1317.000	22.230	400.900
100.730	34.172	82.000	179.100	1895.000	40.900	3.900	549.100
100.630	34.223	58.000	106.000	1554.000	23.620	4.180	611.600
100.590	34.117	75.000	162.000	1875.000	126.900	21.570	579.800
100.640	34.131	128.000	173.500	1997.000	222.300	1.950	567.700
100.630	34.105	101.000	177.300	2112.000	104.900	2.100	548.600
100.680	34.102	82.000	130.200	1784.000	89.700	1.500	556.900
100.590	34.170	49.000	122.900	1704.000	37.300	13.240	578.500
100.570	34.181	36.000	134.900	1703.000	51.500	14.490	554.100
100.570	34.226	83.000	164.400	1697.000	53.400	5.250	580.100
100.600	34.218	73.000	135.700	1636.000	38.900	6.310	547.400
100.680	34.061	174.000	225.700	967.000	475.700	6.380	490.200
100.720	34.056	65.000	100.600	1510.000	111.600	8.250	562.100
100.760	34.182	187.000	414.600	2269.000	293.200	26.520	580.200
100.810	34.207	69.000	104.800	1456.000	51.100	5.860	569.800
100.750	34.206	77.000	131.000	1463.000	160.500	6.210	506.800
100.700	34.211	36.000	96.600	1609.000	31.100	5.400	607.900
100.640	34.255	65.000	135.000	1433.000	44.400	13.200	646.200
100.640	34.310	44.000	153.000	1688.000	446.400	9.720	700.700
100.720	34.267	38.000	81.800	1381.000	18.600	15.110	663.600
100.800	34.288	63.000	83.900	1310.000	25.100	4.440	721.600
100.740	34.318	73.000	159.300	1616.000	38.800	4.270	774.500
100.600	34.030	1.000	0.500	2190.000	4.800	7.960	0.700
100.570	34.003	159.000	310.100	2052.000	259.400	23.490	528.200
100.570	34.051	85.000	145.500	1633.000	69.700	9.150	494.300
100.510	34.044	39.000	116.600	1551.000	23.200	3.840	1027.000
100.530	34.026	35.000	105.200	1544.000	14.500	6.630	894.500
100.580	34.023	124.000	232.000	1945.000	127.400	2.150	616.600
100.420	34.032	52.000	94.600	1433.000	35.000	21.820	423.800
100.440	34.070	39.000	136.600	1728.000	154.800	9.920	595.000
100.450	34.020	37.000	90.100	962.000	31.700	4.740	281.900
100.480	34.018	70.000	113.400	1446.000	351.500	2.940	456.800
100.490	34.060	56.000	145.700	2090.000	50.400	28.100	553.600
100.480	34.078	61.000	115.300	2060.000	53.500	20.010	572.200
100.390	34.087	48.000	109.100	2100.000	70.500	8.490	598.400
100.390	34.050	61.000	126.600	572.000	52.500	12.780	563.400
100.260	34.140	43.000	76.900	65.000	45.800	7.400	216.000
100.320	34.156	32.000	22.700	200.000	133.100	1.690	116.100
100.370	34.149	44.000	72.700	576.000	51.900	3.820	218.500
100.350	34.228	55.000	148.700	2016.000	86.300	3.440	620.800
100.460	34.188	44.000	92.000	1589.000	75.000	14.150	539.900
101.100	34.763	86.000	126.700	1409.000	55.400	10.520	545.100
101.070	34.828	158.000	182.200	1811.000	95.500	17.150	524.000
101.080	34.790	53.000	118.000	1427.000	18.100	11.010	537.600
101.050	34.765	91.000	142.000	1812.000	79.700	7.460	581.600
101.330	34.808	50.000	100.200	1375.000	38.200	10.100	537.700
101.020	34.659	278.000	357.700	3001.000	508.200	3.560	465.700
101.020	34.696	152.000	226.500	2095.000	44.200	15.920	517.200
101.070	34.688	275.000	467.700	3120.000	255.400	7.770	418.800
101.300	34.774	40.000	80.100	1600.000	56.800	5.600	572.400
101.280	34.810	85.000	144.400	1757.000	47.900	13.190	553.300
101.280	34.839	328.000	541.800	3760.000	549.500	5.990	403.900
101.270	34.733	100.000	224.900	2097.000	599.600	8.840	570.500
101.240	34.778	91.000	134.500	1874.000	184.300	10.950	579.100
101.040	34.627	79.000	204.900	1864.000	177.600	6.910	509.800
101.000	34.752	37.000	87.000	1395.000	22.000	8.070	518.900
101.470	34.891	77.000	84.000	1835.000	112.900	18.830	493.600
101.430	34.899	97.000	78.900	1819.000	85.500	15.830	504.600
101.140	34.659	282.000	415.900	2880.000	557.100	5.690	486.600
101.180	34.645	48.000	104.000	1573.000	37.100	6.630	596.600
101.220	34.703	209.000	286.800	2127.000	398.600	5.400	485.800
101.160	34.625	150.000	259.200	1786.000	178.900	13.240	575.300
100.970	34.618	95.000	144.600	1564.000	1127.000	7.410	546.300
100.980	34.587	85.000	127.700	1489.000	69.100	5.580	556.700
101.030	34.465	133.000	144.700	1514.000	114.300	19.200	494.300
101.040	34.410	356.000	138.200	487.000	201.900	21.460	127.400
101.420	34.831	138.000	100.000	1118.000	1416.000	15.830	339.900
101.260	34.667	277.000	136.500	900.000	1075.000	27.520	472.600
101.300	34.665	226.000	81.500	1189.000	1126.000	17.220	304.800
101.300	34.658	42.000	59.200	1356.000	33.700	5.020	550.600
101.240	34.649	34.000	57.700	1198.000	24.600	7.030	626.300
101.250	34.642	25.000	47.700	1280.000	12.900	5.000	621.500
101.190	34.633	93.000	137.500	895.000	884.500	7.180	574.000
100.540	34.778	43.000	99.900	1044.000	35.000	5.090	404.200
100.500	34.799	48.000	112.300	1510.000	53.300	4.220	522.100
100.310	34.845	94.000	123.500	2197.000	246.500	13.700	533.300
100.390	34.812	21.000	30.800	670.000	22.000	3.150	159.000
100.260	34.850	62.000	76.500	1230.000	39.600	6.140	599.400
100.470	34.898	56.000	42.000	130.000	19.600	5.360	97.200
100.380	34.343	65.000	184.300	1687.000	154.500	9.510	955.000
100.330	34.807	33.000	49.700	478.000	192.700	10.980	181.900
100.380	34.456	59.000	96.300	1564.000	431.800	0.800	331.500
100.280	34.394	50.000	128.500	2188.000	65.300	15.240	585.500
100.350	34.392	52.000	144.100	2401.000	203.300	16.320	563.800

