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Climatic Calibration of Pollen Data

A User's Guide for the Applicable Computer Programs in the Statistical Package for Social Scientists (SPSS)

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National Science Foundation

Prepared for
U.S. Nuclear Regulatory Commission

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ABSTRACT

Radiocarbon-dated pollen records are a source of quantitative estimates for climatic variables for the past 9000 years. Multiple regression is the main method for calculation of these estimates and requires a series of steps to gain equations that meet the statistical assumptions of the analysis. This manual describes these steps which include 1) selection of the region for analysis, 2) selection of the pollen types for statistical analysis, 3) deletion of univariate outliers, 4) transformation to produce linear relationships, 5) selection of the regression equation, and 6) tests of the regression residuals. The input commands and the output from a series of SPSS (Statistical Package for Social Scientists) programs are illustrated and described, and, as an example, modern pollen and climatic data from lower Michigan are used to calculate a regression equation for July mean temperature.

CONTENTS

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INTRODUCTION

Pollen data from radiocarbon-dated sediments can provide estimates of past temperature, rainfall, and moisture balance. By revealing the changes in the vegetation over the past 15,000 years, pollen data indirectly record the climatic changes that forced alterations in the vegetation. Because pollen data are quantitative, multiple regression procedures can be used to calibrate the geographic distribution of modern pollen data in terms of temperature or rainfall (Webb and Bryson, 1972; Webb, 1980). The resultant regression equations can then be applied to fossil samples, and time series and maps of past temperature or precipitation patterns can be produced. Our manual describes how these regression equations are produced. Full descriptions of the methods for collecting and counting pollen data appear in Birks and Birks (1980).

Gaining calibration functions that transform pollen percentages into estimates of climatic variables requires a sequence of computer programs. These make a series of calculations that help the analyst select the samples, pollen types, and climatic variables to include in the data set before a multiple regression equation is developed or checked for assumption violations (Webb and Clark, 1977; Howe and Webb, 1977, 1983). Our article describes the sequence of steps and associated computer programs that were in use at Brown University in May, 1981. Bartlein and Webb (1984) have since updated this sequence of programs by introducing programs from BMDP (Biomedical Computer Programs P-Series, Dixon and Brown, 1979). Other procedures exist for the climatic interpretation of pollen data, and some of these do not require use of regression analysis (Iversen, 1974; Grichuk, 1969). These methods have been reviewed and discussed in Webb and Clark (1977), Davis (1978), Webb (1980), Birks and Birks (1980), Birks (1981), Prentice (1983), and Howe and Webb (1983).

The pollen and climate data used for calibration work at Brown University are stored in an SPSS (Statistical Package for Social Scientists, Nie *et al.* 1975) file with 260 pollen types and 100 climatic variables observed at 3300 sites in eastern North America (Webb and McAndrews, 1976). Within SPSS, programs are available for executing the first seven steps (Figure 1) in selecting the data, calculating the multiple regression equations, and checking residuals (observed minus calculated climatic values) generated by the regression equations (Howe and Webb, 1983.) FORTRAN programs designed by S. Howe and R. Arigo can then be used for further testing of the residuals. The steps in the calibration procedure are illustrated by way of an example in which pollen data from lower Michigan are used to estimate the mean July daily temperature (Webb, 1974).

In this description of the calibration procedure, we have assumed that the data are already stored in an SPSS file with associated labels for the pollen types and climatic variables. With the data in a SPSS file, SPSS commands make it relatively easy to select the samples and variables for use in a given analysis. Those researchers who cannot use or do not elect to use SPSS will still find our documentation useful in spelling out the many decisions needed to gain a calibration equation. These analysts can either write their own programs or use available programs to do the operations that we do in SPSS.

Figure 1

FILE OF MODERN
POLLEN and CLIMATE
DATA

|
V

PROGRAMS
IN
SPSS

|
V

I. CONDESCRIPTIVE (Calculates univariate statistics for each variable.)
II. SCATTER DIAGRAMS
III. WRITE OR LIST CASES FOR CANDIDATE OUTLIERS
IV. CONDESCRIPTIVE AND SCATTER DIAGRAMS WITH CANDIDATE OUTLIERS DELETED
V. REGRESSION
VI. RESIDUALS PLOTTED ON MAPS
VII. RESIDUAL MAPS

|
V

FORTRAN
PROGRAMS

1. VORNAI DIAGRAM
2. MORAN STATISTIC (to test for spatial autocorrelation of the residuals).
3. OTHER TESTS OF THE RESIDUALS (for normality, independence, etc.)

Figure 1: Sequence of computer programs used to develop a regression equation for calibrating pollen data in climatic terms.

SELECTION OF POLLEN TYPES AND SAMPLING SITES

Initial Selection of The Samples of Modern Data

Calculation of a calibration function or a set of calibration functions begins with knowing what fossil data are being studied and calibrated. The chosen set of modern samples should, if possible, contain a broad enough range of pollen percentages to match the range of the pollen percentages of the major types within the fossil data (Webb and Bryson, 1972). Such a match is a necessary, although not sufficient, condition for the modern samples to be analogs for the fossil samples (see pp. 248-249 in Neter and Wasserman, 1974). The geographical extent of the modern samples should initially be chosen large enough to yield the desired range in the pollen percentages for each of the major pollen types. Upon later analysis with the scatter diagrams (Step II), the size of the initial region may need to be modified, but selection of modern samples that match the fossil data is good place to start the analysis.

By setting the limiting values for the latitude and longitude of the region (within the SPSS program, use SELECT IF LATITUDE GE 40.0, etc.; see Step I, CONDESCRIPTIVE below), the user chooses the geographic region containing paired observations of pollen and climatic data. The user may also choose the type of pollen sites (e.g. lake, bog, etc.) to be included in the study.

Calculation of Pollen Percentages

SPSS commands are used to calculate pollen percentages. For the pollen data from lower Michigan, the percentages are based on a sum of total pollen minus spores and obligate aquatic types. In order to minimize the effect of human disturbance on the percentages of various pollen types, *Ambrosia* (ragweed) pollen was deleted from the pollen sum. Its current high value in most samples results from human land-clearance and agriculture and creates a no-analog condition between the modern and fossil data. Deleting ragweed pollen helps to minimize this problem (Webb, 1973, Van Zant *et al.*, 1978). After selection of pollen samples and calculation of the pollen percentages, the data are then ready to be processed by the SPSS routine CONDESCRIPTIVE. (The names of the pollen types are listed in Table 1.)

STEP I CONDESCRIPTIVE

Purpose of Using Condescriptive

This program calculates the maximum value for each pollen type and such basic univariate statistics as the mean and variance. The pollen types meeting certain minimum criteria are then selected for further analysis. Our current practice is initially to retain only those types whose mean is greater than 1.0% or whose mean is less than 1.0% but whose maximum value is greater than 5.0%. In general the pollen types that do not meet these criteria have too weak a numerical relationship with the particular climatic variable to be of use in the regression equation (Howe and Webb, 1983).

Computer Commands For Using CONDESCRIPTIVE

COMMAND	*ARGUMENT*	*PROGRAM & TASK: COMMENTS*
RUN NAME	CONDESCRIPTIVE FOR MICHIGAN TEMPERATURE RUN	Label of run (should be well selected for easy reference)
GET FILE	MODERN3D	Modern3d is the SPSS file of modern data used in this example. It contained 256 variables for each of 1312 cases or sites. (The modern file of surface data is frequently updated, and the current version contains many more variables and cases.)
ALLOCATE	TRANSPACE = 16000	This command allocates sufficient space for memory. (Less space may be adequate.)
COMPUTE	OLDSEQ = SEQNUM	SEQNUM is an intrinsic SPSS variable which numbers the cases within a given SPSS system file. When a 'SELECT IF' card is encountered, SPSS renumbers the remaining cases and changes the values of variable SEQNUM accordingly. Because the original values of SEQNUM are used to identify modern site locations, another variable 'OLDSEQ' must be created to preserve those values of SEQNUM.
SELECT IF	(LATITUDE GE 41.5 AND LE 46.0 AND LONGITUD GE -86.5 AND LE -83.0 AND SEQNUM LE 600 AND NE 483)	Selects data from the input file according to constraints listed. In this example, all cases located in the region 41.5 to 46.0° N and 83.0 and 86.5° W (except cases with sequence number 483 or with sequence numbers above 600) are selected from MODERN3D. This particular 'SELECT IF' chooses 64 cases at sites in the Lower Peninsula (LP) of Michigan by selecting first all cases at sites in a region containing the LP, then deleting those in the Upper Peninsula (UP) and one site (seq. num. 483 = Murry Lake) at the same location as Frains Lake. (In tests for spatial autocorrelation, only one of several coincident sites can be used.)

