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A User's Manual for the GEOPACK (Version 1 .O) Geostatistical Software System

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GEOSTATISTICS FOR WASTE MANAGEKENT:

A User's Manual For the GEOPACK (Version 1.0) Geostatistical Software System

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FOREWORD

EPA is charged by Congress to protect the Nation's land, air and water systems. Under a mandate of national environmental laws focused on air and water quality, solid waste management and control of toxic substances, pesticides, noise, and radiation, the agency strives to formulate and implement actions which lead to a compatible balance between human activities and the ability of natural systems to support and nurture life.

The Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the laboratory are responsible for management of research programs to: (a) determine the fate, transport and transformation rates of pollutants in the soil, the unsaturated zone and the saturated zones of the subsurface environment; (b) define the processes to be used in characterizing the soil and subsurface environment as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil, and indigenous organisms; (d) define and demonstrate the applicability and limitations of using natural processes, indigenous to the soil and subsurface environment, for the protection of this resource.

This user's manual serves the purpose of instructing the user in the use of GEOPACK, a comprehensive, user-friendly geostatistical software system. This guide should help the end-user, both novice and sophisticated, to become familiar with the features of GEOPACK. By using GEOPACK, and spending a little time becoming familiar with geostatistics, end-users will be able to include these geostatistical techniques in their work and research environments.

Clinton W. Hall

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SUMMARY

A comprehensive, user-friendlygeostatistical software system called GEOPACK has been developed. The purpose of this software is to make available the Programs necessary to undertake a geostatistical analysis of spatially correlated data. The programs were written so that they can be used by scientists, engineers or regulators with little experience in geostatistical techniques and still satisfy the requirements of more advanced users. Using these programs, and spending a little time becoming familiar with geostatistics the end-user should be able to include these techniques in their work and research environments.

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SECTION 1

INTRODUCTION

To use geostatistical techniques in the analysis of spatially correlated data generally requires the use of a computer to handle the large number of samples and carry out the lengthy calculations. Unless someone is known who is willing to provide the necessary computer programs, one is faced with the difficult task of finding, purchasing or developing the required computer software. Although there are a number of practicing geostatisticians who undoubtedly have access to the necessary programs, these programs are not generally available or are proprietary codes. Often, the programs which are developed for research purposes are subject to limited availability and are difficult for others to use or modify for purposes other than those for which they were originally designed.

GEOPACK has been developed in cooperation with the U.S. EPA's R.S. Kerr Environmental Research Laboratory, Ada, OK. **It was** developed with the philosophy that geostatistical software is needed that can be used as a learning tool by individuals with little or no geostatistical expertise and yet can also satisfy the needs of individuals with more advanced training in geostatistical methods. The specific objectives in creating GEOPACK were to develop: 1) geostatistical software which is easy to use so that those with little training in geostatistical methods can learn these techniques and eventually use them in their work environment: 2) an integrated system which will free the user from excessive file editing and program manipulation; 3) a system which is adaptable in the sense that additional programs can be incorporated into the system by the end user at a later date without having to alter previous programs or recompile the entire system; 4) programs which produce graphic output in a variety of forms and of publishable quality to meet the needs of research scientists and engineers and 4) software which includes on-line help facilities and extensive error checking-in the programs. The on-line help facilities offer information concerning the operation of the system, its capabilities and limitations, how to alter the system as well as programming conventions and definitions.

GEOPACK allows the incorporation of other geostatistical programs, such as GEO-EAS (reference), so the features of this and other programs can be accessed. Examples showing how these geostatistical programs can be used in the analysis of spatially correlated data can be found in Yates et al. (1986 a,b,c), Yates (1986), Yates and Warrick (1987), Yates et al. (1988) and Yates and Yates (1988, 1989). For individuals interested in learning geostatistical techniques, a number of texts are available and include: Clark (1979), Journel and Huijbregts (1978). Journel (1988) and David (1977).

GEOPACK geostatistical software system is a package of programs for conducting analyses of the spatial variability of one or more random functions. The system is menu driven, and simplified so that a minimum number of input data are needed. The programs also limit the amount of intermediate results printed to the screen or the printer.

GEOPACK uses dynamic allocation of memory so that data sets with a wide range of variables and positions can be used without having to alter the program.

A large storage array (currently set to approximately 10000 storage locations) is partitioned based on the number of samples and variables so that there is little wasted space compared to defining the arrays to have a fixed number of samples and variable. One limitation is that GEOPACK allows data base (i.e. a data file) to contain a maximum of 10 variables plus their x and y positions and a sample or position number (the sample number must be a real number). During execution of GEOPACK, whenever additional storage space (i.e. memory) is required by a program, the space is obtained from the large storage array. If attempts are made to use more memory than is available, an error message is printed out giving the memory status. From this information, a decision can be made on how to reduce the memory requirements to allowable limits (i.e. reducing the number of variables or samples considered, etc.).

The GEOPACK system includes programs to do the more common statistical and geostatistical analyses. The system is estimation oriented in that if the ordering in the menu system is followed, a grid of estimates for the selected variable in the data set will result. A description of the various components of the system follows.

Help Facilities

The program includes on-line help facilities to provide the user with information concerning the operation of the program, data requirements, conventions, definitions, run-time errors, missing files, etc. that are encountered during execution. At the menu level, the help information is of a general nature. During execution of a program, the help is more specific, such as defining a term.

User-Defined Programs

GEOPACK includes a feature which makes it simple to access any user-defined program (i.e. program not included with GEOPACK) for generating statistics, line graphics, surface graphics, text editing and data base management systems. The program names are defined in the GEOPACK System Default Settings file (see Section 2.5.c). Other miscellaneous user-defined programs can also be incorporated into GEOPACK using the USER's Menu (see Section 2.5.e).

Basic Statistics

Basic statistics such as the mean, median, variance, standard deviation, skew, kurtosis and maximum and minimum values can be determined for the selected data base (i.e. a file containing one or more random functions plus their x and y coordinates). Programs are also included for linear regression, polynomial regression, Kolomogorov-Smirnov test for distribution and calculating several percentiles of a selected data set (i.e. for a particular random function such as moisture content). GEOPACK can also directly access any commercially available statistics package while running GEOPACK which allows the user to run more comprehensive statistical analyses contained in a commercially available statistics package.

Variography

The sample semivariogram, the cross-semivariogram or a semivariogram for combined random functions [i.e., Z(x) + Y(x)] for a two-dimensional spatially-dependent random function can be determined. The approach used in determining the sample semivariogramis similar to that outlined in Journal and Huijbregts (1978).

A model can be fitted to the sample semivariogram using the nonlinear least-squares fitting procedure of Marquardt (1963). This provides a first estimate for the coefficients to be used in a cross-validation program and helps to automate the model-fitting procedure. If the least-squares technique fails, or other information is available which should be included in the model-fitting process, the traditional iterative method of manually selecting the model coefficients and viewing a graph comparing the sample values to the model can be used.

Linear Estimation

GEOPACK includes programs to calculate the ordinary kriging and cokriging estimators in two dimensions along with their associated estimation variance. Punctual and block kriging and geometric anisotropy are included. There is a cross-validation option which uses the kriging estimator in a jackknifing mode to cross-validate the spatial correlation structure. It is possible to include indicator kriging in an analysis by creating an indicator variable using a data transformation program supplied in GEOPACK.

Nonlinear Estimation

Nonlinear estimators such as the disjunctive kriging and disjunctive cokriging estimators can be determined along with the estimation variance and the conditional probability that the value is greater than a specified cutoff level. Up to 10 cutoff levels are allowed. As with the linear estimation method, this type of an analysis can be done on punctual or block support and may include anisotropy.

Graphics Outputs

Various graphics capabilities are included such as linear or logarithmic line plots, contour and block (i.e., pixel) diagrams. Device drivers for the HP@ Laser Jet@ (series II), HP plotters, and dot matrix printers (similar to Epson@ printers) are included with GEOPACK. Drivers for other printers and plotters can be written and included in GEOPACK. The graphics programs supplied with GEOPACK produce intermediate quality output and are intended for quick and easy, albeit rough, graphic illustrations. For the highest quality graphic output, GEOPACK can be interfaced with any user-defined graphics package so that custom diagrams can be developed. Using the USER's Menu, any commercially available graphics packages can be accessed while running GEOPACK. A particular data file can be plotted using a commercial graphics package by either using an internal editor (if one is included in the commercial graphics package) or by writing a simple format-translation program to create a new output file in the correct format.

SECTION 2

SOFTWARE DESCRIPTION AND OPERATION INSTRUCT&

2.1. COMPUTER REQUIREMENTS

GEOPACK has been written using a combination of Microsoft@ FORTRAN and C programming languages and runs on IBM@-compatible microcomputers such as the PC-AT, Compaq@-286, -386, Zenith@, etc. using an MS-DOS® operating system (ideally version 3.30 or greater) and 640 K memory. GEOPACK does not require a math coprocessor but will use one if it is available. A virtual disk can be used to increase operating efficiency if it is defined to be the temporary storage directory. GEOPACK also requires that the ANSI.SYS driver be installed for the screen output to perform properly. GEOPACK requires hard disk storage of about 4 Mbytes and either a CGA, EGA, VGA or Hercules@ graphics adapter and the appropriate monochrome or color monitor.

2.2. INSTALLING GEOPACK

2.2.a. Installation Instructions.

An installation program is supplied with GEOPACK to facilitate the installation of GEOPACK onto a hard disk. To completely install GEOPACK, at least 4 Mbytes of free space must be available on the hard disk. The installation program can be started by typing either

A:INSTALL <source drive> <destination drive and path>

or

A:INSTALL

If the optional <source drive> and <destination drive and path> are not specified, the program will provide prompts for this information. The source drive can be any legal floppy drive and the default value is A:. The destination drive and path indicates the hard drive and subdirectory for the "root" of the geostatistical programs. The default destination is C:\GEOPACK. It is advisable to specify a destination drive and subdirectory since a number of programs are copied to this subdirectory and could be accidentally deleted if only a drive (i.e., C:) is specified, since typically root directories are used to store a variety of programs. If any of these programs are deleted, GEOPACK may produce unpredictable results.

Before GEOPACK will operate correctly, the computer must have a specific configuration. To install GEOPACK, several modifications to the computer must be made. These are described in more detail in the following sections.

1. A temporary storage directory must be created. This is done automatically.
2. An environment variable must be set. The AUTOEXEC.BAT file must be altered.
3. A system parameter file must be created. This is done automatically.

You will need to modify this file (see Section 2.5.c) to add the names of the editor, line and contour graphics, data base management system, etc. you have available.

4. If you have a HERCULES graphics card, you must run MSHERC.COM prior to starting a GEOPACK session. This program should be put in the AUTOEXEC.BAT file.
5. The ANSI.SYS driver (see your MS-DOS manual) must be installed in the CONFIG.SYS file. This is done by adding a statement like: DEVICE-C:\DOS\ANSI.SYS to the CONFIG.SYS file. Be sure that the correct path for ANSI.SYS is used.

2.2.b. Temporary Storage Directory.

GEOPACK uses a temporary storage directory to hold information such as the data set, intermediate results, output files, etc. The installation procedure automatically creates a temporary directory called TMP to be used to store intermediate results. In general, the temporary storage directory is transparent to the user.

2.2.c. Setting or Changing the GEOPACK Directory Specification.