100.330	34.459	78.000	175.200	2317.000	168.500	20.640	576.100
100.270	34.472	37.000	76.900	864.000	319.000	6.570	216.100
100.300	34.361	70.000	130.600	1449.000	157.900	13.840	584.700
100.280	34.450	46.000	106.200	1234.000	303.400	20.280	375.500
100.350	34.426	47.000	110.100	1556.000	46.600	13.440	609.500
100.520	34.728	89.000	176.300	1563.000	58.600	19.620	466.800
100.570	34.731	32.000	57.500	445.000	32.000	7.420	182.100
100.510	34.668	38.000	107.000	1419.000	177.200	16.570	506.500
100.650	34.672	27.000	71.700	480.000	54.800	11.420	210.900
100.710	34.675	40.000	68.600	937.000	147.100	5.730	320.900
100.470	34.728	28.000	56.100	573.000	46.300	4.680	205.100
100.430	34.690	341.000	149.600	1906.000	711.700	7.030	616.200
100.560	34.652	37.000	76.600	1209.000	70.000	12.430	453.800
100.590	34.679	26.000	30.000	124.000	50.500	2.710	102.500
100.620	34.698	54.000	112.700	1435.000	131.400	10.990	421.300
100.620	34.578	87.000	99.400	1111.000	644.700	13.080	289.500
100.740	34.685	40.000	46.700	614.000	106.400	5.200	142.600
100.800	34.679	47.000	208.000	2162.000	24.700	4.990	507.100
100.900	34.682	88.000	141.200	1856.000	72.600	18.840	436.900
100.890	34.722	53.000	97.900	1287.000	10.700	6.910	293.600
100.620	34.771	54.000	148.800	2333.000	31.400	5.900	515.600
100.960	34.812	72.000	142.300	1469.000	77.300	23.780	530.500
100.820	34.454	82.000	101.700	1130.000	38.700	7.860	625.800
100.580	34.782	107.000	93.900	305.000	189.500	106.900	131.900
100.950	34.760	66.000	115.000	1332.000	35.600	9.510	529.100
100.930	34.754	39.000	75.100	1378.000	37.800	8.000	453.800
101.020	34.883	43.000	78.500	1223.000	16.500	3.360	451.900
100.460	34.650	73.000	167.100	1761.000	202.800	17.050	685.100
100.460	34.592	78.000	168.900	816.000	822.600	0.100	497.400
100.470	34.472	72.000	112.300	1561.000	96.300	31.230	578.000
100.440	34.544	29.000	46.200	703.000	416.000	7.440	171.300
100.430	34.506	96.000	370.400	2606.000	568.900	49.780	504.600
100.810	34.759	69.000	92.800	1425.000	54.400	3.760	510.000
100.550	34.803	65.000	86.100	1463.000	36.300	19.060	496.700
100.660	34.756	12.000	14.700	20.000	24.200	3.120	59.700
100.860	34.752	72.000	104.400	1409.000	60.500	9.480	503.200
100.840	34.781	60.000	115.500	1461.000	31.900	10.880	551.800
100.710	34.643	109.000	169.500	1616.000	15.600	19.400	553.800
100.660	34.609	221.000	495.100	2857.000	360.100	42.360	625.500
100.780	34.777	54.000	98.500	1444.000	26.000	0.780	576.100
100.790	34.716	99.000	174.500	1680.000	86.500	4.850	494.600
100.860	34.710	69.000	101.900	1016.000	25.300	5.710	380.200
100.850	34.557	42.000	56.000	500.000	72.800	5.880	154.500
100.880	34.588	64.000	124.800	1462.000	70.300	7.110	590.000
100.920	34.504	70.000	190.300	1517.000	35.600	18.600	489.900
101.040	34.864	105.000	153.200	1788.000	215.500	0.890	479.200
100.780	34.597	114.000	158.600	1604.000	218.500	13.800	553.500
100.840	34.648	59.000	139.500	1540.000	55.900	3.250	597.100
100.790	34.551	61.000	147.900	1449.000	137.900	5.660	565.200
100.840	34.597	46.000	222.000	1420.000	176.100	5.310	826.600
100.900	34.599	79.000	125.800	1495.000	78.700	11.310	540.800
100.920	34.616	49.000	107.800	1326.000	55.400	2.320	543.300
100.980	34.786	84.000	123.400	1498.000	63.500	5.620	553.000
100.810	34.649	51.000	114.600	1454.000	35.100	6.330	602.200
100.600	34.532	13.000	45.000	137.000	246.400	19.080	61.700
100.670	34.524	50.000	173.000	1351.000	232.200	4.490	781.400
100.560	34.548	48.000	66.500	682.000	328.700	10.460	204.700
100.520	34.644	55.000	106.700	1539.000	76.900	8.580	503.100
100.530	34.662	32.000	59.000	1136.000	22.600	6.900	441.900
101.080	34.903	60.000	72.000	1142.000	468.500	7.000	389.300
101.040	34.816	64.000	92.100	1002.000	16.200	11.210	320.600
101.010	34.834	101.000	323.800	2803.000	285.100	1.220	446.900
101.030	34.780	61.000	77.000	793.000	35.100	5.970	279.000
100.760	34.631	66.000	123.600	1527.000	67.300	9.420	535.400
100.780	34.560	54.000	176.300	1924.000	390.200	10.800	660.700
100.420	34.160	43.000	120.100	1963.000	30.300	13.230	613.800
100.470	34.130	35.000	102.500	1897.000	93.400	4.960	656.300
100.490	34.155	21.000	115.500	2056.000	27.300	13.100	600.900
100.430	34.108	74.000	108.800	2068.000	99.100	22.330	475.800
100.420	34.268	119.000	336.800	2295.000	418.400	14.930	518.900
100.430	34.201	43.000	88.800	1290.000	48.000	6.400	503.500
100.530	34.192	55.000	143.400	1539.000	53.200	22.550	541.700
100.440	34.237	55.000	140.700	1503.000	90.700	3.460	571.600
100.490	34.221	63.000	139.000	1467.000	54.700	9.730	523.600
100.490	34.268	82.000	144.500	1348.000	53.500	28.450	475.200
100.560	34.279	59.000	140.400	1459.000	47.200	11.880	617.700
100.340	34.240	47.000	72.300	957.000	42.900	3.270	395.800
100.340	34.038	25.000	14.100	817.000	63.000	1.980	72.900
100.280	34.070	23.000	12.900	875.000	46.100	1.190	78.200
100.300	34.275	74.000	99.100	1335.000	1174.000	6.020	480.800
100.400	34.236	56.000	132.800	27.000	72.500	4.260	556.700
100.380	34.258	52.000	140.300	1330.000	69.900	8.110	635.000
100.420	34.307	56.000	139.300	1425.000	131.700	5.850	554.100
100.380	34.190	52.000	139.400	1489.000	57.800	8.390	588.200