RECODE	PICEA TO ARTEMISI, IVA TO CYPERACE, MISCHERB TO UNKNOWN (-1,-2,-3=0)	In the list of pollen types (as they are labeled in the SPSS file) PICEA ... ARTEMISI, IVA ... CYPERACE, MISCHERB ... UNKNOWN, all values of -1,-2, and -3 will be made into 0's. The negative values are used in SPSS to indicate missing values, but none exist for these pollen types among the data from lower Michigan.
COMPUTE	TOTAL=0.0	
DO REPEAT	V1=PICEA TO ARTEMISI, IVA TO CYPERACE, MISCHERB TO UNKNOWN	
COMPUTE	TOTAL=TOTAL+V1	
END REPEAT		In the above four steps, the sum of all pollen counts (excluding spores and aquatic pollen) is accumulated in variable TOTAL.
COMPUTE	TOTAL=(TOTAL/100.0)	TOTAL is divided by 100 in order to yield percentages, not proportions.
DO REPEAT	V1=PICEA TO ARTEMISI, IVA TO CYPERACE, MISCHERB TO UNKNOWN	
COMPUTE	V1=V1/TOTAL	This command converts values of pollen counts of all types in the pollen sum to percentages of the TOTAL.
END REPEAT		
WRITE CLASS	(/4X,F4.0,4(2X F6.3), 4X,3(2X,A4)) OLDSEQ,LONDEG,LONMIN, LATDEG,LATMIN,STATE, NAME1,NAME2	This step is optional and gives a listing of the whole data set.
CONDESCRIPTIVE	PICEA TO ARTEMISI, IVA TO CYPERACE, MISCHERB TO UNKNOWN	
STATISTICS	ALL	These two commands give the following statistics for each pollen type in the requested list: mean, variance, range, sum, standard error, kurtosis, minimum value, standard deviation, skewness, and maximum value.
FINISH		End card for SPSS deck