GEOPACK will operate properly only if the environment variable %GEODIR% (the "%" are used to indicate an environment variable) is set to the root of the geostatistical programs. To set this variable the following line should be added to the AUTOEXEC.BAT file

SET GEODIR=C:\GEOPACK

where C:\GEOPACK is the primary subdirectory for the geostatistical programs. In the user-defined menus (described in Section 2.5.d) whenever GEOPACK sees "%GEODIR%" it will substitute "C:\GEOPACK" so that a command: %GEODIR%\SHOWDIR would be the same as C:\GEOPACK\SHOWDIR. Note, the above command can also be typed at the MS-DOS prompt prior to starting GEOPACK. After typing the SET command given above, if the DOS reply: "Out Of Environment Space" appears, the user should consult the DOS manual about SHELL commands.

2.2.e. GEOPACK System Default Settings.

The installation program creates a file that contains the system default settings. This file may require modification before all of the options on the USER and other menus become active. Before making any modifications, see Section 2.5.c.

2.3. SYSTEM OVERVIEW

2.3.a. Program Structure.

The initial program structure of GEOPACK is shown graphically as

```
GEOPACK ───────────┬ DKRG
                   ├ KRIG
                   ├ STAT
                   ├ TMP
                   ├ USER ──────────┬ DATA
                   │                ├ DSTAT
                   │                ├ GEOEAS
                   │                └ UPROG
                   └ VARI
```

where, in the above example, the subdirectory GEOPACK is called the "root" of geostatistical programs. The location of the "root" directory is specified during installation and can be located on any fixed-disk drive and can be anywhere along a subdirectory "tree". It is recommended that the root be the first level subdirectory on a given drive.

The subdirectories: DKRG, KRIG, STAT, USER and VARI, respectively, are used to store the programs for: disjunctive kriging and cokriging (DRKG), ordinary kriging and cokriging (KRIG), basic statistics (STAT), user-defined programs (USER) and variography (VARI). The menu entries for each set of analyses (except for the USER menu) cannot be modified by the end-user. The TMP subdirectory is created to be used as the temporary storage directory during installation.

The subdirectories of the USER directory: DATA, DSTAT, GEOEAS and UPROG are examples of how GEOPACK can be altered to include additional programs. The menu entries for the USER directory and its subdirectories can be modified by the end-user to tailor GEOPACK for an individual's needs. The instructions required to modify the "PACK USER menu are given in Section 2.5.k.

2.3.b. The Function Keys and Cursor Movement.

The function keys: F1, F3, F4, and F5 can be used at any menu in the following manner:

- F1 - Help (At menu and program levels. In programs other F-keys also display help information and are indicated when they are active)
- F3 - Utility Menu
- F4 - View previous screen
- F5 - User Menu (User-defined programs, menus etc. Makes GEOPACK adaptable)

A complete description of the entries on each of the menus that are accessed by the Function keys is given in Section 2.5, The Menu System.,

The cursor (i.e., the light bar or highlighted selection) can be moved by using the following cursor control keys:

Home, End, PgUp, PgDn, Arrow Keys

If these keys are located on the keypad, the NUM-LOCK key must be turned off. A menu entry can also be selected by pressing the letter (or number) that is highlighted in the desired entry.

2.3.c. File-Naming Convention.

Whenever a data set is selected (this data set can be located in any subdirectory on any disk) a file is created in the temporary storage directory and is called "DEFAULT". This file contains two lines, the first gives the selected file name and the second the origination path of the file. A copy of the selected file is written to the temporary storage drive as well. These two files (DEFAULT and the data set) are required before GEOPACK will run properly. All the programs in GEOPACK read the DEFAULT file to obtain the name of the data set. The first part of the data set name (i.e., "TEST" for a data set named "TEST.DAT") is used for many of the intermediate file names. For a data set named "TEST.DAT" which is assumed to contain three variables moist (variable #l), temp (variable #2) and sand (variable #3), the typical file names that reside in the temporary storage directory and a brief description of their purpose follows.

STACKER.		Used by the menu program.
MENUTEMP.BAT	-	Used by the menu program.
DEFAULT.		Contains the name of the data set and path of origination.
TEST.DAT	-	Data set.
TEST.STS		Basic descriptive statistics for all data variables in the data set.
RPLOT.TMP	-	Temporary file containing the data for the last regression or least-squares graph.
GRAPH.DEF		A command file for the graphics program. Contains the commands used to generate the last graph (regression, least-squares, contour plot, etc.).
TEST.V		The default settings file for the semivariogram program. This file is generated when the Default Settings program (on the variogram menu) is executed.

VPLOT.DEF - Temporary file containing the data for the last semivariogram or cross-semivariogram graphed.

VAR11.00 - Contains the sample semivariogram values for variable 1 (i.e., MOIST). First saved file.

VAR11.01 - Contains the sample semivariogram values for variable 1 (i.e., MOIST). Second saved file.

VAR12.00 - Contains the sample cross-semivariogram values for variable 1 with variable 2 (i.e., MOIST vs. TEMP). First saved file.

MVAR11.00 Contains the model coefficients for the sample semivariogram values contained in VAR11.00.

MVAR11.01 Contains the model coefficients for the sample semivariogram values contained in VAR11.01.

MVAR12.00 Contains the model coefficients for the sample cross-semivariogram contained in VAR12.00.

TEST.VAR - Contains the semivariogram and cross-variogram coefficients for use by the kriging and disjunctive kriging programs.

TEST.K - The default settings file for the kriging program. This file is generated-when the Default Settings program (on the kriging menu) is executed.

KPLOT.TMP - Contains the position, the estimate and the estimation variance from the kriging program.

KPLOTl.TMP - Temporary file containing the graphic data for the last kriging contour graph produced.

TEST.D The default settings file for the disjunctive kriging program. This file is generated **when** the Default Settings program (on the disjunctive kriging menu) is executed.

TEST.DCi Contains the input data required by the disjunctive kriging program for variable "i", where "i" is the variable number. This file is created by executing the Hermite Coefficients program on the disjunctive kriging menu.

DPLOT.TMP - Contains the position, the estimate, estimation variance and conditional probabilities (if any) from the disjunctive kriging program.

DPLOTl.TMP - Temporary file containing a contour representation of one of the output data types contained in DPLOT.TMP (i.e., it has the last disjunctive kriging graph produced).

2.4. DATA FILE

2.4-a. Format Instructions.

To operate GEOPACK, a data file must be created in the proper format. Using a text editor or word processor, a data file can be entered or modified for use with GEOPACK. For GEOPACK to function properly, the data set must contain at the minimum: 1) one (or more) spatially-dependent random variable(s) (**i.e.**. soil temperature, moisture, hydraulic conductivity, concentration, etc.) and 2) an x and y position for each value of the random variable(s). A data file **must be** created in ASCII format using the following standard FORTRAN formatting instructions:

RECORDS L-3:		FORMAT(A76/A76/A76)
	TITLE(3)	Three lines of title.
RECORD 4:	.	FORMAT(2I5,F10.3)
	IVAR	The total number of random variables in the data set. These are values of the parameters that will be used in obtaining estimates, etc.
	NDAT	The total number of positions (i.e., X and Y coordinate pairs) in the file.
	CUTOFF	The value given to this variable is the maximum allowed value for the data. Using the CUTOFF, missing data can be excluded from any analysis. To accomplish this, set any missing data in the data file to a large number (e.g. 99999.99). This number must be larger than the numeric value of any variable. To exclude these large numbers, set the CUTOFF value to a number slightly SMALLER than the missing data number (e.g., 99999.00). Then the missing data will not be used by any program.

RECORD 5: FORMAT(13I5)

IINX	The column in the data file that contains the sample number. If no sample is available, the program can be made to read a blank field as zeros. In general, this will not cause any problem in running the programs.
IX	The column in the data file. that contains the X coordinate data. See examples given below for more information.
IY	The column in the data file that contains the Y coordinate data. See examples given below for more information.
IV(1)	The column in the data file that contains one of the random variables. The selection of the first, second, etc. random variable is arbitrary. The easiest way to specify these is to sequentially number the random variables in the order (from left to right) that they appear in the data file. The program uses the order you specify here, as the order the variables will be listed out on the screen. If you want to change the order, then give IV(l) as the 1st variable, IV(2) as the second variable, and so on.
IV(IVAR)	The column in the data file that contains IVAR-th random variable.

RECORD 6: FORMAT(10(4x,A6))

NAM(I)	The variable name for the I-th variable. NOTE: the I-th variable is the variable associated with IV(I) listed above. See examples given below for more information.

RECORD 7: FORMAT(A30)

FMT — Format specification for the data file. This should be of appropriate form to read the data in the file.

e.g.. (F5.0,2F10.3,5X,lE10.2)

RECORD 8-end (see RECORD 7)

DATA VALUES — The data set should have a sample number (or index), X coordinates, Y coordinates and the property(s) to be kriged. Data is read until an end-of-file marker is found. Therefore, there should not be any blank lines in this part of the data file.

Note: The sample no. is assumed to be real.

2.4.b. Examples Of Data Sets.

This is a typical data file. There are 4 random variables: MOIST, TEMP. SAND and OIL-%. There are 119 positions where data was collected (only 4 positions are shown).

```
   4  119
   12       3    5    4    6    7
    MOIST     TEMP      SAND     OIL-%
(G5.0,12F10.3)
    1    6.0000     7.0000   46.8500  999.9990   56.5102    6.5362
    2    6.0000    10.0000   46.2900    5.9250   55.6444    5.2454
          .
                                                              .
  118   24:0000    21:oooo   46.3500  999.9990   54.4012    4.0463
  119   22.0000    24.0000   47.1400  999.9990   52.5845    2.5345
```

Notes:

1) In the above example, the TEMP, MOIST, SAND and OIL are in columns 4,5,6 and 7, respectively. However, if you note line 5 and 6 you'll see that MOIST is specified as variable #l, followed by TEMP, SAND and OIL. This changes the order for the IV(i) and NAM(i) data.

2) Since all the random variables were not sampled at every location, some method for delineating missing data is needed. In the above example, missing data is specified by entering a large number (i.e., 999.9990). When executing a program in GEOPACK, it will ask you the CUTOFF value (for delineating missing data) and you should give a value slightly smaller than 999.9990 but larger than any valid data value, for example, 999. or 900.

```
  This example data file is the same as the one above except there are
  no sample numbers.  To alleviate this problem the first column of the
  data file is specified as the sample number (i.e., they are all 0).
   4  119
   1    2     3    5     4    6     7
    MOIST      TEMP       SAND      oil-%
(Gl.O,F9.3,12F10.3)
    6.0000     7.0000   46.8500  999.9990   56.5102    6.5362
    6.0000    10.0000   46.2900    5.9250   55.6444    5.2454



   22:oooo    24:0000   47.1400  999.9990   52.5845    2.5345
```

2.5. THE MENU SYSTEM

During installation, you are asked for the name you want to use to start the geostatistical programs, where the default *name is* GEOPACK. After starting the program using the selected name, the first menu displayed is the MAIN menu.

2.5.a. Description of the MAIN Menu.

```
Thu Jun 29, 1989 07:47:45 am
Return to MS-DOS, with prompt to save settings and files

GEOSTATISTICAL PROGRAMS: Main Menu

Quit GEOPACK
Data Set Utilities Menu
Statistics Menu
Variogram Menu
Ordinary [Co]Kriging Menu
Disjunctive [Co]Kriging Menu
```

Esc: quit	F1: help	F3: util	F4: view	F5: user menu	↕	Home	End

From the main menu you can select one of several other menus using the cursor keys to move the light bar (or highlighted region) over the desired selection or by typing the highlighted character of the desired selection. The function keys will display menus intended to offer help, utilities and user-defined applications. Selecting an item from the MAIN menu will produce another menu containing programs or other options which are available for undertaking the statistical and geostatistical analyses. A description of the available menus follows.