100.270	34.081	39.000	27.900	196.000	44.700	2.100	102.000
100.240	34.105	54.000	66.200	249.000	53.900	3.080	88.300
100.270	34.122	26.000	23.200	85.000	36.600	1.480	60.400
100.280	34.096	36.000	27.000	37.000	33.000	1.740	61.900
100.260	34.128	33.000	68.700	471.000	33.200	9.900	181.300
100.350	34.101	34.000	39.500	558.000	41.200	4.620	249.200
100.300	34.116	39.000	47.900	975.000	38.100	3.390	424.400
100.220	34.128	89.000	98.900	1174.000	129.800	8.130	372.300
100.400	34.006	37.000	26.100	74.000	64.200	0.400	71.500
100.710	34.088	74.000	103.800	1311.000	38.600	4.910	590.300
100.480	34.112	47.000	102.100	1520.000	15.900	5.890	532.500
100.500	34.191	39.000	127.900	1603.000	16.900	14.480	602.600
100.540	34.259	37.000	105.800	1585.000	21.900	7.570	622.700
100.560	34.308	25.000	59.200	1137.000	37.700	2.470	431.100
100.680	34.275	82.000	161.100	1580.000	1154.000	1.450	606.800
100.690	34.580	113.000	333.200	2074.000	162.000	20.820	654.400
100.700	34.569	84.000	222.500	1700.000	913.600	19.820	621.400
100.670	34.715	77.000	67.300	192.000	93.100	6.260	88.400
100.720	34.722	19.000	18.900	21.000	8.500	2.550	57.100
100.740	34.732	57.000	65.900	1181.000	29.600	7.930	550.000
100.620	34.657	116.000	256.800	1514.000	311.500	14.070	705.600
100.500	34.496	74.000	107.800	742.000	101.600	63.730	514.100
101.430	34.867	196.000	121.500	1404.000	236.900	9.200	598.300
101.040	34.565	330.000	365.900	2349.000	471.600	16.270	562.800
101.020	34.606	85.000	180.900	1590.000	94.200	10.400	625.600
101.060	34.604	34.000	56.700	369.000	12.700	5.840	224.400
100.920	34.561	130.000	209.800	1755.000	150.900	10.950	488.900

APPENDIX 2

Example data

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C*** PROGRAM BESTP                               MAIN   0
C***                                         MAIN   5
C*** OAK RIDGE NATIONAL LABORATORY             MAIN  10
C*** PROGRAM AUTHOR C.L. BEGOVICH            MAIN  15
C*** VERSION 1 SEPTEMBER, 1980                MAIN  20
C***                                         MAIN  25
C*** PROGRAM INPUT                            MAIN  30
C***                                         MAIN  35
C*** CARD 1                                  MAIN  40
C***                                         MAIN  45
C*** COLS 1-80 ALPHANUMERIC TITLE OF THE DATA MAIN  50
C***                                         MAIN  55
C*** CARD 2                                  MAIN  60
C***                                         MAIN  65
C*** COLS 1- 5 NUMBER OF SAMPLES TO BE SELECTED FOR THE VALIDAION MAIN  70
C*** DATA SET                                MAIN  75
C*** COLS 6-10 NUMBER OF VARIABLES FOR EACH DATA POINT(NV)      MAIN  80
C*** COLS 11-15 DATA TRANSFORMATION OPTION        MAIN  85
C***      =0 (DEFAULT) NO TRANSFORMATION          MAIN  90
C***      =1 USE LOGARITHMS OF THE DATA          MAIN  95
C*** COLS 16-20 PRINT OPTION                  MAIN 100
C***      =0(DEFAULT) DO NOT PRINT OBSERVED DATA MAIN 105
C***      =1 PRINT OBSERVED DATA               MAIN 110
C***                                         MAIN 115
C*** CARD 3                                  MAIN 120
C***                                         MAIN 125
C*** COLS 1-10 SEARCH RADIUS (C) FOR INVERSE WEIGHT FORMULA (MI)  MAIN 130
C*** COLS 11-20 APPROXIMATE GRID INTERVAL IN THE LONGITUDE (DEGREES) MAIN 135
C*** COLS 21-30 APPROXIMATE GRID INTERVAL IN THE LATITUDE (DEGREES) MAIN 140
C***                                         MAIN 145
C*** CARD 4                                  MAIN 150
C***                                         MAIN 155
C*** COLS 1- 4 5- 8 9-12 13-16, ETC. ALPHANUMERIC CODES      MAIN 160
C***      FOR THE NV VARIABLES                 MAIN 165
C***                                         MAIN 170
C*** CARD 5                                  MAIN 175
C***                                         MAIN 180
C*** COLS 1-80 FORMAT STATEMENT TO USE TO INPUT THE DATA      MAIN 185
C***                                         MAIN 190
C*** CARD 6 AND FOLLOWING                   MAIN 195
C***                                         MAIN 200
C*** THE DATA SHOULD FOLLOW ACCORDING TO THE FORMAT STATEMENT READ MAIN 205
C*** IN CARD 5. THE DATA IS EXPECTED IN THE FORM LONGITUDE, LATITUDE,MAIN 210
C*** FOLLOWED BY THE NV MEASURED VALUES FOR THAT SAMPLE. MISSING    MAIN 215
C*** DATA ARE INDICATED BY VALUES LESS THAN -90000.                MAIN 220
C*** THE PROGRAM IS DIMENSIONED FOR NV LESS THAN OR EQUAL TO 25,    MAIN 225
C*** AND N LESS THAN OR EQUAL TO 1000. THE NUMBER OF GRID INTERVALS MAIN 230
C*** IN THE X DIRECTION TIMES THE NUMBER OF GRID INTERVALS IN THE  MAIN 235
C*** Y DIRECTION MUST ALSO BE LESS THAN 1000.                      MAIN 240

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C*** THESE LIMITS CAN BE CHANGED BY ALTERING THE FOLLOWING DIMENSION MAIN 245
C*** AND COMMON STATEMENTS. MAIN 250
      DIMENSION TITLE(20),FMT(20),X(1000),Y(1000),CODE(25), DATA(1000, MAIN 255
> 25),IPICK(1000),XM(25),XSD(25),UR(25,17), R(25,17),UXM(25), MAIN 260
> UXSD(25),DATV(17),XMA(25),XSDA(25), UXMA(25),UXSDA(25),NA(25), MAIN 265
> NUA(25) MAIN 270
      COMMON/LOCAT/X,Y,XMIN,XMAX,YMIN,YMAX,GRIDX,GRIDY,FAC,SIGN MAIN 275

      DATA XM/25*0.0D0/,XSD/25*0.0D0/,UXM/25*0.0D0/,UXSD/25*0.0D0/, MAIN 280
> XMA/25*0.0D0/,XSDA/25*0.0D0/,UXMA/25*0.0D0/,UXSDA/25*0.0D0/, MAIN 285
> NA/25*0/,NUA/25*0/
      DOUBLE PRECISION XM,XSD,UXM,UXSD,XMA,XSDA,UXMA,UXSDA,XSDM,XMM, MAIN 290
> UXSDM,UXMM