Sample Output

```
VARIABLE  PICEA      PICEA * SPRUCE

MEAN            0.431        STD ERROR       0.071        STD DEV        0.570
VARIANCE        0.325        KURTOSIS        8.122        SKEWNESS       2.422
RANGE           3.185        MINIMUM         0.0          MAXIMUM        3.185
SUM            27.607

VALID OBSERVATIONS -      64          MISSING OBSERVATIONS -       0

- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

VARIABLE  ABIES      ABIES * FIR

MEAN            0.188        STD ERROR       0.045        STD DEV        0.361
VARIANCE        0.130        KURTOSIS        8.167        SKEWNESS       2.627
RANGE           1.911        MINIMUM         0.0          MAXIMUM        1.911
SUM            12.047

VALID OBSERVATIONS -      64          MISSING OBSERVATIONS -       0

- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

VARIABLE  LARIX      LARIX * LARCH

MEAN            0.012        STD ERROR       0.007        STD DEV        0.057
VARIANCE        0.003        KURTOSIS       24.317        SKEWNESS       4.922
RANGE           0.345        MINIMUM         0.0          MAXIMUM        0.345
SUM             0.771

VALID OBSERVATIONS -      64          MISSING OBSERVATIONS -       0

- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

VARIABLE  JUNIPER    JUNIPERUS,THUJA * JUNIPER, ARBOR VITAE

MEAN            0.751        STD ERROR       0.085        STD DEV        0.682
VARIANCE        0.466        KURTOSIS        2.018        SKEWNESS       1.366
RANGE           2.913        MINIMUM         0.0          MAXIMUM        2.913
SUM            48.083

VALID OBSERVATIONS -      64          MISSING OBSERVATIONS -       0

- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

TABLE 1: Ordered List of Pollen Types
Based on the Output from CONDESCRIPTIVE

NAME	MEAN	STANDARD DEVIATION	MAXIMUM
Quercus	24.726	12.906	51.685
Pinus	23.504	18.688	67.682
Betula	6.435	4.578	19.851
Gramineae	6.247	5.505	29.487
Ulmus	5.494	4.082	29.101
Fagus	3.608	3.238	14.748
Acer	2.960	1.890	8.798
Tsuga	2.828	3.577	16.172
Fraxinus	2.826	2.123	10.582
Polygonaceae	2.270	2.081	10.092
Alnus	1.873	1.363	5.338
Salix	1.544	1.490	8.072
Carya	1.529	1.665	6.969
Populus	1.486	1.577	5.714
Unidentified	1.445	1.284	8.273
Ostrya/Carpinus	1.407	0.862	3.704
Cyperaceae	1.306	2.873	22.192
Chenopodeaceae	1.287	0.742	3.374
Compositae	0.763	0.584	2.667
Juniperus/Thuja	0.751	0.682	2.913
Misc. Herbs	0.629	0.898	4.103
Artemisia	0.622	0.498	1.972
Platanus	0.617	0.649	2.878
Juglans	0.546	0.518	2.158
Plantago	0.535	0.573	2.158
Picea	0.431	0.570	3.185
Myrica	0.387	0.609	2.711
Unknown	0.374	0.579	3.333
Tilia	0.272	0.493	3.175
Rosaceae	0.255	0.380	1.695
Other Trees	0.200	0.317	1.302
Abies	0.188	0.361	1.911
Rhamnus/Vitis	0.184	0.326	1.778
Corylus	0.150	0.232	1.058
Morus	0.125	0.238	0.990
Liquidambar	0.040	0.107	0.360
Celtis	0.032	0.113	0.719
Aquafoliaceae	0.032	0.112	0.704
Thalictrum	0.029	0.080	0.342
Zea	0.019	0.066	0.282
Ericaceae	0.017	0.064	0.277
Larix	0.012	0.057	0.345
Taxus	0.009	0.073	0.587
Ephedra	0.005	0.040	0.324
Sarcobatus	0.004	0.032	0.256

Results of Using CONDESCRIPTIVE

For the pollen data from lower Michigan, the following types satisfied the initial criteria for being included in the further analysis needed to calculate a calibration equation: *Acer* (maple), *Alnus* (alder), *Betula* (birch), *Carya* (hickory), Chenopodiaceae/Amaranthaceae (pigweed/amaranth families), Cyperaceae (sedge family), *Fagus* (beech), *Fraxinus* (ash), Gramineae (grass family), *Ostrya/Carpinus* (hornbeam), *Pinus* (pine), Polygonaceae (buckwheat family), *Populus* (aspen), *Quercus* (oak), *Salix* (willow), *Tsuga* (hemlock), and *Ulmus* (elm). (In SPSS, these pollen types have the following labels: ACER, ALNUS, BETULA, CARYA, CHENOPOD, CYPERACE, FAGUS, FRAXINUS GRAMINEA, OSTRYACA, PINUS, POLYGONA, POPULUS, QUERCUS, SALIX, TSUGA and ULMUS.) The category of Unidentifiable pollen also satisfied the criteria but was excluded because it contains a mixture of pollen types and therefore is an undesirable type to retain as a candidate for the regression equation. Had the categories, Other Trees, Miscellaneous Herbs, or Unknown pollen satisfied the criteria, they would also have been excluded at this stage for this same reason. Including these four types in the CONDESCRIPTIVE step is useful in revealing any sample with high values for one of these categories. Such samples might best be excluded from further analysis. No such samples existed in the data set from lower Michigan.