When leaving GEOPACK (i.e., typing Q at the main menu) another menu is produced which allows you to return to GEOPACK, return to MS-DOS leaving the intermediate data in the temporary storage subdirectory, return to MS-DOS saving the intermediate results to a packed file (see Section 2.5.f) or return to MS-DOS and delete the intermediate results from the temporary subdirectory (see Section 2.5.f).

2.5.b. Description of the HELP Menu (Fl).

```
Thu Jun 29, 1989 07:47:45 am  1
Return to Main Menu

GEOSTATISTICAL PROGRAMS: Main Menu      GEOPACK USER'S MANUAL

Quit GEOPACK                            Return To Main Menu
Data Set Utilities Menu                 Overview Of System
Statistics Menu                         Installation Instructions
Variogram Menu                          File Formatting Instructions
Ordinary [Co]Kriging Menu               Basic System Operation
Disjunctive [Co]Kriging Menu            Menu Help
                                        Utilities in GEOPACK
                                        Adding User Programs and Menus

Esc: quit | Fl: help | F3: util | F4: view | F5: user menu | ↕ | Home | End
```

If the Fl key is pressed from any menu, the HELP Menu is activated. On the HELP Menu there are several help files you can access. In general, the information in the User's Manual and some theory of geostatistics can be found on the HELP menu.

2.5.c. Description of the UTILITY Menu (F3).

```
═══════════════════ Thu Jun 29, 1989 07:47:45 am ═══════════════════
Return to Main Menu

GEOSTATISTICAL PROGRAMS: Main Menu

Quit GEOPACK
Data Set Utilities Menu
Statistics Menu
Variogram Menu
Ordinary [Co]Kriging Menu
Disjunctive [Co]Kriging Menu

                                Utilities Menu

                                Return To Main Menu
                                Change System Default Settings
                                DOS Shell
                                Execute an MS-DOS Command
                                Graph Most Recent Graphic
                                Program Structure

Esc: quit | F1: help | F3: util | F4: view | F5: user menu | ↕ | Home | End
```

If the F3 key is pressed from any menu, the UTILITY Menu is activated. On the UTILITY Menu there are several programs available to alter basic GEOPACK parameters, run MS-DOS commands while inside GEOPACK and view the current GEOPACK program structure. Each utility is described in more detail below.

Change System Default Settings:

This Utility allows you to change the default settings which are used by GEOPACK. The default settings include the path specifications, device names, screen type, default colors and names of default (i.e., user defined) programs. Two files are used: SYSETUP and SYSDEFLT for changing and storing the system default information. SYSETUP is the basic file which MUST be present in the GEOPACK root directory. This file contains the information which is written to the screen by this Utility program, an example is:

System Default Settings File	
RAM-Disk or Temporary Directory	C:\GEOPACK\TMP
Data Storage Directory	C:\GEOPACK\USER\DATA
Text Color Number (O-15)	11
Border Color Number (O-15)	6
Screen Mode (O-Black & White, l-Color)	1
Statistics Program	MICROSTAT
Word Processor or Text Editor	EDT
Line-Type Graphics Program	GRAPHER
Contouring Graphics Program	SURFER
Data Base Management Program	MFOXPLUS

Esc: quit	Fl: help	F2: save	← ↕ →	Home	End	Page Up	Page Down

Since paths are not given for any of the Default programs, it is required that these programs reside in sub-directories on the current MS-DOS PATH (so that they can be found from any sub-directory by using the program name only). It is also possible to specify the entire MS-DOS path and program name. PLEASE NOTE: the programs MICROSTAT, EDT, GRAPHER, SURFER and MFOXPLUS are commercially available programs and are **not included** with the GEOPACK system. The Utility program writes out a file (called SYSDEFLT which is used by the GEOPACK programs. An example of this file is:

```
C:\GEOPACK\TMP
C:\GEOPACK\USER\DATA
           11
            6
            1
    MICROSTAT
          EDT
      GRAPHER
       SURFER
     MFOXPLUS
```

Columns: 1 10 20

This file is used by GEOPACK during operation of the programs. At any time if there is a change in the definition of any item in SYSDEFLT a change needs to be made to this file. The easiest way to do so is to use the Change System Default Settings option on the Utilities Menu (i.e., F3 key).

To manually run the Default Settings program type: DEFLT sysetup sysdeflt from the root directory of GEOPACK. This may be necessary if the sysdeflt file is ever accidentally deleted or modified.

DOS Shell:

This Utility allows you to temporarily exit the GEOPACK system and return to the MS-DOS command-line mode. When you exit to a DOS shell, the text color on the screen will be red. This is to remind you that you are in a DOS shell. Once you are finished running MS-DOS commands you can return to GEOPACK by typing EXIT, which exits you from the DOS Shell.

Please Note: While in a DOS shell, some of the available computer memory is still allocated to GEOPACK and if you try to run a program that requires a lot of memory you may see the message "not enough memory'!. If you must run this program, you should exit the DOS shell (i.e., return to GEOPACK) then exit GEOPACK. This will free up all the available computer memory. Also, it is possible to exit to a DOS shell and restart GEOPACK (this can be done several times). If this is done, the computer may stop operating since there is insufficient memory to contain both the current and pre-installed versions of GEOPACK.

Execute an MS-DOS Command:

This Utility is similar to DOS Shell except that it allows you to run ONE MS-DOS command. Once you have run the MS -DOS command you are returned to the Utility Menu. If you need to run several MS-DOS commands, it is more efficient to exit to a DOS shell.

Please Note: There is slightly LESS available computer memory when Executing an MS-DOS command compared to exiting to a DOS shell.

Graph Most Recent Graphic:

This convenience feature allows you to replot the last graph displayed (or that should have been displayed) on the screen. This feature is useful for computers with insufficient memory to display graphs while in an application program (i.e. the computer doesn't have enough extra memory to run the graphics program). Use this options if you don't see a graph and receive the error message: OUT OF MEMORY.

Program Structure:

This Utility gives a pictorial representation of the current GEOPACK structure (for an example see Section 2.3.a). Changes in the structure of GEOPACK will be reflected in the diagram produced by this program. The USER menu, described in Section 2.5.d, can be modified to include any program, or add another menu. In the above example, the USER menu is used to access four other menus, DATA, DSTAT, GEOEAS and PROG. These menus are for, respectively, available data sets, default statistics program, GEO-EAS geostatistical software and user-defined programs. Additional menus and programs can be added by following the instructions on modifying the USER MENU given in Section 2.5.j.

2.5.d. Description of the View Feature. (F4)

If for some reason you are located at one of the menus and you need to see the last screen of output from a program that has just been completed, you can toggle between the menu screen and the program screen by typing F4 provided your monitor and graphics card allows multiple screens.

2.5.e. Description of the USER Menu. (F5)

```
Thu Jun 29, 1989 07:47:45 am   1
Return to Main Menu

GEOSTATISTICAL PROGRAMS: Main Menu

Quit GEOPACK
Data Set Utilities Menu
Statistics Menu
Variogram Menu
Ordinary [Co]Kriging Menu
Disjunctive [Co]Kriging Menu

                                  User Menu

                          Return To Main Menu
                          EPA GEO-EAS
                          Graphics Menu
                          Statistics Package    (Default)
                          Data Base Management (Default)
                          User Programs

Esc: quit | Fl: help | F3: util | F4: view | F5: user menu | ↕ | Home | End
```

If the F5 key is pressed from any menu, the USER's Menu is activated. The USER's Menu allows GEOPACK to be modified to include other programs and menus which are defined by the user. The instructions which tell GEOPACK which program to run or menu to display are in a file called: USER.MEN, which is located in the root directory of the geostatistical programs (i.e., if the default directory was chosen, it would be C:\GEOPACK). The necessary information for modifying the GEOPACK program is given under the heading "Adding User Defined Programs and Menus" on the User's Manual Help screen (i.e., type Fl).

A brief description of the menu options which are provided with the original GEOPACK system follows.

Statistics Package (Default):

This feature allows you to run a default statistics package during a GEOPACK session. The default statistics package is defined (i.e., the path and name specified by using the system default setting program). To start this program type F3 and select "Change System Default Settings". In the present example, it is assumed that the GEOPACK data set will have to be modified to a format that the default statistics package can read. Therefore, selecting this option will produce another menu which will let you create a file in the proper format (Note: this program may have to be changed for other statistics programs) and run the statistic program. The default statistics menu is located in the subdirectory: %GEODIR%\USER\DSTAT under the file name: DSTAT.MEN.

Graphics Menu:

This feature allows you to run one of several graphics programs during a GEOPACK session. When this option is selected another menu is produced which has three options. The first is to execute the GEOPACK graphics program and the other two are the default line and contour graphics programs.

Data Base Management System (Default):

This feature allows you to run a default data base management system during a GEOPACK session.

GEO-EAS:

This feature allows you to run,GEO-EAS during a GEOPACK session.

Available Data Sets:

This option allows you to select a data set from a subdirectory used solely for storing data sets. The subdirectory specification is %GEODIR%\USER\DATA and the program SDATA.EXE is used for displaying and selecting the data sets located in the directory (for additional information see Select a Data Set in Section 2.5.f).

2.5.f. Description of the Data Set Utilities Menu.

```
Thu Jun 29, 1989 07:47:45 am
Return To Main Menu

GEOSTATISTICAL PROGRAMS: Main Menu

    Data Set Utilities Menu

Q- Return To Main Menu
Select a Data Set
Modify an Existing Data Set
Pack Temporary Directory into File
Unpack Temporary Directory from File
Extract a File From a Packed File
List Temporary Directory and View File
Edit a Data Set
Delete All Files in Temporary Directory
```

Esc: quit	Fl: help F3: util	F4: view	F5: user menu	↕	Home	End

If the highlighted key "U" is typed or the light bar placed over the menu option "Data Set Utilities Menu" on the MAIN Menu and the enter key pressed, the Data Set Utilities Menu is activated. On this menu there are several utilities which can be used to select, edit or modify an existing data set, to pack the contents of the temporary directory **into an** ARCHIVE file for later use or to extract all or part of the files from the archive.

Select a Data Set:

This program allows the selection of an existing data set. The data set must be properly formatted for use with GEOPACK. To create a new file, see the editing program described below.

Select a Data File

C:\GEOPACK\USER\DATA\..

..\
C912.DAT
ECSAR.DAT
TEST.DAT
VIRUS.DAT

Esc: exit	Fl: help	F2: list	← ↕ →	Pg UP	Pg Down	Home	End

A data set can be selected by either 1) typing in the file name or 2) by moving the light bar over the desired data set and typing the ENTER key. Other subdirectories can be accessed in a similar manner to data files. Please note that the symbol ..\ above indicates the subdirectory C:\GEOPACK\USER and if a directory entry is preceeded by a "\", then the entry is a directory specification.

This program copies the requested data from its current path to the temporary directory, creates a file called DEFAULT which contains the program name and its origination path. GEOPACK uses the DEFAULT file to determine the proper name of the data file. Both files (i.e, the data file and DEFAULT) must exist on the temporary directory before GEOPACK will work properly.

GEOPACK requires that a cutoff value be supplied during execution of the programs. The cutoff value is used to indicate missing data. The cutoff value is a specified value that is larger than any of the "true" data in the data set.

For example, if you have a variable that is missing a value at a point in space, in the data set you place a value which is larger than any of the "true" data and larger than the cutoff value which you must specify. During execution of a program you will give a value (called the cutoff value) which is used by the program to determine which values to ignore. Any value in the data set that is greater than the cutoff value will be ignored by the program. It is imperative that the cutoff value you specify is appropriate for given data set; if not, the resulting calculations will be inaccurate.