C      DATA BL/1H /,STAR/1H*/ MAIN 295
C*** CARD 1 MAIN 300
      READ(5,10000) TITLE MAIN 305
C*** CARD 2 MAIN 310
      READ(5,10100) NTRY,NV,ITRAN,IPRINT MAIN 315
C*** CARD 3 MAIN 320
      READ(5,10200) DIST,GRIDX,GRIDY MAIN 325
C*** CARD 4 MAIN 330
      READ(5,10000) (CODE(I),I=1,NV) MAIN 335
C*** CARD 5 MAIN 340
      READ(5,10000) FMT MAIN 345
C*** READ AND COUNT THE DATA VALUES MAIN 350
      N=1 MAIN 355
10     READ(5,FMT,END=30) X(N),Y(N),(DATA(N,I),I=1,NV) MAIN 360
      DO 20 I=1,NV MAIN 365
C*** SUM TO GET SUMMARY STATISTICS ON ENTIRE DATA SET MAIN 370
      IF (DATA(N,I).LE.-90000.) GO TO 20 MAIN 375
      NA(I)=NA(I)+1 MAIN 380
      XMA(I)=XMA(I)+DATA(N,I) MAIN 385
      XSDA(I)=XSDA(I)+DATA(N,I)*DATA(N,I) MAIN 390
20     CONTINUE MAIN 395
      N=N+1 MAIN 400
      GO TO 10 MAIN 405
30     N=N-1 MAIN 410
      WRITE(6,10300) TITLE MAIN 415
      SIGN=-1. MAIN 420
      IF (NTRY.NE.-1) GO TO 40 MAIN 425
      NTRY=N MAIN 430
      SIGN=1. MAIN 435
40     CONTINUE MAIN 440
      WRITE(6,10400) NTRY MAIN 445
      IF (ITRAN.NE.0) WRITE(6,10500) MAIN 450
      IF (IPRINT.NE.0) WRITE(6,10600) MAIN 455
      WRITE(6,10700) DIST,GRIDX,GRIDY MAIN 460
      WRITE(6,10800) N,NV MAIN 465
      IF (N.GT.1000) GO TO 370 MAIN 470
      IF (NV.GT.25) GO TO 380 MAIN 475
C*** TRANSFORM DATA IF OPTION REQUESTED (ITRAN .NE. 0) MAIN 480
      IF (ITRAN.EQ.0) GO TO 70 MAIN 485
      DO 50 I=1,NV MAIN 490
      UXMA(I)=XMA(I) MAIN 495
      XMA(I)=0.0 MAIN 500
      UXSDA(I)=XSDA(I) MAIN 505
      XSDA(I)=0.0 MAIN 510
      NUA(I)=NA(I) MAIN 515
      NA(I)=0 MAIN 520
      DO 50 J=1,N MAIN 525
      IF (DATA(J,I).LE.0.0) GO TO 60 MAIN 530
      NA(I)=NA(I)+1 MAIN 535
      DATA(J,I)= ALOG(DATA(J,I)) MAIN 540
      XMA(I)=XMA(I)+DATA(J,I) MAIN 545
      XSDA(I)=XSDA(I)+DATA(J,I)*DATA(J,I) MAIN 550
50     CONTINUE MAIN 555
      GO TO 70 MAIN 560
60     DATA(J,I)=-99999. MAIN 565
      GO TO 50 MAIN 570
70     CONTINUE MAIN 575
      XMAX=-1.E20 MAIN 580
      XMIN=1.E20 MAIN 585
      YMAX=-1.E20 MAIN 590
      YMIN=1.E20 MAIN 595
      DO 80 J=1,N MAIN 600
      IF (X(J).LT.XMIN) XMIN=X(J) MAIN 605
      IF (X(J).GT.XMAX) XMAX=X(J) MAIN 610
      IF (Y(J).LT.YMIN) YMIN=Y(J) MAIN 615
      IF (Y(J).GT.YMAX) YMAX=Y(J) MAIN 620
80     CONTINUE MAIN 625
C*** FIND CONVERSION FACTOR FOR DEGREES TO DISTANCE MAIN 630
C*** BASED ON MIDPOINT IN LATITUDE MAIN 635
      FAC=COS((YMIN+YMAX)/114.591559) MAIN 640