For the types that were retained, the next question was to find out what type of quantitative relationship that they have with July mean temperature (TMEANJUL) and whether any sites contain outlier values (i.e. anomalous values). For some of the types with means less than 1.0%, the samples with values above 5.0% may be outliers. If so, removal of these samples will mean that these types must be deleted from futher analysis. Scatter diagrams help to answer these questions and aid the decision of which types and which sites to retain for the regression analysis.

STEP II PLOTTING SCATTER DIAGRAMS WITH THE SCATTERGRAM PROGRAM

Purpose Of Plotting The Scatter Diagrams

One purpose of plotting scatter diagrams (Figure 2) is to identify candidate outliers. A case is a candidate outlier if, for at least one pollen type, the paired pollen percentage and TMEANJUL value are 'very' different from those for most other cases. More information about candidate outliers is obtained in Step III (WRITE or LIST CASES) by listing the name, location, and type of the site along with its pollen percentages and climatic value.

A second purpose of printing the scatter diagrams is to identify the type of relationship between the climatic variable (TMEANJUL) and each pollen type. This relationship (after exclusion of the candidate outliers) may be:

1. linear (see *Quercus* in Fig. 2),
2. curvilinear, which can be made linear by proper transformation of the pollen type (see *Carya* and Gramineae in Fig. 2), or
3. neither of the above.

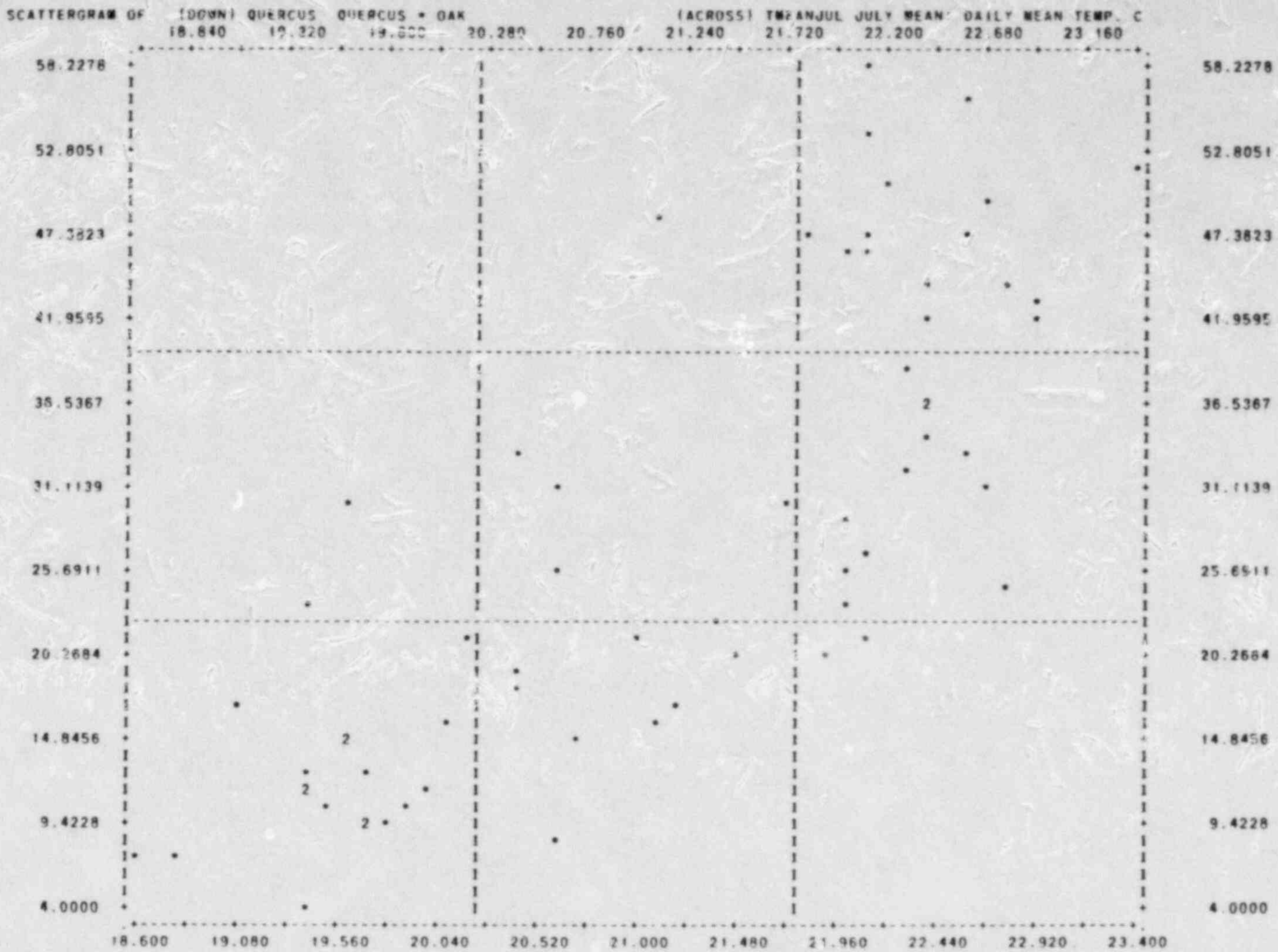
Pollen types with linear or curvilinear relationships are most likely to appear as terms in the regression equation, whereas pollen types of category three probably will not appear. Knowledge of these relationships can be helpful in the interpretation of the regression equation.

Computer Commands for Plotting the Scatter Diagrams

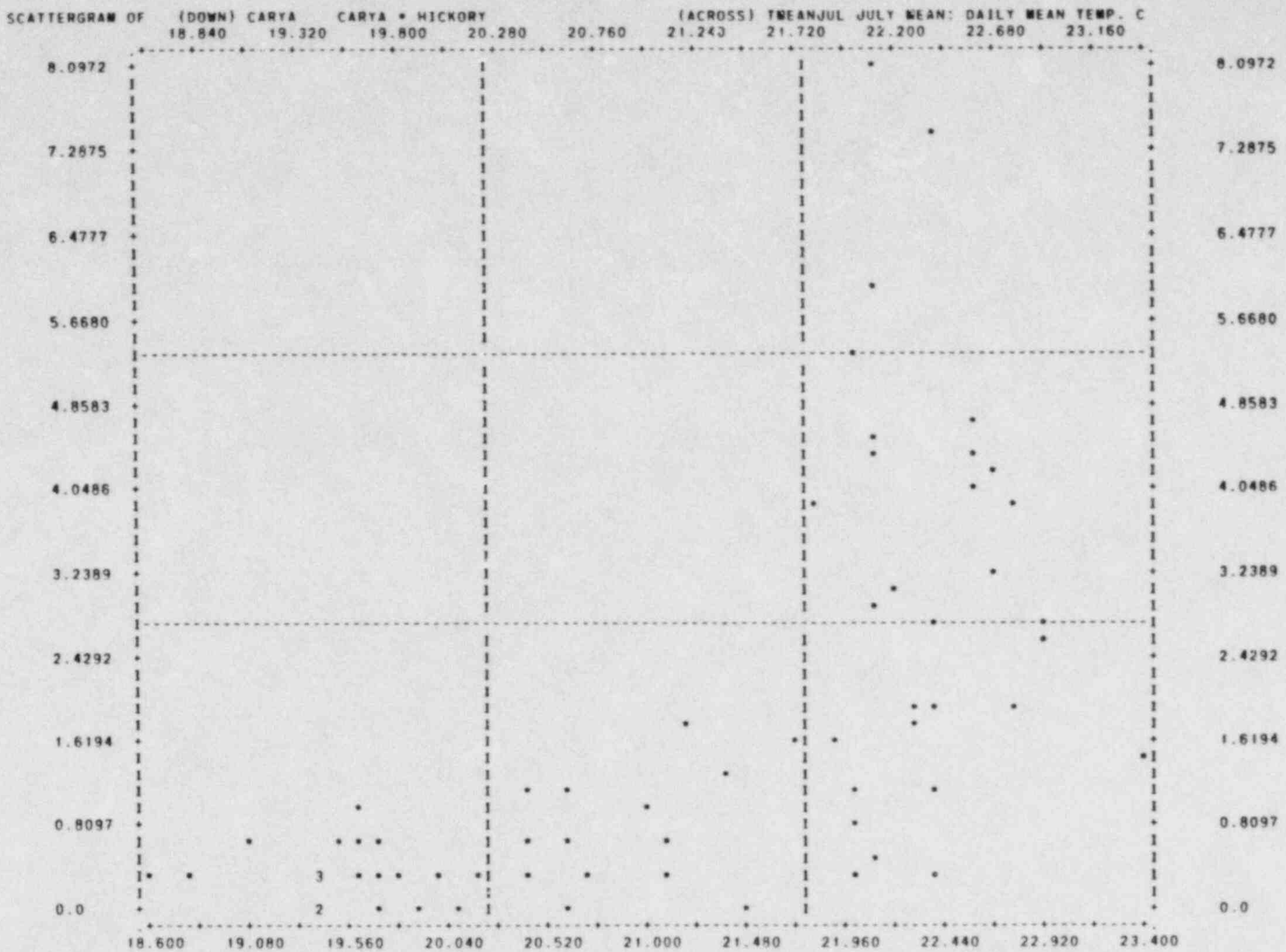
COMMAND	*ARGUMENT*	*PROGRAM & TASK: COMMENTS*
RUN NAME	SCATTER DIAGRAMS FOR...	
GET FILE	MODERN3D	
ALLOCATE	TRANSPACE =	
SELECT IF	(LATITUDE GE 41.5 ... ... 483)	
RECODE	PICEA to ... (-1,-2,-3 = 0)	
COMPUTE	TOTAL = 0.0	
DO REPEAT	V1 = ACER,ALNUS,BETULA, CARYA,CYPERACE,FAGUS, FRAXINUS,GRAMINEA, OSTRYACA,PINUS,POLYGONA, POPULUS,QUERCUS,ULMUS, SALIX,TSUGA	
COMPUTE	TOTAL = TOTAL + V1	
END REPEAT		These commands calculate percentages based on the X types selected for the pollen sum in the previous CONDESCRIPTIVE step. The types that have not been deleted are arranged in alphabetical order for easy access.
COMPUTE	TOTAL = TOTAL/100.0	
DO REPEAT	V1 = ACER,ALNUS,BETULA, CARYA,CYPERACE,FAGUS, FRAXINUS,GRAMINEA, OSTRYACA,PINUS,POLYGONA, POPULUS,QUERCUS,ULMUS, SALIX,TSUGA	
COMPUTE	V1 = V1/TOTAL	
END REPEAT		

SCATTERGRAM	LATITUDE WITH LONGITUD	This command maps the sites associated with the cases retained by the SELECT IF statement.
SCATTERGRAM	V1=ACER,ALNUS,BETULA, CARYA,CYPERACE,FAGUS, FRAXINUS,GRAMINEA, OSTRYACA,PINUS,POLYGONA, POPULUS,QUERCUS,ULMUS, SALIX,TSUGA	This command plots scatter diagrams for each type listed in the scattergram (on Y-axis) against TMEANJUL (mean July temperature) on X-axis. (Note that our practice has been to plot the dependent regression variable along the X-axis and therefore differs from conventional statistical practice.) V1 gives the label for the scatter diagrams.
STATISTICS	ALL	
FINISH		

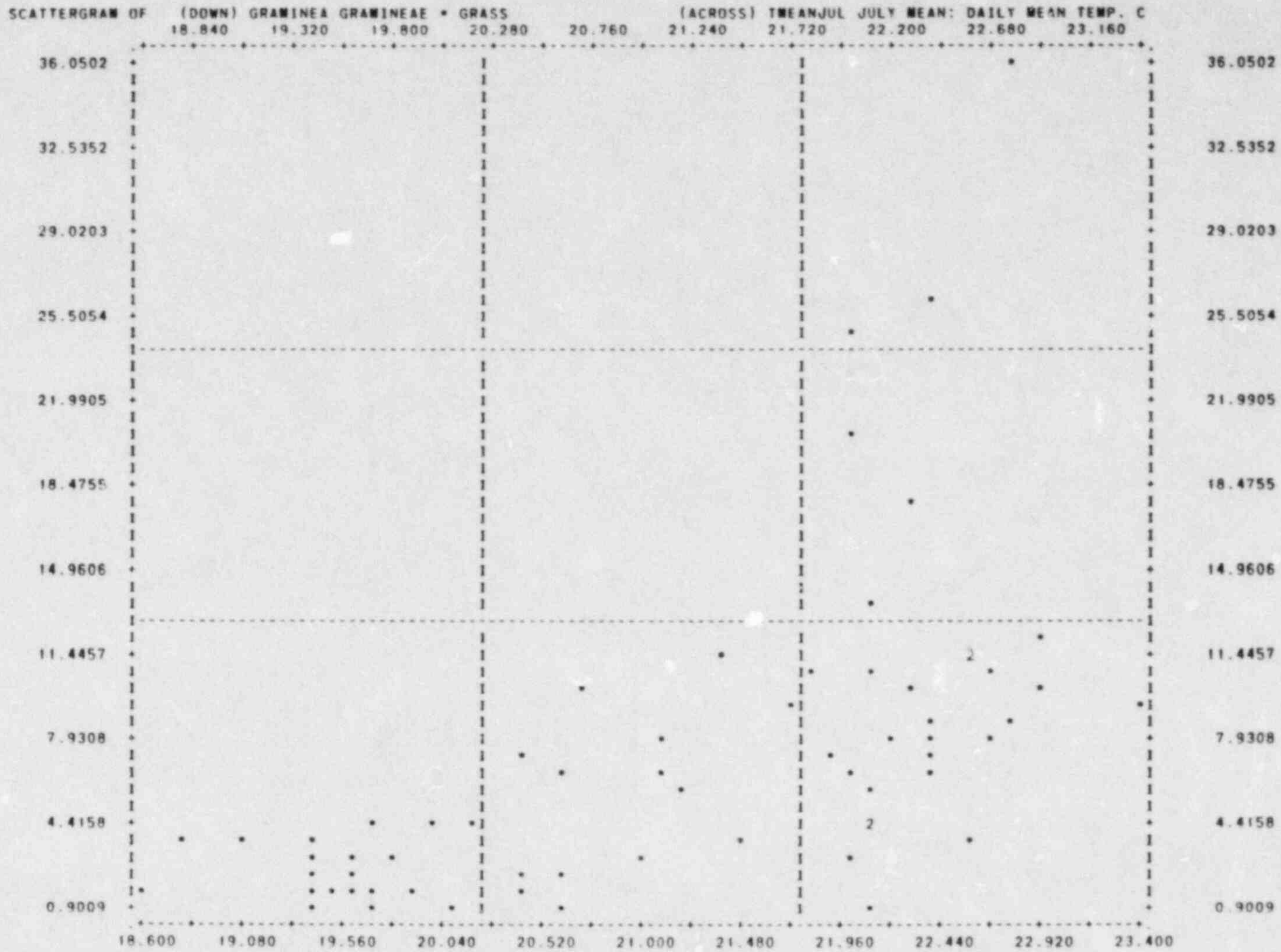
Sample Output



Sample Output



Sample Output



Sample Output

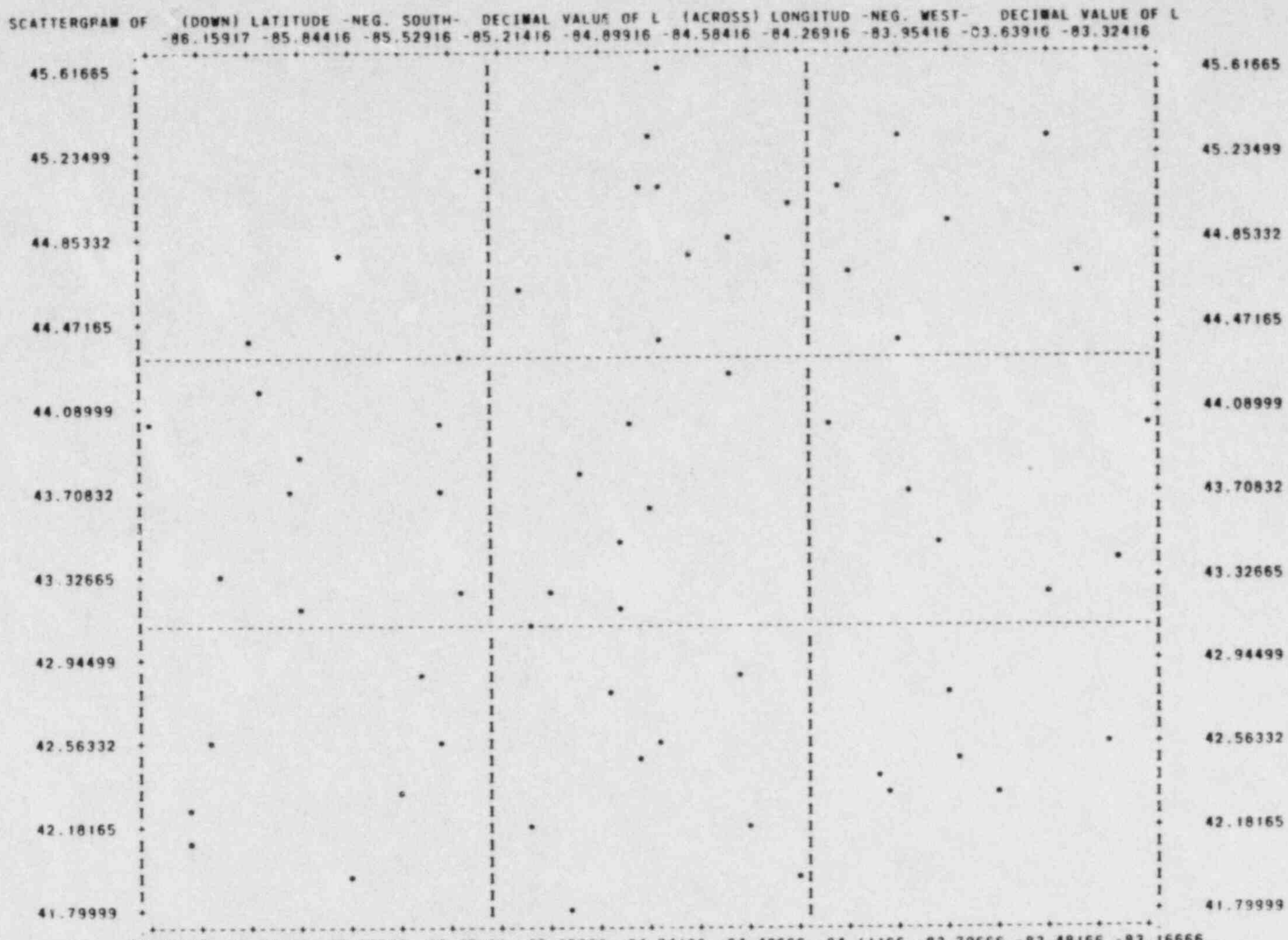


Figure 2: Scatter Diagrams of Quercus, Carya, and Gramineae versus July mean temperature and of latitude versus longitude for Lower Michigan

STEP III WRITE CASES FOR CANDIDATE OUTLIERS

Preparation For Write Cases For Candidate Outliers Run

The purpose of using the WRITE CASES program is to obtain more information about candidate outliers. Candidate outliers are identified on the scatter diagrams. In the scatter diagram (Figure 2) of GRAMINEA (grass pollen) vs. TMEANJUL (mean July temperature), for example, the case plotted near the top right corner could be an outlier. This case is identified in a WRITE CASES run by having both TMEANJUL and GRAMINEA greater than 20. For every type with a candidate outlier, a sequence of commands similar to the following example for the GRAMINEA (8 letter name for Gramineae in the SPSS file) variable can be executed:

```
*SELECT IF        (TMEANJUL GT 20 AND
                  GRAMINEA GT 20)

WRITE CLASS       (/4X,F4.0,4(2X,F6.3),
                  4X,3(2X,A4),2F7.3)
                  OLDSEQ,LONDEQ,LONMIN,
                  LATDEG,LATMIN,STATE,
                  NAME1,NAME2,TMEANJUL,
                  GRAMINEA
```

Computer Commands for Using WRITE CASES

COMMAND	*ARGUMENT*	*PROGRAM & TASK: COMMENTS*
RUN NAME	WRITE CANDIDATE OUTLIERS	
GET FILE	MODERN3D	
ALLOCATE	TRANSPACE=1600	
COMPUTE	OLDSEQ=SEQNUM	This COMPUTE card is needed to insure that the numbering or sequencing of the input files is not altered internally by SPSS during a SELECT IF command. (See note about this command in CONDESCRIPTIVE Stage.)
SELECT IF	(LATITUDE ... ... NE 483)	
RECODE	PICEA ... (-1,-2,-3=0)	
COMPUTE	TOTAL ...	
END REPEAT		
COMPUTE	TOTAL	
DO REPEAT	V1= ... ...TSUGA	
COMPUTE	V1=V1/TOTAL	
END REPEAT		
WRITE CASES	(/4X,F4.0,4X,2A4,4X,F4.2, /12X,8(F6.3,2X) /12X,8(F6.3) MODSEQ,NAME1,NAME2,TMEANJUL ACER,ALNUS,BETULA,CARYA, CYPERACE,FAGUS,FRAXINUS, GRANMINEA,OSTRYACA,PINUS, POLYGONA,POPULUS,QUERCUS SALIX,TSUGA,ULMUS	The first line of the WRITE CASES command gives the printing format for the variables listed on the following lines.
FINISH		

STEP IV CONDESCRIPTIVE AND SCATTER DIAGRAMS WITH OUTLIERS DELETED

Purpose Of Using Condescriptive And Plotting Scatter Diagrams With Outliers Deleted

The purpose of recomputing the CONDESCRIPTIVE statistics and scatter diagrams is to check the pollen types that remain in the data set in light of the new pollen sum and the deletion of the outliers. If no types are deleted from the pollen sum as a result of the Steps II and III, this step may not be necessary. In the example from lower Michigan, five sites and four pollen types Chenopodiaceae/Amaranthaceae, Polygonaceae, Gramineae, and Cyperaceae were deleted. After study of the scatter diagrams, the first three types were judged to be like *Ambrosia* pollen in primarily reflecting human disturbance. Cyperaceae pollen was judged to be of wetland origin and not useful in climatic calibration. The pollen sum was reduced to 13 pollen types.

Pollen types identified as having a curvilinear relationship with the climatic variable are transformed as part of this step, and the transformed variable is plotted against TMEANJUL to verify that the relationship is linear. (The transformed variables are also used in STEP V, the REGRESSION ANALYSIS.) In the data from lower Michigan, square root transformations were chosen for *Fraxinus*, and *Carya*, and a cubic root for *Carya* was also included.

Preparation For Using Condescriptive And Plotting Scatter Diagrams With Outliers Deleted

After study of the scatter diagrams and the listed cases, the outliers are chosen and deleted from the analysis. If a site is to be deleted, adjust the first SELECT IF command to delete it. If the whole taxon is to be deleted, remove the variable name from the two DO REPEAT loops that compute the sums.

The cases that appear to be outliers on the scatter diagrams may be deleted from the subsequent analysis if as samples they are anamalous or contain errors. Reasons for deleting sites with unusual values include:

1. anomalous basin features (e.g. dammed river, cattle trough, when all other samples are from lakes),
2. anomalous edaphic features (e.g. the only sample in an area of sandy outwash),
3. anomalous elevations, and
4. errors in the data (correction is preferable).

Computer Commands for Condescriptive and Scatter Diagrams

With Outliers Deleted

COMMAND	*ARGUMENT*	*PROGRAM & TASK: COMMENTS*
RUN NAME	...	
GET FILE	...	
ALLOCATE	...	
SELECT IF	(LATITUDE LONGITUD... SEQNUM ... NE 454 AND 459 AND 461 AND 462 AND 467 AND 483)	From the analy... of the previous runs, we are deleting sites 454, 459, 461, 462, and 467 in addition to site 483, which was deleted in the previous runs also.
RECODE	... (-1,-2,-3=0)	
COMPUTE	OLDSEQ . .	
COMPUTE	TOTAL= ...	
DO REPEAT	V1=ACER,ALNUS,BETULA, CARYA,FAGUS,FRAXINUS, OSTRYACA,PINUS,POPULUS, QUERCUS,SALIX,TSUGA,ULMUS	Notice CHENOPOD, CYPERACE, GRAMINEA, POLYGONA, were totally deleted from the pollen sum.
COMPUTE	TOTAL ...	
END REPEAT		
COMPUTE	TOTAL=	
DO REPEAT	V1=ACER,ALNUS,BETULA, CARYA,FAGUS,FRAXINUS, OSTRYACA,PINUS,POPULUS, QUERCUS,SALIX,TSUGA,ULMUS	
COMPUTE	V1=V1/TOTAL	
END REPEAT		Notice again, CHENOPOD, CYPERACE, GRAMINEA, POLYGONA were deleted from the pollen sum.

CONDESCRIPTIVE	ACER,ALNUS,BETULA,CARYA, FAGUS,FRAXINUS,OSTRYACA, PINUS,POPULUS,QUERCUS, SALIX,TSUGA,ULMUS	
STATISTICS	ALL	Compute the statistics for the remaining pollen types from the remaining sites.
SCATTERGRAM	ACER,ALNUS,BETULA,CARYA, FAGUS,FRAXINUS,OSTRYACA, PINUS,POPULUS,QUERCUS, SALIX,TSUGA,ULMUS WITH TMEANJUL	
STATISTICS	ALL	Make scatter diagrams for TMEANJUL vs. each remaining pollen type.
FINISH		

STEP V REGRESSION

Purpose of the Multiple Regression Program

The purpose of this program is to calculate a series of multiple regression equations, from which one is chosen as a candidate equation for calibrating pollen data in the pollen diagrams that are being studied. The regression program in SPSS uses a forward-selection stepwise multiple regression procedure. Backwards elimination and other procedures for multiple regression might also be used, if programs for these procedures are available (see Bartlein and Webb, 1984). Once a regression equation is chosen, the program is rerun to gain a scatter plot for checking the residuals of this equation.

Preparation For The Regression Run

Included among the possible independent variables in the regression analysis are all types in the pollen sum as well as any of those transformed variables that exhibit an approximately linear relationship with TMEANJUL. For example, CARYA, the square root of CARYA, or the cube root of CARYA may be in the list of candidate variables. (In Bartlein and Webb, 1984, only one entry for each pollen type is used, that was judged to yield the best linear relationship.)

Computer Commands for REGRESSION ANALYSIS

COMMAND	*ARGUMENT*	*PROGRAM & TASK: COMMENTS*
RUN NAME	REGRESSION RUN FOR MICHIGAN TEMPERATURE REGRESSION	
GET FILE	MODERN3D	
ALLOCATE	TRANSPACE=1600	
SELECT IF	(LATITUDE ... LONGITUD ... SEQNUM ... NE ... AND ...)	
RECODE	PICEA TO ARTEMISI ... (-1,-2,-3=0)	
COMPUTE	OLDSEQ=SEQNUM	
COMPUTE	TOTAL=0.0	
DO REPEAT	V1= ... FRAXINUS ... POPULUS ...	
COMPUTE	TOTAL= ...	
END REPEAT		Same 13 pollen types as previous run, and also same sites
COMPUTE	TOTAL= ...	
DO REPEAT	V1= ... FRAXINUS ... QUERCUS	
COMPUTE	V1= ...	
END REPEAT		Same pollen types as above
COMPUTE	SCARYA=SQRT(CARYA)	This command calculates the square root of CARYA to try to eliminate the curvature when *Carya* percentages are plotted against mean July temperature.

COMPUTE	CCARYA=CARYA**(1./3.)	Calculates the cube root of CARYA.
COMPUTE	SFRAX=SQRT(FRAXINUS)	Calculates the square root of FRAXINUS to try to eliminate curvature when *Fraxinus* percentages are plotted against TMEANJUL.
SCATTERGRAM	SCARYA,CCARYA,SFRAX WITH TMEANJUL	Makes scatter diagrams of SCARYA vs. TMEANJUL, CCARYA vs. TMEANJUL, SFRAX vs. TMEANJUL to illustrate whether the curvature remains.
STATISTICS	ALL	This command gives all the statistics to go along with the scattergrams.
REGRESSION	VARIABLES=TMEANJUL, ACER,ALNUS,BETULA,CARYA, FAGUS,FRAXINUS,OSTRYACA, PINUS,POPULUS,QUERCUS, SALIX,TSUGA,ULMUS, SCARYA,CCARYA,SFRAX, LATITUDE,LONGITUD/ REGRESSION=TMEANJUL WITH ACER,ALNUS,BETULA,CARYA, FRAGUS,FRAXINUS,OSTRYACA, PINUS,POPULUS,QUERCUS, SALIX,ULMUS,SCARYA,CCARYA, SFRAX (1) LATITUDE,LONGITUD (0) RESID=0	This command for stepwise forward multiple regression first identifies the variables and then designates TMEANJUL as dependent variable and all variables listed after WITH as independent variables. The code 1 indicates that the variables preceding the (1) are to be entered sequentially. At each step the variable that enters the regression has the highest F-to-enter value. LATITUDE and LONGITUD have code 0, so their F-to-enter values are given, but the variables never enter the regression. These values indicate how much spatial dependency remains in the data set during the regression.
STATISTICS	6	
FINISH		

Sample Output