For example: given the following data:

index	x 10.0	y 11.2	variable 1	variable 2	variable 3
3			12.55	45.66	1002.321
15	14.9	1.9	11.83	48.19	1032.209
5	18.7	7.7	12.91	36.98	1200.500
7	5.2	14.5	9.50	9999.99	1002.321
45	46.4	16.4	16.82	45.66	1002.321

the value used to indicate missing data is 9999.99. Note that this value is greater than any value of ALL the variables. An appropriate cutoff value to input into GEOPACK would be greater than 2000, since 1200.5 is the largest "true" data value.

Modify an Existing Data Set:

This program allows the creation of new variables in an existing data set. The data set **must** reside on the temporary directory prior to starting this program and be properly formatted for use with GEOPACK. The newly created variables can be added to the file. For example, assume the data set has one variable called the moisture content. If a new variable log(moisture content) is to be created it can be added to the file.

Pack Temporary Directory into File:

This program allows the archiving of the files residing in the temporary directory. This is used if you want to store the intermediate results from GEOPACK for use at a later time. Each file is "PACKED" into a new file in the selected directory under a name you provide. If a file with the same name exists, you will be asked if you want to overwrite it. The screen is similar to the screen shown in the section "Select A Data Set" described above.

Unpack Temporary Directory from File:

This program allows you to retrieve the files that were previously packed using the program described above. If you want to retrieve only a few of the files then use the program described below under EXTRACT A FILE. The screen is similar to the screen shown in the section "Select A Data Set" described above.

Extract a File From a Packed File:

This program allows you to retrieve one or more of the files that were previously packed using the PACK program described above. Please note that you must retrieve the DEFAULT file if you plan to use GEOPACK. If you fail to do so the program will print an error message alerting you to this error (the program does not explicitly state that the DEFAULT file is missing, however). The screen is similar to the screen shown in the section "Select A Data Set" described above.

List Temporary Directory and View File:

This program allows you to list all the files that currently reside in the temporary directory. To "VIEW" a file place the light bar on the desired file and type return. Also, by typing the F2 key, additional information about the file is available. The screen is similar to the screen shown in the section "Select A Data Set" described above.

Edit a Data Set:

This program allows you to edit a file. Any file can be edited whether it exists or not. Once this program is started, you will see the directory listing of the XGEODIRX directory (i.e., the root of the geostatistical programs) and you can select a file from this directory, supply an alternate file (and path) or give a new directory name to see the listing of the new directory.

Remove All Files in Temporary Directory:

This command allows you to remove all the files in the temporary directory. PLEASE NOTE: THE TEMPORARY DIRECTORY SHOULD BE USED ONLY FOR THE GEOSTATISTICAL PROGRAMS SINCE THIS COMMAND WILL REMOVE ALL PROGRAMS IN THIS DIRECTORY (or subdirectory).

Before you can select a second data set to work on, the temporary directory must be cleared of a previous data set. If you want to save the intermediate or final results from this previous data set, use the PACK data set program described above.

2.5.g. Description of the Statistics Menu.

```
═══════════════════ Thu Jun 29, 1989 07:47:45 am ═══════════════════
 Return To Main Menu

 GEOSTATISTICAL PROGRAMS: Main Menu

              Statistics Menu

  Return To Main Menu
  Sample Statistics
  Regression Analysis
  Kolomogorov Test of Distribution
  Least Squares Polynomial
  Percentiles of Data


  Variogram Menu
  Ordinary [Co]Kriging Menu
  Disjunctive [Co]Kriging Menu
```

Esc: quit	Fl: help	F3: util	F4: view	F5: user menu	↕	Home	End

If the highlighted key "S" is typed or the light bar placed over the menu option "Statistics Menu" on the MAIN Menu and the enter key pressed, the Statistics Menu is activated. On the Statistics Menu there are several programs from which you can choose. These programs are intended to do the most basic statistical analyses and are not intended to replace comprehensive statistical packages which are available commercially. Since it is anticipated that there will be a need for accessing a more complete statistical package, GEOPACK has built in capabilities to call (i.e., run) a user-defined statistical program from the USER's MENU (access to the USER's MENU is obtained by typing F5). Since the data format requirements of GEOPACK may be different from the commercial statistics package, an interface may be necessary to rewrite the data file in the appropriate format. When this is necessary, it is advisable to have the Default Statistic Package option on the USER menu call up another menu which has the interface and start commands on it. An example is provided in the file %GEODIR%\USER.MEN.

Sample Statistics:

This program calculates the descriptive statistics for the data set. These statistics include: the number of samples used, the mean, median, variance, standard deviation, skew, kurtosis, maximum and minimum values of the data set.

Regression Analysis:

This program calculates the linear regression coefficients, A and B, for the linear model

$$\text{variable}(i) = A + B \times \text{variable}(j) \qquad j \neq i$$

A plot of the data and regression line is provided as well as the coefficient of determination, and a comparison between the estimates and data values.

Rolomogorov Test of Distribution:

This program calculates the Kolomogorov-Smirnov test statistic for a normal distribution. Other distributions can be tested for by transforming the variable of interest using the Modify a Data Set command on the DATA SET UTILITIES MENU.

Least Squares Polynomial:

This program calculates the nonlinear regression coefficients C(i) for the polynomial model

$$\text{variable}(i) = c(1) + C(2) \times \text{variable}(j) + C(3) \times \text{variable}(j)^2 + \ldots$$

A plot of the data and regression line is provided as well as a comparison between the estimates and data values.

Percentiles of Data:

This program sorts the data set and gives several pre-defined percentiles of the data.

2.5.h. Description of the Variogram Menu.

Thu Jun 29, 1989 07:47:45 am

Return To Main Menu

GEOSTATISTICAL PROGRAMS: Main Menu

Variogram Menu

Return To Main Menu
Set Program Parameters
Variogram Calculation (Sample)
Automatic Model Fit
Manual Model Fit, Select Model(s)
Edit Variogram Model File

Statistics Menu
Ordinary [Co]Kriging Menu
Disjunctive [Co]Kriging Menu

Esc: quit	Fl: help	F3: util	F4: view	F5: user menu	↕	Home	End

If the highlighted key "V" is typed or the light bar placed over the menu option "Variogram Menu" on the MAIN Menu and the enter key pressed, the Variogram Menu is activated. The programs on the Variogram Menu are intended to do the variogram analyses and should include the programming needed in the majority of cases. Using the F5 key and interfacing to GEO-EAS allows you to use the variogram program included in GEO-EAS. In some cases the GEO-EAS program may include some feature not found in GEOPACK so it is advisable to check GEO-EAS if you want a feature not currently supported in GEOPACK. Since the data format requirements of GEOPACK are different from GEO-EAS, an interface is necessary and has been written into the GEOPACK system. You must remember the names you give to various files while running GEO-EAS since it doesn't have a specified naming convention. When GEOPACK writes a file which is in GEO-EAS format it always has the extension EPA (i.e., <name>.EPA).

GEOPACK will save up to 15 sample semivariograms using the following naming convention:

<RAM drive>\VARij.OO	first saved sample semivariogram for variable i with j (i,j=l,..,IVAR) if variable 1 is MOIST, 2 is TEMP and 3 is SAND, then if i-l and j-2 VARij.00 is the first cross-variogram between MOIST and TEMP saved by GEOPACK.

```
<RAM drive>\VARij.01      second saved sample semivariogram
<RAM drive>\VARij.02      third saved sample semivariogram
                .  .03
                .  .
                .  .
                .  .
<RAM drive>\VARij.14      fifteenth saved sample semivariogram
```

Set Program Parameters:

GEOPACK provides you with a program for setting the variogram parameters to facilitate using GEOPACK in an efficient manner. This program allows you to specify a value for any of the parameters used to calculate the sample semi-variogram or cross-semivariogram. You can specify any or all of these parameters and once they are specified, the program will not ask for interactive input during execution. For example, if you want to run the program five times and are planning to change only one parameter each time, you would give a "?" in the parameter field for that parameter. During execution you will be asked to provide only that value. In this manner, you will only have to answer the necessary questions during execution.

Spatial Correlation Function Parameter Settings File

Data File Name:		(FNAME)	TEST.DAT
Enable Graphics Options (i.e., -G)	(Y/N)		Y
Save All Sample Variogram Functions	(Y/N)		Y
Data Cutoff Value:		(CUTOFF)	100.0
Number of Lagged Distances		(NLAG)	12
Distance Between Lagged Distances:		(BLAG)	?
Width of Lagged Interval:		(WLAG)	0.0
Width of Angle Class:		(DALF)	90.0
Number of Directions:		(NDIR)	1
Angle for Direction Number-1			0.0
Angle for Direction Number-2			30.0
Angle for Direction Number-3			60.0
Angle for Direction Number-4			90.0

↑up	↓down	Home	PgUp	PgDn	End	F2=Save	Esc-Exit

Variogram Calculation (Sample):

This program calculates the sample semivariogram or cross-semivariogram for a spatially-dependent, two-dimensional random function.

There are two ways that the results from the sample semivariogram program can be saved. The easiest method is to specify in the Parameter Settings file to save all sample semivariograms (i.e., Place a "Y" in the appropriate field). When this is done, every time the sample semivariogram program is run, the results will be stored on the temporary subdirectory. Since 15 files may be saved at any time, you will most likely never run the program more than 15 times so saving every file will not produce a problem. If you should create 15 files and wish to save additional sample semivariograms, you can delete files that you do not expect to use.

An alternative method for saving the output from the semivariogram program is to save the output from only those runs tha-t produce "reasonable" results. This can be done by selecting OPTION KEY: "S" at the end of the Sample Variogram Calculation program. The OPTION KEYS appear at the lower right hand corner.of the screen during execution of a program. The "S" option only appears at (or near) the end of the program and generally after a graphic plot of the sample semivariogram has been produced.

Fit Model Automatically To Sample Variogram:

This program allows you to fit a mathematical model (e.g., a gaussian, exponential, linear, spherical or power model) to a sample semivariogram. The fitting method uses the nonlinear least squares minimization technique of Marquardt (1963).

Sample Autocorrelation Functions Saved

MOIST / MOIST : 00 01 02 03 04
MOIST / TEMP : 00 01
MOIST / SAND :
TEMP /TEMP : 00
TFMP /SAND :
SAND /SAND :

Fl: view	Enter: select	D: delete	←↕→	Home	End	Pg UP	Pg Dn

To specify a sample semivariogram (first step in running this program), a screen is produced which shows all the saved variograms for each random function and all the cross-variograms for each pair of random functions. This screen displays the random function name, such as:

MOIST / MOIST	for a direct semivariogram for MOIST
MOIST / TEMP	for a cross-semivariogram for MOIST and TEMP

followed **by** a series of numbers, such as

MOIST / MOIST	00 01 02 03
MOIST / TEMP	00 03

The numbers indicate the 00th (or Olth, etc.) saved sample semivariogram for the specified random function(s). Given in Section 2.3 is a description of the naming convention used by GEOPACK. The numbers (i.e., 00 or 01, etc.) are the extension of the sample semivariogram file name (i.e., VARij.00).

Typing RETURN selects the particular sample semivariogram file for use by the fitting program. Typing Fl gives some information about the sample semi-variogram file that the cursor is highlighting. This help information is supplied to help you determine which file you want to use when you have a number of files from which to choose. The output from the fitting program is stored on the temporary drive (or subdirectory) using a naming convention similar to the sample semivariograms. After a sample semivariogram has been modeled (and the results saved -- SEE SECTION ABOVE ON SAVING THE SAMPLE SEMIVARIOGRAM) the model coefficients are saved in a file

<RAM drive>\mVARij.OO	first saved semivariogram model coefficient file. This file corresponds to <RAM>\VARij.OO
<RAM drive>\mVARij.Ol	second-file saved
<RAM drive>\mVARij.02	third file saved
<RAM drive>\mVARij.l4	fifteenth file saved where the "m" is used to designate the MODEL semivariogram file.