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FAC=FAC*FAC                                MAIN 645
DO 90 IR=1,17                               MAIN 650
DO 90 K=1,NV                                MAIN 655
R(K,IR)=0.0                                 MAIN 660
UR(K,IR)=0.0                                 MAIN 665
90 CONTINUE                                  MAIN 670
IF (IPRINT.EQ.0) GO TO 100                  MAIN 675
WRITE(6,11000)TITLE                         MAIN 680
WRITE(6,11100)                               MAIN 685
100 IF (SIGN.GT.0.0) GO TO 110               MAIN 690
***   FIND THE VALIDATION DATA SET          MAIN 695
CALL PICK(IPICK,DATA,N,NV,NTRY)             MAIN 700
GO TO 130                                   MAIN 705
110 DO 120 K=1,N                           MAIN 710
IPICK(K)=K                                 MAIN 715
120 CONTINUE                                 MAIN 720
130 DO 150 K=1,NTRY                         MAIN 725
***   ESTIMATE THE VALIDATION SAMPLE IPICK(K)  MAIN 730
CALL TRVP(IPICK(K),DATA,CODE,DIST,N,NV,R,UR,ITRAN,IPRINT)  MAIN 735
***   SUM TO GET STATISTICS ON VALIDATION DATA SET  MAIN 745
DO 140 I=1,NV                             MAIN 750
XM(I)=XM(I)+DATA(IPICK(K),I)              MAIN 755
XSD(I)=XSD(I)+DATA(IPICK(K),I)*DATA(IPICK(K),I)  MAIN 760
IF (ITRAN.EQ.0) GO TO 140                 MAIN 765
UXM(I)=UXM(I)+EXP(DATA(IPICK(K),I))        MAIN 770
UXSD(I)=UXSD(I)+EXP(DATA(IPICK(K),I))*EXP(DATA(IPICK(K),I))  MAIN 775
140 CONTINUE                                MAIN 780
150 CONTINUE                                MAIN 785
160 WRITE(6,12200)TITLE                     MAIN 790
IF (ITRAN.NE.0) WRITE(6,12000)             MAIN 795
WRITE(6,10900)                             MAIN 800
FN=1./FLOAT(NTRY)                         MAIN 805
***   CALCULATE THE RESIDUAL MEAN SQUARE ERROR (MSR(P))  MAIN 810
DO 180 K=1,NV                             MAIN 815
DO 170 IR=1,17                            MAIN 820
R(K,IR)=R(K,IR)*FN                        MAIN 825
DATV(IR)=SQRT(R(K,IR))                   MAIN 830
170 CONTINUE                                MAIN 835
WRITE(6,11600) CODE(K),DATV               MAIN 840
180 CONTINUE                                MAIN 845
WRITE(6,11700) NTRY                      MAIN 850
WRITE(6,12300)TITLE                       MAIN 855
IF (ITRAN.NE.0) WRITE(6,12000)             MAIN 860
WRITE(6,10900)                             MAIN 865
***   CALCULATE THE NORMALIZED DIFFERENCE BETWEEN MSR(P) AND MSR(2)  MAIN 870
DO 200 K=1,NV                             MAIN 875
DO 190 IR=1,17                            MAIN 880
DATV(IR)=100.*(R(K,IR)-R(K,7))/R(K,7)  MAIN 885
190 CONTINUE                                MAIN 890
WRITE(6,11600) CODE(K),DATV               MAIN 895
200 CONTINUE                                MAIN 900
WRITE(6,11700) NTRY                      MAIN 905
WRITE(6,11200) TITLE,NTRY                MAIN 910
DO 230 K=1,NV                             MAIN 915
IF (N.EQ.NTRY) GO TO 210                 MAIN 920
XMM=XMA(K)-XM(K)                         MAIN 925
XSDM=XSDA(K)-XSD(K)                      MAIN 930
XMM=XMM/FLOAT(NA(K)-NTRY)                MAIN 935
XSDM=DSQRT((XSDM-XMM*XMM*FLOAT(NA(K)-NTRY))/FLOAT(NA(K)-NTRY-1))  MAIN 940
NDIFF=NA(K)-NTRY                         MAIN 945
210 XMA(K)=XMA(K)/FLOAT(NA(K))           MAIN 950
XSDA(K)=DSQRT((XSDA(K)-XMA(K)*XMA(K)*FLOAT(NA(K)))/FLOAT(NA(K)-1))  MAIN 955
XM(K)=XM(K)*FN                          MAIN 960
XSD(K)=XSD(K)-XM(K)*XM(K)*NTRY          MAIN 965
SD=DSQRT(XSD(K)/FLOAT(NTRY-1))          MAIN 970
DO 220 IR=1,17                            MAIN 975
***   FINISH CALCULATIONS FOR S(P) IN EQUATION 8            MAIN 980
R(K,IR)=NTRY*R(K,IR)/XSD(K)              MAIN 985
220 CONTINUE                                MAIN 990
WRITE(6,12500) CODE(K),XM(K),SD,XMA(K),XSDA(K),NA(K)  MAIN 995
IF (N.NE.NTRY) WRITE(6,12600) XMM,XSDM,NDIFF  MAIN 1000
230 CONTINUE                                MAIN 1005
WRITE(6,12700)                             MAIN 1010
***   FIND MINIMUM S(P) AND PRINT THE TABLE FOR S(P) IN EQUATION 8  MAIN 1015
WRITE(6,12400)TITLE                       MAIN 1020
IF (ITRAN.NE.0) WRITE(6,12000)             MAIN 1025
WRITE(6,10900)                             MAIN 1030
DO 250 K=1,NV                             MAIN 1035
IM=1                                      MAIN 1040
DATV(1)=BL                                MAIN 1045
XMIN=R(K,1)                                MAIN 1050
DO 240 IR=2,17                            MAIN 1055
DATV(IR)=BL                                MAIN 1060
IF (R(K,IR).GT.XMIN) GO TO 240            MAIN 1065

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IM=IR
XMIN=R(K,IR)
240 CONTINUE
DATV(IM)=STAR
WRITE(6,11400) CODE(K),(R(K,IR),IR=1,17)
WRITE(6,11500) DATV
250 CONTINUE
WRITE(6,11800)
WRITE(6,11700) NTRY
C*** REPEAT CALCULATIONS FOR BACK-TRANSFORMED DATA
IF (ITRAN.EQ.0) GO TO 360
WRITE(6,12200)TITLE
WRITE(6,12100)
WRITE(6,10900)
DO 270 K=1,NV
DO 260 IR=1,17
UR(K,IR)=UR(K,IR)*FN
DATV(IR)=SQRT(UR(K,IR))
260 CONTINUE
WRITE(6,11600) CODE(K),DATV
270 CONTINUE
WRITE(6,11700) NTRY
WRITE(6,12300)TITLE
WRITE(6,12100)
WRITE(6,10900)
DO 290 K=1,NV
DO 280 IR=1,17
DATV(IR)=100.*(UR(K,IR)-UR(K,7))/UR(K,7)
280 CONTINUE
WRITE(6,11600) CODE(K),DATV
290 CONTINUE
WRITE(6,11700) NTRY
WRITE(6,11300) TITLE,NTRY
DO 320 K=1,NV
IF (N.EQ.NTRY) GO TO 300
UXMM=UXMA(K)-UXM(K)
UXSDM=UXSDA(K)-UXSD(K)
UXMM=UXMM/FLOAT(NUA(K)-NTRY)
UXSDM=DSQRT((UXSDM-UXMM*UXMM*FLOAT(NUA(K)-NTRY))/FLOAT(NUA(K)-
> NTRY-1))
NDIFF=NUA(K)-NTRY
300 UXMA(K)=UXMA(K)/FLOAT(NUA(K))
UXSDA(K)=DSQRT((UXSDA(K)-UXMA(K)*UXMA(K)*FLOAT(NUA(K)))/
> FLOAT(NUA(K)-1))
UXM(K)=UXM(K)*FN
UXSD(K)=UXSD(K)-UXM(K)*UXM(K)*NTRY
SD=DSQRT(UXSD(K)/FLOAT(NTRY-1))
DO 310 IR=1,17
UR(K,IR)=NTRY*UR(K,IR)/UXSD(K)
310 CONTINUE
WRITE(6,12500) CODE(K),UXM(K),SD,UXMA(K),UXSDA(K),NUA(K)
IF (N.NE.NTRY) WRITE(6,12600) UXMM,UXSDM,NDIFF
320 CONTINUE
WRITE(6,12700)
WRITE(6,12400)TITLE
WRITE(6,12100)
WRITE(6,10900)
DO 340 K=1,NV
IM=1
DATV(1)=BL
XMIN=UR(K,1)
DO 330 IR=2,17
DATV(IR)=BL
IF (UR(K,IR).GT.XMIN) GO TO 330
IM=IR
XMIN=UR(K,IR)
330 CONTINUE
DATV(IM)=STAR
WRITE(6,11400) CODE(K),(UR(K,IR),IR=1,17)
WRITE(6,11500) DATV
340 CONTINUE
WRITE(6,11800)
WRITE(6,11700) NTRY
350 CONTINUE
360 STOP
370 WRITE(6,12800)
STOP
380 WRITE(6,12900)
STOP
10000 FORMAT(20A4)
10100 FORMAT(4I5)
10200 FORMAT(3F10.0)
10300 FORMAT(1H1,20A4/)
10400 FORMAT(54H0THE NUMBER OF SAMPLES IN THE VALIDATION DATA SET ARE
> 15/)