```
* * * * * * * * * * * * * * * * * * * * * *   M U L T I P L E   R E G R E S S I O N   * * * * * * * * * * * * *   VARIABLE LIST  1
                                                                                                                REGRESSION LIST  1
DEPENDENT VARIABLE..    TMEANJUL   JULY MEAN: DAILY MEAN TEMP. C

VARIABLE(S) ENTERED ON STEP NUMBER  4..    TSUGA      TSUGA - HEMLOCK

MULTIPLE R          0.92890                   ANALYSIS OF VARIANCE    DF      SUM OF SQU[illegible]ES      MEAN SQUARE          F
R SQUARE            0.86286                   REGRESSION               4.        [illegible]          21.78607       84.93692
ADJUSTED R SQUARE   0.85270                   RESIDUAL                54.        13.85142           0.25651
STANDARD ERROR      0.50647
```

----------------- VARIABLES IN THE EQUATION ------------------

VARIABLE	B	BETA	STD ERROR B	F
QUERCUS	0.42814670D-01	0.61079	0.00560	58.523
FAGUS	0.92282510D-01	0.29098	0.01753	27.728
ULMUS	0.77738060D-01	0.21926	0.02187	12.631
TSUGA	-0.65669860D-01	-0.20600	0.02345	7.839
(CONSTANT)	19.02248			

------------- VARIABLES NOT IN THE EQUATION -------------

VARIABLE	BETA IN	PARTIAL	TOLERANCE	F
ACER	-0.02509	-0.05689	0.70510	0.172
ALNUS	-0.05454	-0.12750	0.74952	0.876
BETULA	-0.07017	-0.10746	0.32162	0.619
CARYA	-0.11610	-0.18755	0.35788	1.932
FRAXINUS	0.04792	0.08727	0.45480	0.407
OSTRYACA	0.03640	0.08471	0.74277	0.383
PINUS	0.04985	0.03598	0.07146	0.069
POPULUS	0.06823	0.18073	0.96223	1.790
SALIX	0.01989	0.04238	0.62230	0.095
SCARYA	-0.09100	-0.13357	0.29544	0.963
CCARYA	-0.07125	-0.11345	0.34768	0.691
SFRAX	0.07296	0.13055	0.43915	0.919
LATITUDE	-0.59066	-0.49243	0.09532	16.966
LONGITUD	-0.06539	-0.15720	0.79258	1.343

Use Of Regression Output

One regression equation is selected. Inspection of the ADJUSTED R SQUARE and STANDARD ERROR values often helps this choice. For example, the equation is selected for the regression step (often when three to six pollen types are in the equation) at which changes in these two values stabilize to two or three percent or to 0.1 or 0.2 °C. The size of these limiting numbers depends upon the size of the study area and the strength of the pollen/climate relationship. In the example, regression equation 4 was chosen with variables QUERCUS, FAGUS, ULMUS, TSUGA because addition of another variable, POPULUS, in regression equation 5 only little changed the ADJUSTED R SQUARE or the STANDARD ERROR.

STEP VI RESIDUAL CHECK

Plot of the Residuals versus Dependent Variable

Once the regression equation is chosen, the regression program should be rerun to print out a diagram of the standardized residuals (y-axis) versus the standardized magnitude of the dependent variable (mean July temperature along the x-axis). The residuals are standardized by dividing each by the standard deviation of all residuals, and the dependent variable is standardized by subtracting its mean and dividing by its standard deviation. This scatter plot shows whether or not the variance of the residuals is homogenous and therefore similar for all values of the dependent variable (Neter and Wasserman, 1974). If the variance is inhomogenous because the largest positive residuals only occur for low values of the dependent variable, then the regression equation is biased and may need recalculation (Howe and Webb, 1983). The plot of residuals for the lower Michigan data showed the variance to be homogenous.

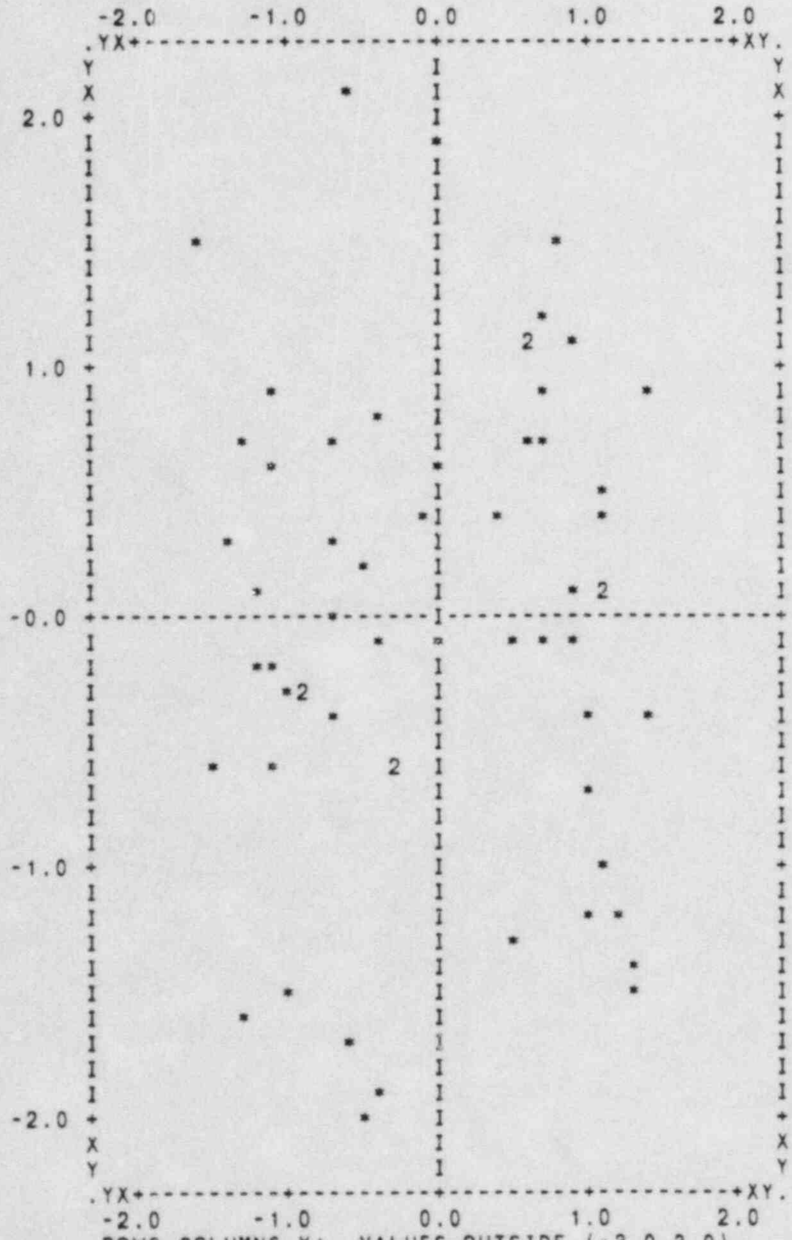
Computer Commands for Plotting the Residuals