Save Model(s), Fit Model Manually:

This program displays the model semivariogram coefficients that have been modeled using the automatic fitting program and allows the user to select the "best" model to be saved in a file for use by the kriging program. The program allows you to save, view and manually model the semivariogram. Each operation is described below.

Saving a Semivariogram. The semivariogram model can be saved to the file which then becomes available to the Ordinary [Colkriging and Disjunctive [Colkriging programs. This must be done prior to kriging, otherwise the kriging program will not have a variogram model to use in the calculations. If the semivariogram models were fitted to the sample semivariogram using the "least-square" method (i.e., automatic fitting procedure), then the semivariogram model should be cross-validated prior to kriging. To do this, use the Cross Validation option on the Ordinary [Co]Kriging menu. To save the a semivariogram: type "S", "RETURN" and give the line number of the model you want saved. If no semivariogram model coefficients are saved, the kriging program will not work properly and an error message will be printed out stating that no semivariogram model coefficients were found.

Viewing a Semivariogram. This option allows you to view a saved semivariogram. You might want to do this if you have saved many semivariograms and are trying to determine the one you want to use for kriging.

To view the a semivariogram: TYPE "V", "RETURN" and give the line number of the model you want plotted. If you want to view several semivariogram then give the line numbers using-the format: "1,2,3" for lines 1 to 3. Note, you can only view 3 or less models on one graph.

Manually Modeling a Semivariogram. This option allows you to alter the coefficients of a saved semivariogram. You must **use** the automatic fitting program prior to manually modeling a semivariogram since this gives you a good starting point for the coefficients. If several model files are available, you can see the sample semivariogram from which the model was derived by typing the Fl key.

If you choose to manually model the semivariogram, you MUST place the model coefficients into the variogram model file manually, as well (unless you decide to use the automatically fitted values listed on the screen>.

To manually model a semivariogram: TYPE "M", "RETURN", change the coefficients shown at the bottom of the screen, and type "ESC" to have the model and sample semivariograms plotted.

Edit Variogram Model File:

This program allows the user to directly edit the file which stores the models for the semivariogram. If a model is fitted to a sample semivariogram manually, then the model coefficients must be manually entered into the variogram model file using this program.

Variogram Editor: File: G:\TEST.VAR

Variables		Model	Nugget	Sill-Nugget	Range	#
MOIST / MOIST	:	Exponential	0	1.371	8.001	00
MOIST / TEMP	:	Exponential	0	-2.999	9.994	00
MOIST / SAND	:	None	0	0	0	00
TEMP / MOIST	:	Exponential	0	-2.999	9.994	00
TEMP / TEMP	:	Exponential	2.001	15.003	4.513	00
TEMP /SAND	:	None	0	0	0	00
SAND / TEMP	:	None	0	0	0	00
SAND /SAND	:	None	0	0	0	00

Esc: Exit	Fl: Help	F2: Save	← ↕ →	Home	End	Page Up	Page Down

If no semivariogram model coefficients are saved, the kriging program will not work properly and an error message will be printed out stating that no semivariogram model coefficients were found. To correct this error, use the Save Model(s), Fit Model **Manually** program to save the semivariogram model coefficients for the random functions of interest.

2.5.i. Description of the Kriging Menu.

```
═══════════════ Thu Jun 29, 1989 07:47:45 am ═══════════════
 Return To Main Menu                                        1

 GEOSTATISTICAL PROGRAMS: Main Menu

       Ordinary [Co]Kriging Menu

 Return To Main Menu
 Set Program Parameters
 Cross Validation
 Ordinary [Co]Kriging
 Line Contour Diagram
 Block Contour Diagram


 Statistics Menu
 Variogram Menu
 Disjunctive [Co]Kriging Menu
```

Esc: quit	Fl: help	F3: util	F4: view	F5: user menu	↕	Home	End

If the highlighted key "0" is typed or the light bar placed over the menu option "Ordinary [Co]Kriging Menu" on the MAIN Menu and the enter key pressed, the Kriging Menu is activated giving access to several programs for calculating estimates of the selected random function(s) in space. You can use the F5 key to interface to GEO-EAS (or other programs) which allows you to use the ordinary kriging program for one random function included in GEO-EAS.

Set Program Parameters:

Information on using the setting of the program parameters for kriging is similar to that given in Section 2.5.i. An example of the screen generated by the Set Program Parameters program is given below. More information about the parameters can be found by starting this program and using the Fl key.

Kriging Parameter Settings File			
Est Loc in File (Y/N):	N	Anisotropy Ratio:	1.0
Maximum Search Radius:	20.00	Anisotropy Angle:	0.0
Contour File: (Y/N)	Y	Number Contour Levels:	4
Enable Graphic Option:	Y	Save Intermed. Results	N
ESTIMATE GRID: (P/B)	P	ORIGIN	0.0,0.0
No. of Points · X	30	Width Betw. Pts · X	?
No. of Points · Y	30	Width Betw. Pts · Y	?
No. OF VARIABLES:	?	No. NEAREST NEIGHBORS	
Estimate Var #l	1	Estimate Var #l	10
Auxiliary Var #l	2	Auxiliary Var #l	10
Auxiliary Var #2	3	Auxiliary Var #2	10
Auxiliary Var #3	?	Auxiliary Var #3	10
Auxiliary Var #4	?	Auxiliary Var #4	10
BLOCK KRIGING DISCRETIZATION		BLK COVAR. (0 default)	0.0
No. of Cells · X	3	Width of Cell · X	?
No. of Cells · Y	3	Width of Cell · Y	?

←left	right→	↑up	↓down	Home	PgUp	PgDn	End	F2=Sav	Esc-Exit

Cross-Validation:

GEOPACK provides you with a program that allows you to cross-validate the model for the spatial correlation structure. The cross-validation technique used is a semi-quantitative technique based on kriging and is used to evaluate whether the covariance function (or variogram) is appropriate for the experimental data. The method involves estimating the value of the random function of interest at every known sampling location but excluding the known value from the estimation process (the known value is excluded because kriging is an exact interpolator). Using all the pairs of actual and estimated values, various quantities can be calculated and used as an indication of the "quality" of the model spatial correlation function.

Ordinary Kriging and Cokriging:

The program GEOKRIG is used for kriging and cokriging. GEOPACK allows up to 10 variables to be used for cokriging although it is advisable to use 4 or less random functions in practice. If more than 5 random functions are used, the default settings program cannot be used while running the kriging program, since it only allows you to input 1 primary and 4 auxiliary random functions. A large static array of 10000 words is partitioned for storage of input data, the kriging matrix, etc. so there is a limit to the size of problem that can be executed with this program.

GEOPACK allows you to create estimated values in one of two manners, either on a grid system or by reading a file of x and y coordinates. This latter method is useful if irregularly spaced estimates are required.

Estimates on a Grid. The first method is to create a grid system with estimated values and estimation variances at each of the nodal points. To do this, you must supply the following information:

The origin of the grid system (usually the origin for the collected data is used).
The number of columns of estimates in the X direction
The distance between columns in the X direction
The number of rows of estimates in the Y direction
The distance between rows in the Y direction

case, the total number of estimates is -(Number of **columns)·(Number** of

Read Locations From a File. An alternative method for determining the placement for calculating estimates is to create a file which contains a list of the desired X and Y coordinates for the placement of the estimates. When using this option, GEOPACK will prompt you for the file name and use the file to determine the placement of estimates.

Line Contour Diagram:

A contouring package is provided with GEOPACK so that the output files from the kriging program can be graphically illustrated. The output file from the kriging program is in the temporary storage directory with a name: KPLOT.TMP. The contouring program reads this file and produces an output file KPLOTl.TMP which can be used by the graphics program to draw a contour plot ***on*** any device for which a device driver is supplied.

Block Contour Diagram:

The pixel contour program is similar to the line contouring program described above except that the estimation grid ***is*** presented on the screen and each cell is filled with a color and/or pattern in correspondence to the estimated value of the particular cell. This provides another method for viewing the results of the data and gives a better feel of the coarseness of the grid system. The pixel diagram which results from using ***this*** program can be printed by using the GRAPHICS.COM utility supplied with MS-DOS and the PRINT-SCREEN key.

2.5. j. Description of the Disjunctive Kriging Menu.

```
═══════════════ Thu Jun 29, 1989 07:47:45 am ═══════════════
 Return To Main Menu

   GEOSTATISTICAL PROGRAMS: Main Menu

        Disjunctive [Co]Kriging Menu

    Return To Main Menu
    Set Program Parameters
    Hermite Coefficients       (DK Step 1)
    Estimates, [Co]Kriging     (DK Step 2)
    Line Contour Diagram
    Block Contour Diagram


    Statistics Menu
    Variogram Menu
    Ordinary [Co]Kriging Menu


 Esc: quit | F1: help | F3: util | F4: view | F5: user menu | ↕ | Home | End
```

If the highlighted key "D" is typed or the light bar placed over the menu option "Disjunctive Kriging Menu" on the MAIN Menu and the enter key pressed, the Disjunctive Kriging Menu is activated giving access to several programs for calculating estimates and conditional probabilities of the selected random function(s) in space.

Set Program Parameters:

Information on the setting of program parameters for disjunctive kriging can be found in Sections 2.5.h and 2.5.i (i.e., variograms and kriging). One difference between this program and the previous programs is that there are two screens of parameters that can be set for disjunctive kriging. To toggle to the next screen type Ins.

Calculate Hermite Coefficients:

The first step in disjunctive kriging is the definition of a transform variable. The transform variable is assumed to be bi-variate normally distributed. The program calculates the transformed values of the data set which are used in the disjunctive [co]kriging program. For each random function that will be used for kriging, a transformed data set must be calculated (i.e., run this program for each data set selected). As a check on the transform process, a comparison between the mean and variance of the data and the transformation is given and should be approximately the same.

Calculate Estimates:

The program GEODK is used to disjunctive kriging and cokriging. The disjunctive kriging program allows up to 10 variables to be used for cokriging. Up to 10 cutoff values can be specified for which the program will calculate the conditional probability that the estimated value is greater than the cutoff level. During execution, the output to the screen will use as heading designators the letters A through J. Typing the FlO key will bring up a window that gives the definitions of the headings in terms of the cutoff values and transformed cutoff values.

Line and Block Contour Diagrams:

Line and block contour diagrams are also available from the Disjunctive Kriging Menu. For more information concerning these programs, see the description under the Kriging Menu, above.

2.5.k. Modifying and Adding Menus.

It is possible to tailor GEOPACK to an individual's needs by adding programs or menus to the USER menu (accessed through the F5 key). If the program to be added to the system requires the use of the data set or any of the output files produced by GEOPACK, read the help information under the heading SYSTEM OPERATION on the main HELP menu. The information concerning the files, their contents, formats, naming conventions, etc. is given by this help sequence.

The following steps are used to add a program or menu to GEOPACK. Several examples are included in GEOPACK and can be found by typing the *.MEN files. It is usually easier to start with copy of an existing *.MEN file (or portion thereof) as a template and make the required modification(s) to the template. To add a single executable program is very easy, since only a few lines must be added to an existing *.MEN file. To add an additional menu requires creation of a complete *.MEN file, and therefore is somewhat more difficult. If a new menu is to be created, it is generally a good idea to place the *.MEN and executable files is a new subdirectory.