MAIN1070
MAIN1075
MAIN1080
MAIN1085
MAIN1090
MAIN1095
MAIN1100
MAIN1105
MAIN1110
MAIN1115
MAIN1120
MAIN1125
MAIN1130
MAIN1135
MAIN1140
MAIN1145
MAIN1150
MAIN1155
MAIN1160
MAIN1165
MAIN1170
MAIN1175
MAIN1180
MAIN1185
MAIN1190
MAIN1195
MAIN1200
MAIN1205
MAIN1210
MAIN1215
MAIN1220
MAIN1225
MAIN1230
MAIN1235
MAIN1240
MAIN1245
MAIN1250
MAIN1255
MAIN1260
MAIN1265
MAIN1270
MAIN1275
MAIN1280
MAIN1285
MAIN1290
MAIN1295
MAIN1300
MAIN1305
MAIN1310
MAIN1315
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MAIN1325
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MAIN1375
MAIN1380
MAIN1385
MAIN1390
MAIN1395
MAIN1400
MAIN1405
MAIN1410
MAIN1415
MAIN1420
MAIN1425
MAIN1430
MAIN1435
MAIN1440
MAIN1445
MAIN1450
MAIN1455
MAIN1460
MAIN1465
MAIN1470
MAIN1475
MAIN1480
MAIN1485
MAIN1490

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10500 FORMAT(48H0THE CONCENTRATION IS TRANSFORMED BY LOGARITHMS.)      MAIN1495
10600 FORMAT(49H0RESULTS FROM EACH VALIDATION SAMPLE ARE PRINTED.)      MAIN1500
10700 FORMAT(26H0THE SEARCH RADIUS (C) IS ,G9.3,4H MI./                MAIN1505
  > 40H0THE GRIDING INCREMENT FOR LONGITUDE IS ,G9.3/
  > 39H0THE GRIDING INCREMENT FOR LATITUDE IS ,G9.3/)                 MAIN1510
10800 FORMAT(11H THERE ARE ,I5,13H SAMPLES FOR ,I2,10H VARIABLES,        MAIN1515
  > 23H IN THE TOTAL DATA SET.)                                         MAIN1520
10900 FORMAT(10H0 VARIABLE/6X,7HAVERAGE,7H P=.5, 7H P=1, 7H P=1.25,       MAIN1525
  > 7H P= 1.5, 7H P=1.75,7H P= 2,7H P=2.25,7H P= 2.5,7H P=2.75,       MAIN1530
  > 7H P= 3, 7H P= 3.5,7H P= 4,7H P= 4.5,7H P= 5,7H P= 5.5,          MAIN1535
  > 7H P= 6 /)                                                       MAIN1540
11000 FORMAT(1H1,20A4/21H0VALIDATION DATA SET:)                         MAIN1545
11100 FORMAT(10H0 VARIABLE/6X,14H OBS AVERAGE, 7H P=.5,7H P=1,             MAIN1550
  > 7H P=1.25,7H P=1.5, 7H P=1.75,7H P=2,7H P=2.25,7H P=2.5,           MAIN1555
  > 7H P=2.75,7H P=3, 7H P=3.5,7H P=4,7H P=4.5,7H P=5,                  MAIN1560
  > 7H P=5.5,7H P=6 /)                                                 MAIN1565
11200 FORMAT(1H1,20A4/19H0SUMMARY STATISTICS//1X,                           MAIN1570
  > 23HVALIDATION DATA SET(N'=,I4,1H),9X,14HTOTAL DATA SET, 13X,        MAIN1575
  > 19HPREDICTION DATA SET/ 1H+,10X,28(1H_),2X,28(1H_),2X,28(1H_)/      MAIN1580
  > 9H VARIABLE,5X,4HMEAN,9X,4HS.D.,13X,4HMEAN,8X,4HS.D., 6X,1HN,6X,      MAIN1585
  > 4HMEAN,8X,4HS.D.,5X,4HN-N'/ 1H+,12X,6H_____,7X,6H_____,11X,          MAIN1590
  > 6H_____,6X,6H_____, 4X,3H_____,3X,6H_____,6X,6H_____,3X,            MAIN1595
  > 6H_____/)                                                       MAIN1600
11300 FORMAT(1H1,20A4/41H0SUMMARY STATISTICS OF UNTRANSFORMED DATA//1X,MAIN1605
  > 23HVALIDATION DATA SET(N'=,I4,1H),9X,14HTOTAL DATA SET, 13X,        MAIN1610
  > 19HPREDICTION DATA SET/ 1H+,10X,28(1H_),2X,28(1H_),2X,28(1H_)/      MAIN1615
  > 9H VARIABLE,5X,4HMEAN,9X,4HS.D.,13X,4HMEAN,8X,4HS.D., 6X,1HN,6X,      MAIN1620
  > 4HMEAN,8X,4HS.D.,5X,4HN-N'/ 1H+,12X,6H_____,7X,6H_____,11X,          MAIN1625
  > 6H_____,6X,6H_____, 4X,3H_____,3X,6H_____,6X,6H_____,3X,            MAIN1630
  > 6H_____/)                                                       MAIN1635
11400 FORMAT(IX,A4,1X,17F7.3)                                              MAIN1640
11500 FORMAT(1H+,6X,17(6X,A1))                                             MAIN1645
11600 FORMAT(1X,A4,1X,17F7.2)                                              MAIN1650
11700 FORMAT(///I5,30H VALIDATION SAMPLES WERE USED ,                      MAIN1655
  > 20HFOR THE ABOVE TABLE.)                                               MAIN1660
11800 FORMAT(//37H0ASTERISK DENOTES MINIMUM S(P) VALUE.)                     MAIN1665
11900 FORMAT(17H1ESTIMATED VALUES)                                           MAIN1670
12000 FORMAT(10H LOG SCALE)                                                 MAIN1675
12100 FORMAT(22H BACKTRANSFORMED SCALE)                                       MAIN1680
12200 FORMAT(1H1,20A4/22H0TABLE OF SQRT(MSR(P))/)                          MAIN1685
12300 FORMAT(1H1,20A4/32H0TABLE OF (MSR(P)-MSR(2))/MSR(2)/)              MAIN1690
12400 FORMAT(1H1,20A4/14H0TABLE OF S(P)/)                                    MAIN1695
12500 FORMAT(4X,A4,5X,G9.4,6X,G9.4,6X,G9.4,3X,G9.4,1X,I3)               MAIN1700
12600 FORMAT(1H+,71X,G9.4,3X,G9.4,1X,I3)                                 MAIN1705
12700 FORMAT(///47H0NOTE: N MAY NOT BE THE SAME FOR ALL VARIABLES ,        MAIN1710
  > 20HDUE TO MISSING DATA.)                                              MAIN1715
12800 FORMAT(34H THERE ARE MORE THAN 1000 SAMPLES.,                         MAIN1720
  > 43H RECOMPILE PROGRAM WITH LARGER DIMENSIONS.)                         MAIN1725
12900 FORMAT(39H THERE ARE MORE THAN 25 MEASUREMENTS. ,                      MAIN1730
  > 41HRECOMPILE PROGRAM WITH LARGER DIMENSIONS.)                         MAIN1735
END                                                                           MAIN1740
                                                                           MAIN1745