```
COMMAND         ARGUMENT

RUN NAME        REGRESSION RUN FOR MICHIGAN TEMPERATURE REGRESSION
GET FILE        MODERNED
ALLOCATE        TRANSPACE=16000
SELECT IF       (LATITUDE GE 41.5 AND LE 46.0 AND
                LONGITUD GE -86.5 AND LE -83.0 AND
                SEQNUM LE 600 AND
                NE 454 AND 459 AND 461 AND 462
                AND 467 AND 483)
RECODE          PICEA TO ARTEMISI,IVA TO CYPERACE,MISCHERB TO UNKNOWN
                (-1,-2,-3=0)
COMPUTE         OLDSEQ=SEQNUM
COMPUTE         TOTAL=0.0
DO REPEAT       V1=ACER,ALNUS,BETULA,CARYA,FAGUS,
                FRAXINUS,OSTRYACA,PINUS,
                POPULUS,QUERCUS,SALIX,TSUGA,ULMUS
COMPUTE         TOTAL=TOTAL+V1
END REPEAT
COMPUTE         TOTAL=TOTAL/100.0
DO REPEAT       V1=ACER,ALNUS,BETULA,CARYA,FAGUS,
                FRAXINUS,OSTRYACA,PINUS,POPULUS,
                QUERCUS,SALIX,TSUGA,ULMUS
COMPUTE         V1=V1/TOTAL
END REPEAT