STEP 1: Determining Whether a Menu or a Program Will be Added:

The first step is to determine whether a menu or a program is to be added to GEOPACK. If it appears that the application to be added may require several programs or batch files, it is better to create a new menu containing these items. An example of creating a menu is the GEOEAS.MEN file contained in the subdirectory %GEODIR%\USER\GEOEAS, where %GEODIR% is used by GEOPACK to designate the root directory of the geostatistical programs. The reason for creating a menu rather than specifying a program is that to run the program GEOEAS requires rewriting the GEOPACK data file in a format that can be read by GEOEAS.. This requires an interfacing program to create a new file in the proper format.

Next on this menu are the commands for starting the GEOEAS programs. This is followed by a program which takes the output of the kriging program (in GEOEAS) and rewrites the output in a format that GEOPACK can read. This enables the user to utilize the GEOPACK routines on the GEOEAS output. Since each of these commands concerns the use of GEOEAS it is better to put them into a menu specifically to run the GEOEAS program, rather than including all these commands on the USER menu, since space is limited to 11 entries on any one menu.

Step 2: Altering the USER.MEN:

The second step is to alter USER.MEN to include another or alter an existing heading. Once the program or menu to be added to GEOPACK has been created it can be accessed through the USER menu (i.e., F5 key) by adding or modifying an entry to the menu file. Entries to the USER menu are added by editing the USER.MEN file located in the root of the geostatistical programs (i.e., %GEODIR%\USER.MEN). An example of a menu entry is:

```
Line
 1:        %lE@User Menu
 2:        *_GEO-EAS
 3:        #message
 4:
 5:        ^%GEODIR%\user.men
 6:        +%COMSPEC% /c cd %GEODIR%\user\geoeas
 7:
 8:        ^%GEODIR%\user\geoeas\GEOEAS.MEN
```

where the symbols have the following meaning:

% in column 1 indicates that the next two hexadecimal numbers indicate the Menu colors, where the first and second numbers are the background and foreground colors, respectively, and the colors are given by the color-numbers given below (for example a dark blue background with light yellow lettering is specified by using "%lE" in line 1, above)

0 - Black	8 - Grey
l Blue	9 - Light Blue
2 - Green	A Light Green

3 - Cyan	B - Light Cyan
4 - Red	C - Light Red
5 - Magenta	D - Light Magenta
6 - Brown	E - Light Yellow
7 - White	F - Light White

In any other column the "%" is used for different purposes.

@ print the following text as the menu title

* print the following text as menu selection heading

print following text in the information box at the top of the menu

tells the menu program to hold the-menu on the screen as long as possible before switching screens. This helps to improve the visual appeal of the menu program but should only be used when "popping" (i.e., adding) or "pushing" (i.e., deleting) a menu and not when running an executable program. **It** should be placed prior *to* the menu to be added or deleted.

\+ indicates that the remainder of the line is to be executed. THE MENU PROGRAM WILL ONLY RUN EXECUTABLE FILES AND NOT BATCH FILES OR BATCH COMMANDS. To run a BATCH command the following method must be used:

```
+%COMSPEC% /c cls         - this will clear the screen
+%COMSPEC% /c echo . . .  - this will echo . . .
+%COMSPEC% /c cd c:\      - this will call the directory c:\
```

The name of the file to be executed must be either in the current directory, include a full path specification or the file must be in a directory on the DOS path. It is generally a good idea to include the full path of every program whether you expect the program to be in the current directory or not, since it may not be obvious what the current directory is. You can always change the current directory using "%COMSPEC% /c CD\<new subdirectory>".

^ tells the menu program to add a menu to the screen where the name following "^" is the file containing the menu instructions. (Pop the menu on the screen)

/ tells the menu program to remove the "top-most" menu from the screen. Sometimes the remove menu instruction (i.e., "/") is given on two consecutive lines. This is done so that two "quit menu" key strokes are not needed to return to the proceeding menu (this is only done when an additional copy of the User's Menu is popped on the screen to move it from the right hand side of the screen to the left hand side; which is done to improve visual appeal.).. (Push the menu off the screen).

the underscore before the "G" on line 2 is used to designate the highlighted character. This character will activate the menu option. If there are two (or more) menu options with the same highlighted character, the cursor bar will move to the next one, each time the highlighted character is entered.

STEP 3: If Another MENU Is Being Added:

It is often best to place the new program into a separate subdirectory. An example of this is the GEO-EAS subdirectory which stores the executable programs for the GEO-EAS geostatistical software system. Once the subdirectory is named and created, the newly developed program(s) and auxiliary files should be copied into it. A new data file containing the entries for the newly created menu must be created using the methods described above. It is probably best to start with an existing menu command file (e.g., USER.MEN, GEOEAS.MEN or equivalent) to act as a template, changing only those lines that are needed. This will provide a guide for setting up the command file.

In the USER.MEN file, the call to the new menu is made as follows (assuming that a new subdirectory called "NEWDIR" has been created with the following path: %GEODIR%\USER\NEWDIR and that the command file for the new menu is called "NEWMEN.MEN"):

```
#place a descriptive message for the menu here
* _NEWMEN Menu
~

^%GEODIR%\user.men
+%COMSPEC% /c cd %GEODIR%\user\newdir

"%GEODIR%\user\newdir\NEWMEN.MEN
```

The commands necessary to run one (or more) programs from the new menu are as follows (it is assumed that the new program is called NEWPRG):

```
#Quit Menu
*_Quit
/
/
*Run _NEWPRG
#place a descriptive message for what the program does here
+%GEODIR%\user\newdir\NEWPRG
```

The above instructions should be adequate for modifying GEOPACK to include the new menu and program(s).

2.5.1. Trouble Shooting.

If an error should occur while attempting to add a program or menu to GEOPACK try one of the remedies listed below.

1. The newly created USER menu entry does not show up on the USER menu. This might occur if the wrong menu data file was altered. The proper file to alter is %GEODIR%USER.MEN. Also, only 11 entries can be placed on one menu. If you wish to have more than 11 entries you will have to create an additional menu or move some of the programs to other menus, if they exist.

2. The newly created menu does not run when selected from the USER menu. This is probably due to an improper path-file name combination. Make sure that the path and file names are correct. If an error message is printed out by the program, it is often "lost" because the menu reappears on the screen too quickly. The error message (or other information) can be seen by typing the F4 key.

3. The newly created menu does not have any entries on it and an error message: Abort Menu: Menu Data Not Found is printed to the screen. This is caused because the menu program cannot find the newly created menu data file. This may be due to changing directories before the new menu is placed on the screen. You should check to make sure that the commands in the User Menu and the new menu are appropriate for what you are trying to do.

4. To get back to the USER MENU (located at the right-hand side of the screen, you have to type two "quits". This is caused because you have popped an additional USER.MEN on to the screen and the newly created menu only deletes one of the USER.MEN when you quit the menu. To delete two USER.MEN place two '/' in the newly create menu file each on a separate line.

2.6. GEOPACK Enhancements

2.6.a. Running GEO-EAS Geostatistical Software.

The GEO-EAS geostatistical software can be executed from within GEOPACK. The GEO-EAS programs are accessed by typing the F5 key and selecting the GEO-EAS option. Since the data set required by GEO-EAS is formatted differently than GEOPACK, there is an interface supplied to create a data set in GEO-EAS format. This data set will have the file extension ".EPA". There is also an interface program to take the output from the GEOEAS kriging program and convert it to GEOPACK format. This enables results to be printed and plotted using GEOPACK graphics capabilities.

2.6.b. Description of GEOPACK Utility Programs.

GEOPACK contains a number of utility programs which can be used separately from the system to aid in alteration of the system or for use in a "command-line" mode (i.e., running the program without using the menu system). A brief description of the function of each program and their use follows.

Program Name	Description
HELP.EXE	This program is used to call a particular help information section from a file. For example, if you want to print the help information concerning "Theory of Variograms" the HELP program could be used as follows: C:\HELP VARI.HLP THEORY.HLP where VARI.HLP is the help information desired and THEORY.HLP is the file containing VARI.HLP.
GEOPACK.EKE	This program displays the first screen giving the GEOPACK name. This program also determines where the call to GEOPACK is made (i.e., the subdirectory where GEOPACK is typed) so that after leaving the program you will be returned to that directory.
MSDOS.EXE	This program allows you to execute a DOS command while running GEOPACK.
DOSSHELL.EXE	This program allows you to leave GEOPACK in a DOS shell and temporarily suspend execution of GEOPACK. When finished executing DOS commands you reenter GEOPACK by typing EXIT
MENU2.ExE	This is the menu program.
EVOKE.EXE	This program is used to execute a program when it is desired that system parameters be passed to the program. (Note: system parameters are set by the user and are difficult to "hard" program). This program is particularly useful when altering.(i.e., adding additional programs) GEOPACK since it enables you to pass system parameters to other programs without having to know their value. For example, to run a "C" program and passing the location of the temporary directory, the border color and the text color use:

EVOKE <prog name> $(TEMPDIR) $(BORD) $(TEXT)

EVOKE.EXE substitutes the "true" values for $(TEMPDIR), $(BORD) and $(TEXT) in the spawning process, i.e., the above command is equivalent to <prog name> g:\ 1 11 provided that the system is setup so that the temporary directory is g:\, and the border and text colors are 1 and 11, respectively. The list of parameters EVOKE.EKE can pass follows:

EDITOR - Default text editor
TEMPDIR - Temporary directory
PRINTER - Printer device
PLOTTER - Plotter device
ROWS - Maximum number of rows on screen
COLS - Maximum number of rows on printed page
TEXT - Text color
BORD - Border color
MODE - Screen mode (O-mono, l-color) This only works in FORTRAN programs

DSTAT - Default statistics package
LGRAPH - Default line graph package
GRAPH - Default contour, 3-D graphics pkg
DBASE - Default data base management system

Examples: Try these examples in the *root* of the geos-tatistical programs

```
EVOKE defgraf $(LGRAPH) $(TEMPDIR) $(BORD) $(TEXT)
EVOKE defgraf $(GRAPH) $(TEMPDIR) $(BORD) $(TEXT)
EVOKE $(DBASE) EVOKE DOSSHELL $(BORD) $(TEXT)
EVOKE SDATA $(TEMPDIR) $(BORD) $(TEXT)
EVOKE $(EDITOR)
EVOKE edit $(EDITOR) <dir name> $(BORD) $(TEXT)
```

SDATA.EXE This program allows you to declare a data file active by copying it to the temporary directory (e.g., RAM drive) and creating the DEFAULT file which contains the data file name and origination path. To use type: SDATA from root of the geostatistical programs.

PACK-EXE This program allows you to take the files on the temporary subdirectory (e.g., RAM drive) and store them in an archive file. These files may be retrieved at a later time using one of the programs: EXTRACT.EXE, SDATA.EXE or UNPACK.EXE.

To use type: PACK from root of the geostatistical programs.

UNPACK.EXE This program allows you to take an archived file and remove all the stored files back to the temporary storage drive (i.e., RAM disk).

To **use** type: UNPACK from *root* of the geostatistical programs.

EXTRACT.EXE This program allows you to take one *or more* stored files out of an archived file and place them on the temporary storage drive (i.e., RAM drive). You must extract the data file and the DEFAULT file before attempting to run GEOPACK.

To use type: EXTRACT from root of the geostatistical programs.

EDIT.EXE This program along with EVOKE allows you to call up the default text editor for editing the data base. See examples for using EVOKE for use instructions.

LISTDIR.EXE This program allows you to list the contents of any directory on a floppy or hard drive. The program also allows you to view a file.