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SUBROUTINE PICK(IPICK,DATA,N,NV,NTRY)                                     PICK  0
C*** SUBROUTINE PICK SELECTS THE VALIDATION DATA SET FOR NTRY SAMPLESPICK 10
C*** BY DIVIDING THE AREA UNDER STUDY INTO GRIDS.                         PICK 15
C*** AT THE FIRST STEP, ONE SAMPLE IS SELECTED FROM EACH GRID              PICK 20
C*** (IF AT LEAST ONE EXISTS). -IF THE NUMBER OF SAMPLES SELECTED          PICK 25
C*** ARE GREATER THAN THE INPUT SIZE OF THE VALIDATION DATA SET,           PICK 30
C*** SAMPLES ARE SELECTED RANDOMLY FROM THIS SELECTION. IF THERE AREPICK 35
C*** NOT ENOUGH SAMPLES THE PROGRAM CONTINUES SELECTING SAMPLES ON          PICK 40
C*** A GRID BY GRID BASIS UNTIL THE VALIDATION DATA SET IS COMPLETED.PICK 45
C*** IT IS ASSUMED THE INITIAL DATA SET IS RANDOMLY SORTED.                PICK 50
C*** DIMENSION IPICK(1),DATA(1000,1)                                         PICK 55
COMMON/LOCAT/X(1000),Y(1000),XMIN,XMAX,YMIN,YMAX,GRIDX,GRIDY, FAC,PICK 60
> SIGN
NPICK=0
NX=(XMAX-XMIN)/GRIDX+1.
NY=(YMAX-YMIN)/GRIDY+1.
NTOTAL=NX*NY
IF (NTOTAL.GT.1000) GO TO 160
DO 10 J=1,NTOTAL
 10 IPICK(J)=0
C*** THE FIRST STEP DETERMINES THE GRID LOCATION OF EACH SAMPLE,          PICK 105
C*** SELECTING ONE SAMPLE FROM EACH GRID.                                  PICK 110
C*** ONCE A SAMPLE IS SELECTED THE LONGITUDE IS NEGATED TO DENOTE          PICK 115
C*** THAT IT IS A VALIDATION SAMPLE.                                       PICK 120
DO 70 I=1,N
XCHK=XMIN+GRIDX
DO 20 IX=1,NX
  IF (X(I).LE.XCHK) GO TO 30
  XCHK=XCHK+GRIDX
20 CONTINUE
IX=NX

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30 YCHK=YMIN+GRIDY          PICK 160
DO 40 IY=1,NY               PICK 165
IF (Y(I).LE.YCHK) GO TO 50   PICK 170
YCHK=YCHK+GRIDY             PICK 175
40 CONTINUE                  PICK 180
IY=NY                       PICK 185
C*** AT THIS POINT SAMPLE I IS IN GRID IX,IY      PICK 190
50 ICNT=(IX-1)*NY+IY         PICK 195
IF (IPICK(ICNT).NE.0) GO TO 70   PICK 200
DO 60 J=1,NV               PICK 205
IF (DATA(I,J).LE.-90000.) GO TO 70   PICK 210
60 CONTINUE                  PICK 215
IPICK(ICNT)=I               PICK 220
X(I)=-X(I)                 PICK 225
NPICK=NPICK+1               PICK 230
70 CONTINUE                  PICK 235
C*** NOW COMPRESS THE DATA INTO THE FIRST NPICK    PICK 240
C*** LOCATIONS IN IPICK           PICK 245
80 NZERO=0                  PICK 250
DO 100 J=1,NTOTAL           PICK 255
IF (IPICK(J).EQ.0) GO TO 90   PICK 260
IPICK(J-NZERO)=IPICK(J)     PICK 265
GO TO 100                   PICK 270
90 NZERO=NZERO+1            PICK 275
100 CONTINUE                 PICK 280
IF (NPICK.LT.NTRY) GO TO 130  PICK 285
IF (NPICK.EQ.NTRY) RETURN    PICK 290
C*** AT THIS POINT MORE THAN ENOUGH VALIDATION SAMPLES WERE CHOSEN,    PICK 295
C*** SO DELETE AS MANY AS NECESSARY CHOOSING THEM AT RANDOM.          PICK 300
NDEL=NPICK-NTRY             PICK 305
DO 120 J=1,NDEL             PICK 310
110 XU=RANF(J)              PICK 315
IU=NPICK*XU+.5              PICK 320
IF (IPICK(IU).EQ.0) GO TO 110  PICK 325
IPICK(IU)=0                 PICK 330
120 CONTINUE                  PICK 335
NPICK=NTRY                  PICK 340
GO TO 80                   PICK 345
C*** AT THIS POINT THERE ARE NOT ENOUGH VALIDATION DATA SAMPLES      PICK 350
C*** SO CONTINUE TO ADD TO THE LIST BY SELECTING ONE                  PICK 355
C*** FROM EACH GRID (IF POSSIBLE) UNTIL THERE ARE ENOUGH            PICK 360
C*** SAMPLES.              PICK 365
130 ILEFT=0                  PICK 370
DO 150 I=1,NX               PICK 375
DO 150 J=1,NY               PICK 380
DO 140 K=1,N                PICK 385
IF (X(K).LE.0.0) GO TO 140   PICK 390
ILEFT=ILEFT+1               PICK 395
IPX=(XMAX-X(K))/GRIDX+1.     PICK 400
IF (IPX.NE.1) GO TO 140     PICK 405
IPY=(YMAX-Y(K))/GRIDY+1.     PICK 410
IF (IPY.NE.1) GO TO 140     PICK 415
NPICK=NPICK+1               PICK 420
X(K)=-X(K)                 PICK 425
IPICK(NPICK)=K              PICK 430
IF (NTRY.EQ.NPICK) RETURN    PICK 435
GO TO 150                   PICK 440
140 CONTINUE                 PICK 445
150 CONTINUE                 PICK 450
IF (NPICK.LT.NTRY.AND.ILEFT.GT.0) GO TO 130   PICK 455
WRITE(6,10000)NTRY           PICK 460
STOP                         PICK 465
160 WRITE(6,10100) NTOTAL    PICK 470
STOP                         PICK 475
10000 FORMAT(40H THERE WERE NOT ENOUGH SAMPLES TO CHOSE , I5,      PICK 480
> 20H VALIDATION SAMPLES.)          PICK 485
10100 FORMAT(37H THE TOTAL NUMBER OF GRIDS REQUESTED,,I6,        PICK 490
> 43H IS GREATER THAN DIMENSIONED VALUE OF 1000./        PICK 495
> 42H RECOMPILE PROGRAM WITH LARGER DIMENSIONS.)        PICK 500
END                         PICK 505
SUBROUTINE TRYP(IPICK,DATA,CODE,DIST,N,NV,R,UR,ITRAN,IPRINT)    TRYP  0
C*** SUBROUTINE TRYP FINDS THE ESTIMATES OF S(P) FOR A VALIDATION    TRYP  5
C*** DATA SAMPLE FOR ALL VALUES OF P.                                TRYP 10
INTEGER P                  TRYP 15
COMMON/LOCAT/X(1000),Y(1000),XMIN,XMAX,YMIN,YMAX, GRIDX,GRIDY,FAC,TRYP 20
> SIGN                         TRYP 25
DIMENSION DATA(1000,1),TOT(25,17),HDATA(25,17), PVAL(16),R(25,1), TRYP 30
> UR(25,1),CODE(1)           TRYP 35
DATA PVAL/.5,1.,1.25,1.5,1.75,2.,2.25,2.5,2.75,3.,3.5, 4.,4.5,5., TRYP 40
> 5.5,6./                     TRYP 45
DO 10 IR=1,17                TRYP 50
DO 10 K=1,NV                 TRYP 55
TOT(K,IR)=0.0                TRYP 60
HDATA(K,IR)=0.0               TRYP 65