REGRESSION      VARIABLES=TMEANJUL,
                FAGUS,
                QUERCUS,TSUGA,
                ULMUS/
                REGRESSION=TMEANJUL WITH
                FAGUS,QUERCUS,TSUGA,ULMUS
                (2)
                RESID=0
STATISTICS      6
```

Sample Output

PLOT: STANDARDIZED RESIDUAL (DOWN) -----
PREDICTED STANDARDIZED DEPENDENT VARIABLE (ACROSS)

DEPENDENT VARIABLE: TMEANJUL VARIABLE LIST 1



ROWS,COLUMNS Y: VALUES OUTSIDE (-3.0,3.0)
ROWS,COLUMNS X: VALUES IN (-3.0,-2.05) OR (2.05,3.0)

STEP VII RESIDUAL PLOT AND RESIDUAL MAPS

Purpose Of Plotting Residuals on Maps

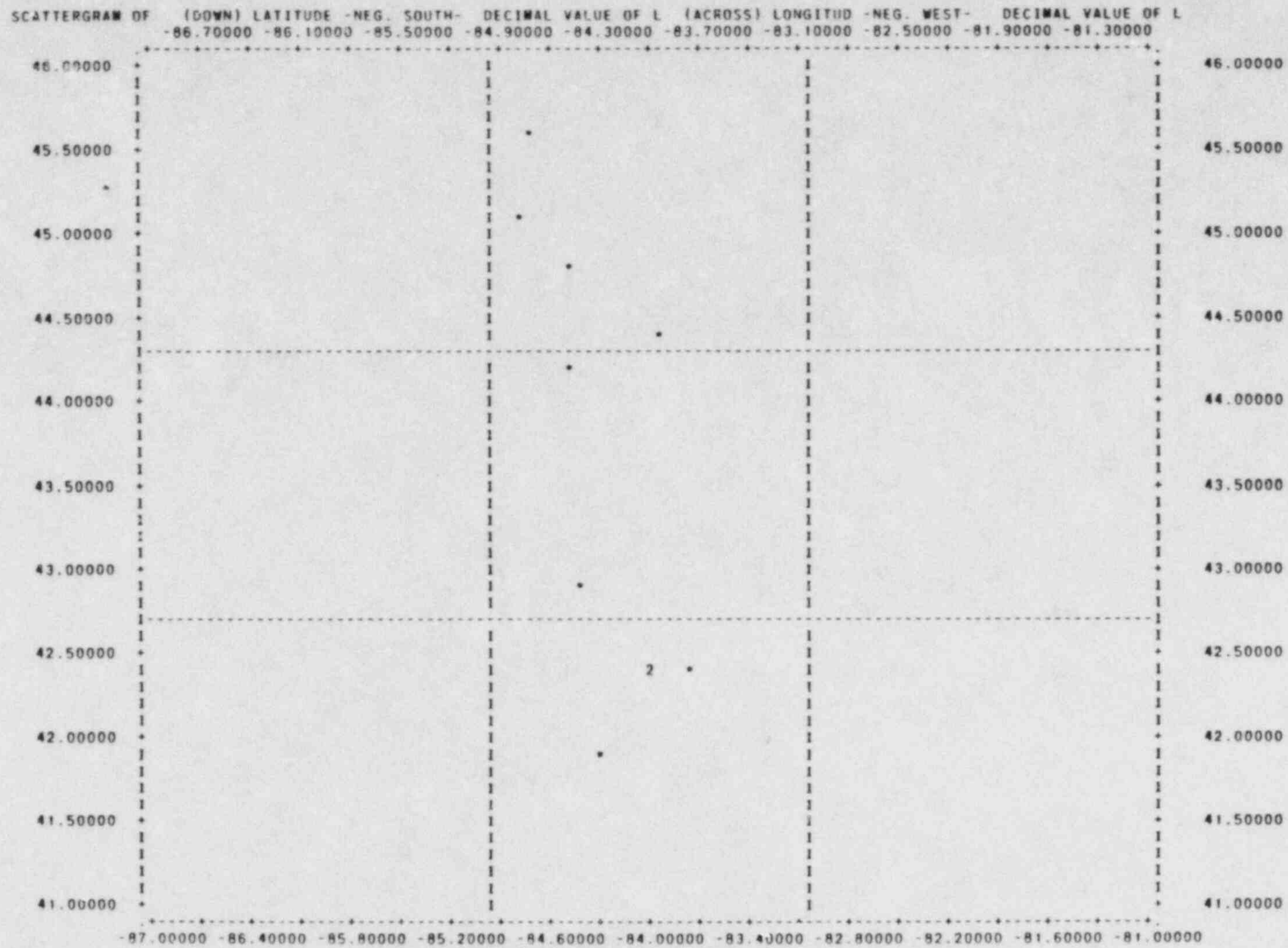
This program computes the residuals associated with the regression equation chosen in the previous step. It produces a sequence of maps of these residuals showing the spatial distribution of residuals in intervals, such as (-inf.,-2], (-2,-1], etc. It then splits the residuals into subsets and maps each of these subsets. If the residuals in these subsets are distributed somewhat evenly, then the regression equation chosen is a good one, because it exhibits little spatial autocorrelation in its residuals. Calculation of the Moran Statistic (Cliff and Ord, 1981) provides an explicit statistical test for spatial autocorrelation among the residuals. We have written a FORTRAN program that calculates the Moran statistic.

Computer Commands for Plotting the Residual Maps

COMMAND	ARGUMENT	PROGRAM & TASK: COMMENTS
RUN NAME	RESIDUAL ANALYSIS FOR MICHIGAN ...	
GET FILE	MODERN3D	
ALLOCATE	TRANSPACE=1600	
SELECT IF	(LATITUDE ... LONGITUD ... SEQNUM ... NE 454 ... AND 467 ...)	
RECODE	PICEA ... (-1,-2,-3=0)	
COMPUTE	OLDSEQ= ...	
COMPUTE	TOTAL= ...	
DO REPEAT	V1=ACER ... FRAXINUS ... POPULUS ...	
COMPUTE	V1= ...	
END REPEAT		
COMPUTE	EST=19.02248 +0.0428*QUERCUS +0.0922*FAGUS +0.0777*ULMUS -0.0656*TSUGA	This command computes the temperature estimate for each case, and the next command calculates the standardized residuals.
COMPUTE	SRES=(TMEANJUL-EST)/0.50647	

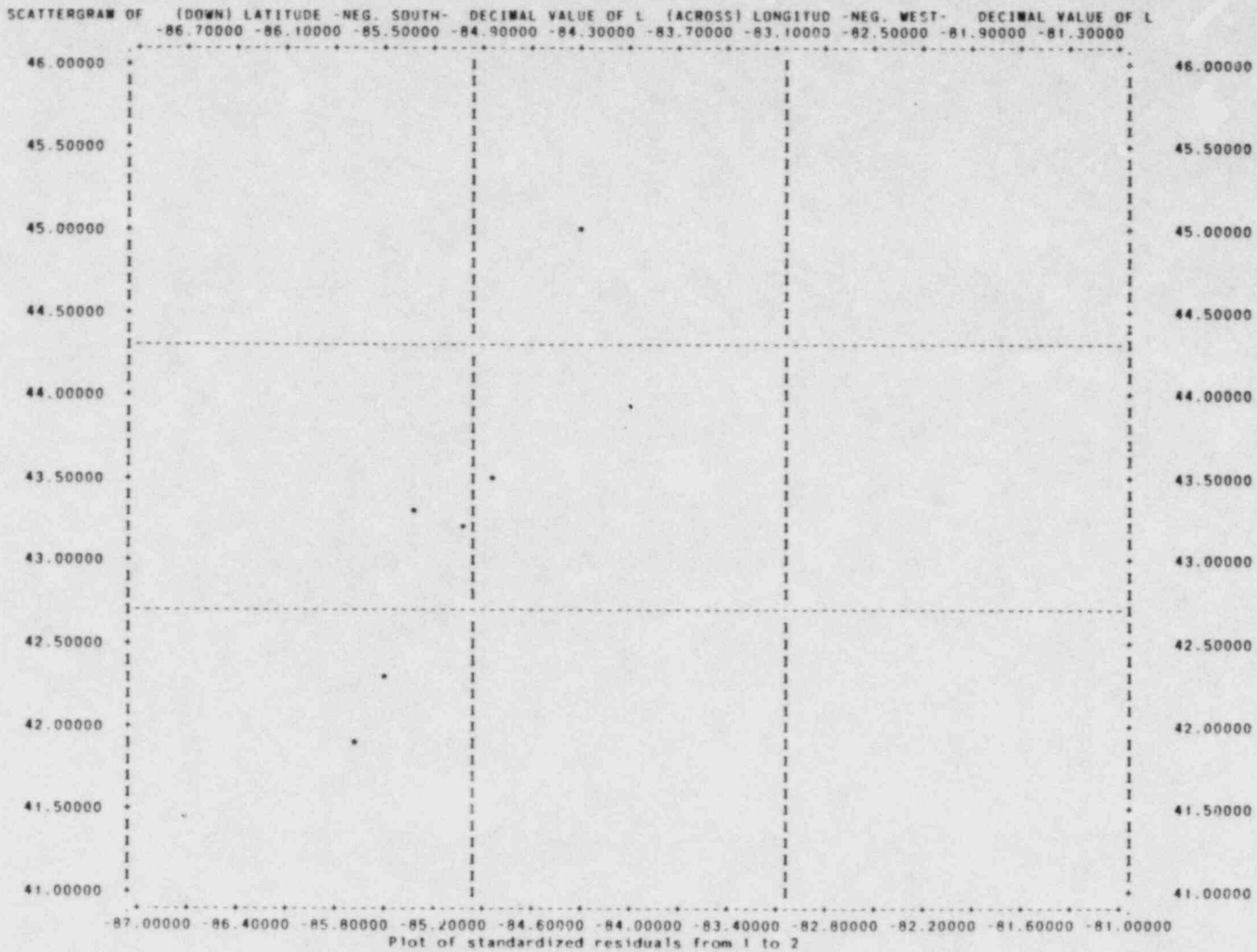
SCATTERGRAM	SRES WITH EST	The estimated mean July daily temperature is EST=..., the regression equation selected from the regression runs. SRES gives the standardized residual TMEANJUL-EST. The scatter diagram of SRES vs. EST shows how the residuals are distributed.
SCATTERGRAM	LATITUDE (41.0,46.0) WITH LONGITUD (-87.0,-81.0)	Map of the sites.
*SELECT IF	(SRES LT -2.0)	
SCATTERGRAM	LATITUDE (41.0,46.0) WITH LONGITUD (-87.0,-81.0)	Map of the sites associated with residuals less than -2.
*SELECT IF	(SRES GT -2.0 AND LT -1.0)	
SCATTERGRAM	LATITUDE ...	Map of the sites associated with residuals between -2 and -1.
*SELECT IF	(SRES GT -1.0 AND LT 0.0)	
SCATTERGRAM	LATITUDE (41.0 ...	
*SELECT IF	(SRES GT 0.0 AND LT 1.0)	
SCATTERGRAM	LATITUDE ...	
*SELECT IF	(SRES GT 1.0 AND LT 2.0)	
SCATTERGRAM	LATITUDE ...	
*SELECT IF	(SRES GT 2.0)	
SCATTERGRAM	LATITUDE ...	
FINISH		

Sample Output



Plot of standardized residuals from -2 to -1

Sample Output



SUMMARY

The above sequence of programs are those required to gain a multiple regression equation that can be used to calibrate fossil pollen data in terms of climatic estimates. An important task within these steps is the close examination of the data used in calculating the regression equation. The final regression equation is most likely to be useful 1) if the pollen types or transformed pollen types are linearly related to the dependent climatic variable, 2) if outliers are identified and deleted that may disproportionately influence the regression results, and 3) if the large residuals are carefully checked to indicate whether they cause a poor or biased performance of the regression equation (Howe and Webb, 1983). This careful checking of the modern data will help produce a robust unbiased regression equation. Further tests for finding the best regression equation are still being developed (Bartlein and Webb, 1984), and we are continuing to improve our sequence of programs to incorporate these tests (Figure 1).

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NRC FORM 335 (11-81) U.S. NUCLEAR REGULATORY COMMISSION **BIBLIOGRAPHIC DATA SHEET**	1. REPORT NUMBER *(Assigned by DDC)* NUREG/CR-3847
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16. ABSTRACT *(200 words or less)*

Radiocarbon-dated pollen records are a source of quantitative estimates for climatic variables for the past 9000 years. Multiple regression is the main method for calculation of these estimates and requires a series of steps to gain equations that meet the statistical assumptions of the analysis. This manual describes these steps which include (1) selection of the region for analysis, (2) selection of the pollen types for statistical analysis, (3) deletion of univariate outliers, (4) transformation to produce linear relationships, (5) selection of the regression equation, and (6) tests of the regression residuals. The input commands and the output from a series of SPSS (Statistical Package for Social Scientists) programs are illustrated and described, and, as an example, modern pollen and climatic data from lower Michigan are used to calculate a regression equation for July mean temperature.

17. KEY WORDS AND DOCUMENT ANALYSIS

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17b. IDENTIFIERS/OPEN-ENDED TERMS

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CLIMATIC CALIBRATION OF POLLEN DATA

JUNE 1984