To use type: C:\LISTDIR <dir name> <border color> <text

color>. where the colors are given by the color-numbers given below:

0 - Black	8 - Grey
1 - Blue	9 - Light Blue
2 - Green	10 - Light Green
3 - Cyan	11 - Light Cyan
4 - Red	12 - Light Red
5 - Magenta	13 - Light Magenta
6 - Brown	14 - Light Yellow
7 - White	15 - Light White

VIEW.EXE — This program allows you to view the contents of a file. To use this program type the following: C:\VIEW -<border color> +<text color> <file name> where the border and text colors are given in above. Colors are either decimal as described above or hexadecimal using a format such **as:** 0x1E.

VED.EXE — This program allows you to manually edit the semi-variogram coefficient file (see the variogram menu and associated help screens for more information) if it exists.

AUTO.EXE — This program operates with the menu system and executes the necessary commands to create the hard-coded and user-definable menus.

MGEOEAS.EXE — This is an example of a user-written interface to couple the GEO-EAS geostatistical software to the GEOPACK system. This program modifies that GEOPACK data file so the GEO-EAS can read its contents.

MGEOCNVT.EXE — This is an example of a user-written interface to couple the GEO-EAS geostatistical software to the GEOPACK system. This program modifies the GEO-EAS output file so that GEOPACK can use the results for further analysis.

SHOWDIR.EXE — This program allows you to see a diagram of all the sub-directories that branch off the current (or specified) subdirectory. To use type: SHOWDIR <any dir>.

DEFLT.EXE — This program allows you to alter the system settings for the parameters listed under EVOKE.

To use this program type: DEFLT SYSETUP SYSDEFLT.

SECTION 3

EXAMPLES

3.1 VIRUS DECAY RATES IN TUCSON GROUND WATER

Description of Data

Water samples were obtained from 71 continuously pumping public water supply wells in the Tucson Basin. The water samples were taken to the laboratory and viruses were added. The samples were incubated at the <u>in situ</u> ground-water temperature. At predetermined times, subsamples were withdrawn and assayed to determine the number of virus particles remaining in the water. The decay rate was calculated as the slope of the line drawn through the data using linear regression and has the units of $\log_{10}$(virus particles)/day.

Geostatistical Calculations

The data set was configured in the following way according to GEOPACK requirements and is included in the directory %GEODIR%\USER\DATA under the name, VIRUS.DAT.

Ground Water Data for the Tucson Basin

```
    2   71     500.00
    12     3     4     5
     TEMP      DECAY   -
(f5.0,4F10.3)
    1      8.498     7.458  20.00000  -0.82800
    2     14.129     6.453  20.00000  -0.94600
    3     14.330     8.263  20.00000  -0.92400
    4      5.280     8.665  20.00000  -1.16400
    5      5.079     8.464  20.00000  -1.06700
    6      6.084     7.056  23.00000  -0.79700
    7      7.291     6.855  23.00000  -0.98900
    8      5.883     5.045  23.00000  -0.89200
    9     17.951     6.654  23.00000  -0.88900
   10      2.263     8.866  24.50000  -0.69500
   11     -0.151     9.671  24.50000  -0.85500
   12      5.280     7.458  24.50000  -0.73400
   13      6.285     6.654  24.50000  -0.76900
   14      3.671     7.660  24.50000  -0.80200
   15     14.934     5.447  24.50000  -0.69600
   16     11.716     6.654  24.50000  -0.67600
   17     14.129     4.240  24.50000  -0.96300
   18     14.934     4.442  24.50000  -0.81000
   19     -4.374    11.682  24.50000  -0.80500
   20     -5.983    12.889  24.50000  -0.81400
   21     -1.961    10.475  26.00000  -0.79600
   22      5.280     6.252  26.00000  -0.69900
   23      9.906     4.643  26.00000  -0.76000
```

24	8.096	5.246	26.00000	-0.64000
25	8.096	5.849	26.00000	-0.94800
26	10.107	5.246	26.00000	-0.48800
27	15.135	3.436	26.00000	-0.59900
28	15.738	4.240	26.00000	-0.57600
29	16.543	3.235	26.00000	-0.94500
30	12.520	2.430	26.00000	-0.75400
31	16.744	0.620	26.00000	-0.67600
32	-5.581	11.280	26.00000	-0.79700
33	-5.581	11.481	26.00000	-0.54400
34	3.269	6.855	27.00000	-0.39800
35	3.269	7.257	27.00000	-0.37100
36	5.481	5.447	27.00000	-0.81600
37	10.710	3.034	27.00000	-0.31700
38	8.096	3.838	27.00000	-0.67800
39	7.492	4.643	27.00000	-0.65800
40	8.297	4.643	27.00000	-0.76500
41	9.101	4.240	27.00000	-0.78700
42	11.917	-1.592	27.00000	-0.73400
43	11.515	3.034	27.00000	-0.68900
44	11.314	3.838	27.00000	-0.73400
45	15.537	3.034	27.00000	-0.62900
46	15.135	2.430	27.00000	-0.68400
47	15.939	1.425	27.00000	-0.33900
48	15.537	2.430	27.00000	-0.77200
49	16.744	0.419	27.00000	-0.53400
50	16.543	1.023	27.00000	-0.23600
51	5.079	5.447	28.25000	-0.60400
52	4.878	4.643	28.25000	-0.46800
53	6.285	3.637	28.25000	-0.65600
54	6.285	4.240	28.25000	-0.71300
55	9.302	1.626	28.25000	-0.58400
56	10.509	2.430	28.25000	-0.79400
57	13.526	3.235	28.25000	-0.66400
58	17.951	2.430	28.25000	-0.72700
59	1.056	7.458	30.50000	-0.19400
60	-1.961	8.665	30.50000	-0.67000
61	-1.357	7.660	30.50000	-0.66000
62	1.861	2.833	30.50000	-0.53800
63	3.068	2.631	30.50000	-0.33400
64	3.470	5.447	30.50000	-0.63800
65	3.470	6.051	30.50000	-0.55200
66	4.274	5.246	30.50000	-0.15100
67	2.665	1.626	30.50000	-0.50500
68	3.872	1.023	30.50000	-0.43900
69	5.682	0.821	30.50000	-0.53300
70	5.883	2.028	30.50000	-0.62900
71	2.062	4.039	30.50000	-0.41400

Several steps are required for conducting the geostatistical analysis and are described below. The data set was created following the format instructions given in Section 2.4.a. All user inputs are shown in Boldface **type**.

Step 1: Select a Data Set

To use GEOPACK a data set must be available. Therefore the first step in using this program is to create a data set (which is assumed to have been done) and then start GEOPACK and *select it.*

1) Select Data Set Utilities Menu at Main Menu.
2) Select Select a Data Set at Data Set Utilities Menu.
3) To select the data set, either use the cursor keys to find the entry VIRUS.DAT or type the name of the file on the keyboard. If a number of files exist in this directory, it is possible to move the cursor to the first (or next) file beginning with a specific letter by typing ALT-letter (i.e., hold the ALT key and type the desired letter). Note: the Select Data program automatically looks in the "data" directory. This directory *is* specified in the SYSDEFLT file which can be altered using the Change System Default Settings program (i.e., type F3 then C, its the second line on the screen that follows). Once the file VIRUS.DAT has been selected, GEOPACK reads in the data file, and outputs *to* the screen the cutoff level and the number of available data points for the variables. You are returned to the Main Menu.

Step 2: Check Distribution of Data

The next step in the analysis is to determine if the data are normally distributed. Although the kriging technique does not required the data to have a normal distribution (and is a best linear unbiased estimator regardless of the distribution of the data) the estimator is optimal whenever the data is normally distributed.

4) Select Statistics Menu.
5) Select Kolomogorov Test of Distribution.
6) Select the appropriate data set, in this case, B, decay. The calculations are output to the screen. At this time, you may type J to jump ahead. The results of the Kolomogorov-SmirnovTest for Distribution are output to the screen. In this case, we accept the null hypothesis at the 0.05 level and thus there is some evidence that the data are normally distributed. If the data were not normally distributed, it would be possible to transform the data into a new data set with a normal distribution. A logarithmic transformation is a common technique for transforming data into a normal distribution. You are returned to the Statistics Menu.

Step 3: Determining the Variogram

Next the sample spatial correlation structure (i.e., the sample semi-variogram) must be determined. Without this functional relationship between the distance and the variance it is not possible to use the kriging techniques.

7) Select Variogram Menu.
8) Select Variogram Calculation (Sample).
9) Select type of correlation function, in this case, A, semivariogram.

10) Select the principal function, in this case, B, decay.
11) You will now be asked several questions about how you want the calculations performed, unless you have set up the default settings fiie in such a manner as to avoid this. When responding to the questions, you may either type in a number or push Enter to select the default value which is shown on the lower left-hand side of the screen.
12) After all of these questions have been answered, the variogram is calculated. The progress of the calculations is output to the screen as Percent Completion on the lower right-hand side.
13) Both a table of values and a plot of the sample variogram are printed to the screen. For this data set, the output appears as shown in Figure 3.1.1 (Note: the following figures use the device drivers supplied with GEOPACK. Publication quality figures can be created using an appropriate graphics package and the USERS MENU (F5).
14) You are now given several options. Select Options to add labels to your graph. Upon Exiting this menu, you are returned to the Variogram Menu.
15) Select Automatic Model Fit.
16) You will again be asked several questions, then allowed to choose the autocorrelation function you wish to model.
17) Select a model type, in this case, D, spherical. The input parameters are printed to the screen, as well as the input data. If you wish to delete any of the data, type D, Enter, the Observation number, and Enter. You need to repeat this step for each line you want to delete. In this case, we delete lines 8 through 12.
18) Several screens will be printed, detailing the results of the model variogram calculations. The model fit to the data will then be printed to the screen. For this example, the output is as shown in Figure 3.1.2.
19) Once again, you are given the opportunity to add labels, etc. to the graph.
20) Upon Exiting the screen, you are asked if you want to rerun the program. If No, you are returned to the Variogram Menu.
21) Select Manual Model Fit, Select Model(s).
22) You now select the desired file by hitting Enter.
23) A summary of the models that you have run on that data file is then shown. Type S to save the correlation model that you want to krig.
24) You are returned to the Variogram Menu.

Step 4: Create a Grid of Estimates Using Ordinary Kriging

The final step in this example is to obtain a grid of estimates using the data set and the model of the spatial correlation structure. An estimate can be made at any point in the field of interest. In general, estimates made far from any data points will have a higher estimation variance (i.e., there is less confidence that the estimate is close to the true value) compared to estimates made close to data points. If an estimate is made at the same coordinates as one of the data points in the data set, the estimated value will exactly equal the data value at that point and the estimation variance will be zero. This behavior indicates that kriging is an exact interpolator.

25) Select Ordinary Kriging. You will be asked several questions unless you have modified the Default Settings file to avoid this.

26) Several screens showing the output from the kriging calculations will be output to the screen. Once again, at the Kriging Estimates for Decay screen, you are given the opportunity to Jump ahead and bypass seeing the output of this program.

27) When the program is finished, you are returned to the Ordinary Kriging Menu, where you select Line Contour Plot.

28) You are given the choice of plotting the estimated value or the variance. In this case, we choose A, and the following contour plot is shown on the screen:

29) You are given the option to add labels to the plot as before.

30) After Exiting this program, you are returned to the Ordinary Kriging Menu.

31) This time, we select Block Contour Plot.