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10 CONTINUE                                TRYP  70
NTRY=0                                     TRYP  75
RDIS=DIST                                    TRYP  80
20 DO 50 J=1,N                               TRYP  85
C***   IF THE LONGITUDE IS LESS THAN 0 THEN IT IS A VALIDATION SAMPLE. TRYP  90
      IF (X(J).LE.0.0) GO TO 50                TRYP  95
      IF (X(J).EQ.SIGN*X(IPICK).AND.Y(J).EQ.Y(IPICK)) GO TO 50    TRYP 100
C***   IF THE SAMPLE IS WITHIN THE CUTOFF DISTANCE DO THE COMPUTATIONS. TRYP 105
C***   CALCULATE THE DISTANCE BETWEEN SAMPLES IN MILES               TRYP 110
      DIFF=(X(J)-SIGN*X(IPICK))*(X(J)-SIGN*X(IPICK))*FAC+ (Y(J)-Y(IPICK))TRYP 115
      > )*(Y(J)-Y(IPICK))                         TRYP 120
      DIFF=SQRT(DIFF)*60.*1.516                  TRYP 125
C***   CHECK TO SEE IF DISTANCE IS WITHIN SEARCH RADIUS              TRYP 130
C***   (C IN EQUATION 5)                                 TRYP 135
      IF (DIFF.GT.RDIS) GO TO 50                TRYP 140
      DO 40 K=1,NV                               TRYP 145
C***   CHECK FOR MISSING VALUES                      TRYP 150
      IF (DATA(J,K).LE.-90000.) GO TO 40        TRYP 155
C***   HDATA IS THE SUMMATION OF WEIGHTS * PREDICTION VALUES          TRYP 160
C***   W(I)*Z(I) IN EQUATION 5                   TRYP 165
C***   TOT IS THE SUMMATION OF WEIGHTS W(I) IN EQUATION 6             TRYP 170
      DO 30 IR=1,16                             TRYP 175
      HDATA(K,IR+1)=(DIFF**(-PVAL(IR)))*DATA(J,K)+HDATA(K,IR+1)    TRYP 180
      TOT(K,IR+1)=(DIFF**(-PVAL(IR)))+TOT(K,IR+1)                  TRYP 185
30 CONTINUE                                  TRYP 190
C***   SUMMATIONS FOR P=0 (AVERAGE)                 TRYP 195
      TOT(K,1)=1.0*TOT(K,1)                     TRYP 200
      HDATA(K,1)=HDATA(K,1)+DATA(J,K)           TRYP 205
40 CONTINUE                                  TRYP 210
50 CONTINUE                                  TRYP 215
C***   IF THERE ARE NO PREDICTION VALUES INSIDE THE SEARCH            TRYP 220
C***   RADIUS, INCREASE THE RADIUS BY A SMALL AMOUNT FOR             TRYP 225
C***   THIS SAMPLE.                                         TRYP 230
      DO 60 K=1,NV                               TRYP 235
      IF (TOT(K,1).EQ.0) GO TO 80                TRYP 240
60 CONTINUE                                  TRYP 245
C***   R IS THE SUMMATION OF RESIDUALS FOR EACH VALIDATION SAMPLE       TRYP 250
C***   UR IS THE SUMMATION OF RESIDUALS IN THE BACK-TRANSFORMED DATA     TRYP 255
      DO 70 IR=1,17                           TRYP 260
      DO 70 K=1,NV                               TRYP 265
      HDATA(K,IR)=HDATA(K,IR)/TOT(K,IR)         TRYP 270
      R(K,IR)=R(K,IR)+(HDATA(K,IR)-DATA(IPICK,K))* (HDATA(K,IR)-
      > DATA(IPICK,K))                         TRYP 275
      IF (ITRAN.NE.0) UR(K,IR)=UR(K,IR)+(EXP(HDATA(K,IR))-
      > (EXP(DATA(IPICK,K))))*(EXP(HDATA(K,IR))-(EXP(DATA(IPICK,K))))    TRYP 280
      70 CONTINUE                                TRYP 285
      IF (IPRINT.EQ.0) RETURN                  TRYP 290
      XVAL=SIGN*X(IPICK)                      TRYP 295
      WRITE(6,10000)XVAL,Y(IPICK)              TRYP 300
      WRITE(6,10100) (CODE(K),DATA(IPICK,K), (HDATA(K,IR),IR=1,17),K=1,    TRYP 305
      > NV)                                     TRYP 310
      RETURN                                    TRYP 315
80 CONTINUE                                  TRYP 320
      RDIS=RDIS*2.                            TRYP 325
      NTRY=NTRY+1                            TRYP 330
      WRITE(6,10200) RDIS,X(IPICK),Y(IPICK)    TRYP 335
      IF (NTRY.GT.10) STOP 10                  TRYP 340
      GO TO 20                                TRYP 345
10000 FORMAT(11H LOCATION: ,2F10.3)          TRYP 350
10100 FORMAT(1X,A4,1X,18F7.2)                TRYP 355
10200 FORMAT(37H THE DISTANCE HAD TO BE INCREASED TO ,G10.3,
      > 54H TO PICK UP AT LEAST 1 SAMPLE WITHIN RADIUS OF SAMPLE:,    TRYP 360
      > 2G10.3)                                TRYP 365
      END                                     TRYP 370

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