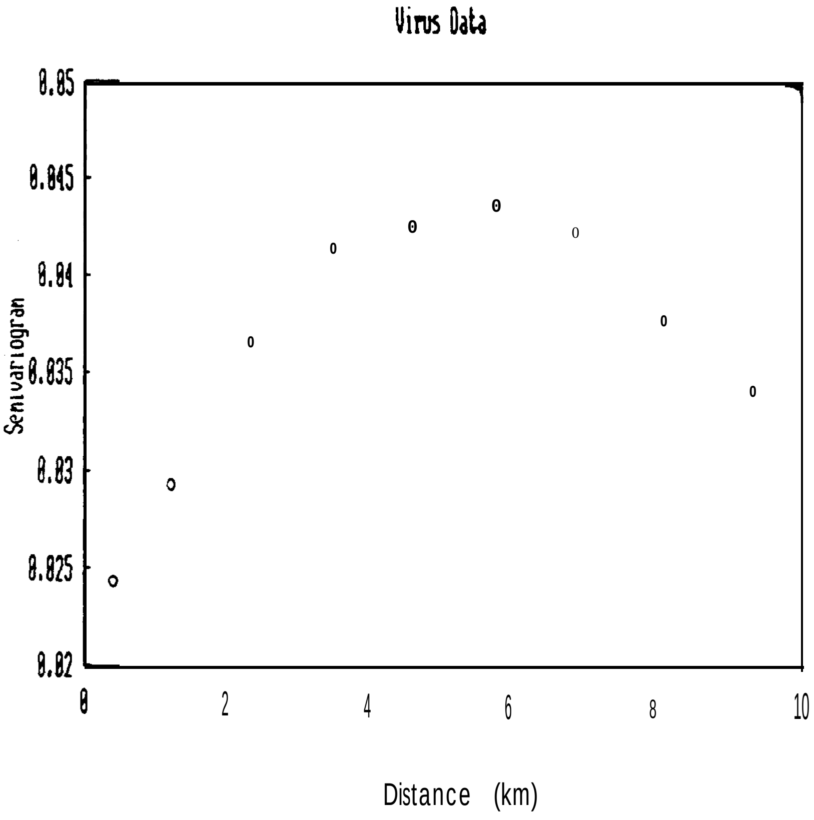
32) Again we choose A to plot the estimated values, and the output looks like the following:

e= .0•	SEMIVARIOGRAM CALCULATION	δθ = ± 90.0'
DATE: 09/01/1989		**TIME: 09:06 am**

A

LAG	No. OF COUPLES	DISTANCE	SEMIVARIOGRAM DECAY	DRIFT DECAY
1	11	.41	.0243	-.I444
2	125	1.23	.0292	-.0649
3	232	2.30	.0366	-.1125
4	230	3.54	.0415	-.1355
5	249	4.65	.0426	-.1603
6	241	5.03	.a437	-.1633
7	216	6.95	.0424	-.1621
8	193	8.17	.0379	-.1557
9	160	9.38	.0342	-.1586
10	175	10.50	.0406	-.1680
11	137	11.66	.0574	-.2497
12	146	12.77	.0426	-.1555

Strike a key when ready ... |X|R|O|H|



B

Fieure 3.1.1. Example output from **Variogram Calculation (Sample)** program for the data set, VIRUS.DAT. In A and B, respectively, **are** the tabular **values and a plot** of the semivariogram function.

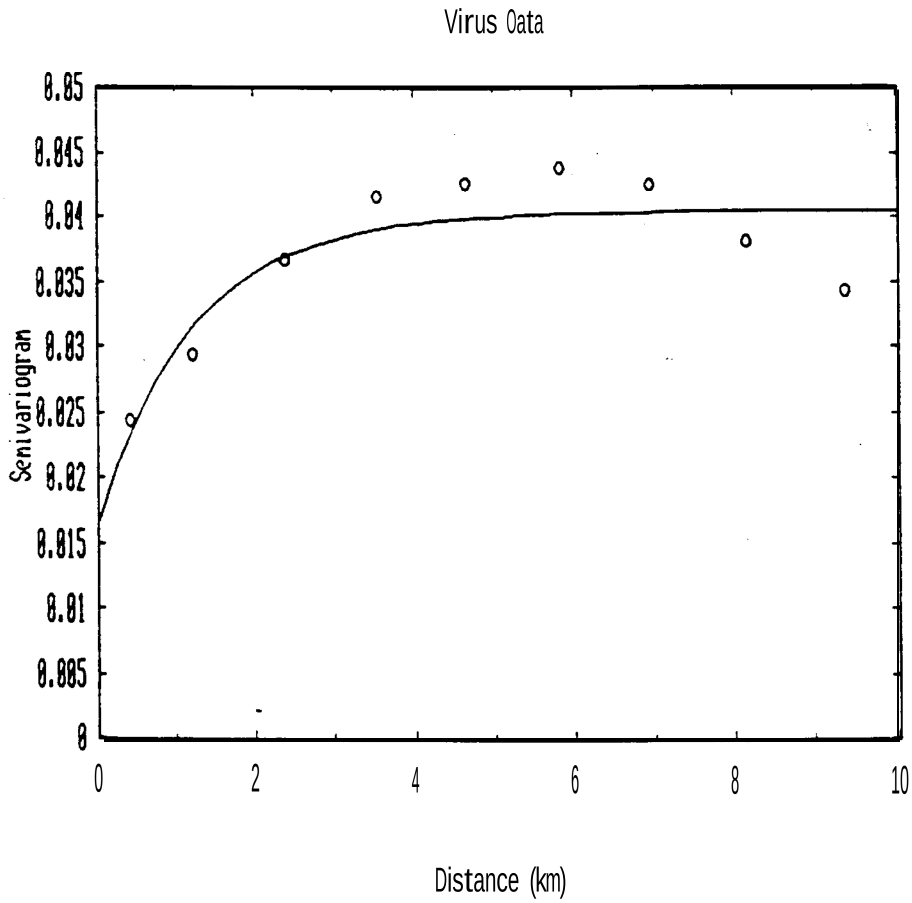


Figure 3.1.2. Example output from the Automatic Model Fit program. The solid line is an spherical model that was fitted to the sample semivariogram.

A

SUMMARY OF SPATIAL CORRELATION MODELS

Line No.	No. Pts	DIR	MODEL	NUGGET	Sill - NUGGET	RANGE	SSQ
1	10	.OO	EXPON	.0165	.0240	1.2286	.00008
				[2.33]	[3.55]	[2.001	
2	10	.00	SPHER	.0207	.0197	3.8252	.00007
				[5.341	[4.98]	[3.52]	
3	10	.00	POWER	.0000	0311	.1297	.00016
				[.00]	[.16]	1 .19]	

Esc: Exit | F1: Help | S: Save | V: View | M: Model (Manual Mode)

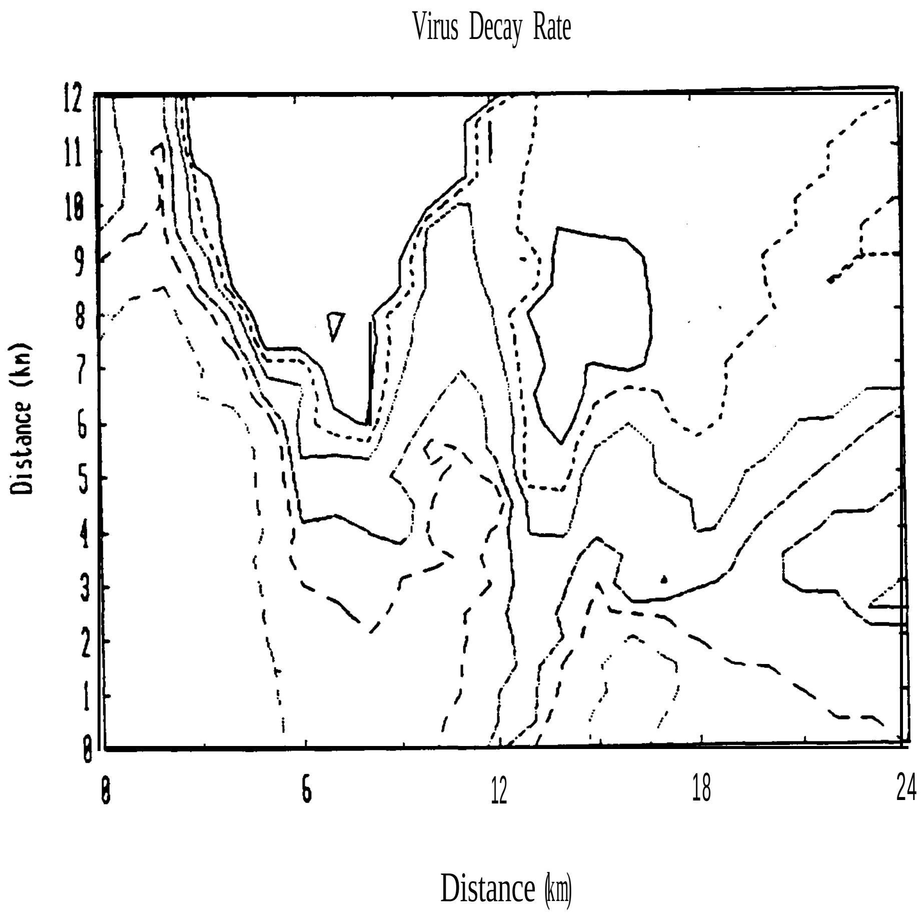
B

Variogram Editor: File: G:\VIRUS.VAR

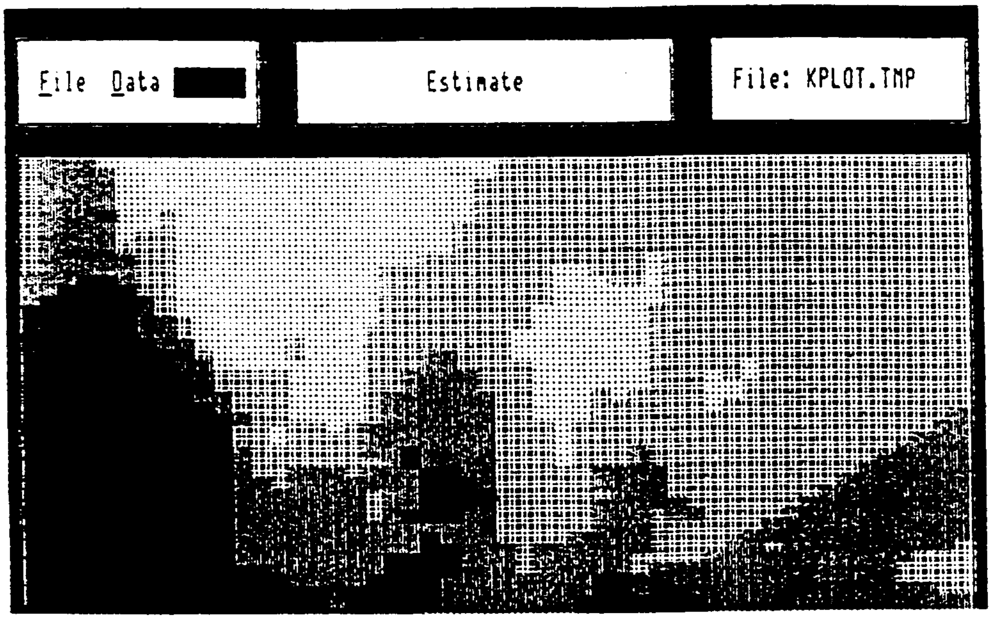
Variables	Model	Nugget	Sill-Nugget	Range	#
TEMP /TEMP :	None	0	0	0	
TEMP /DECAY:	None	0	0	0	
DECAY/TEMP :	None	0	0	0	
DECAY / DECAY :	Spherical	0.021	0.02	3.825	00

ESC: Exit | Fl: Help | F2: Save | ↕ →| Home | End | ,Page Up | Page Down |

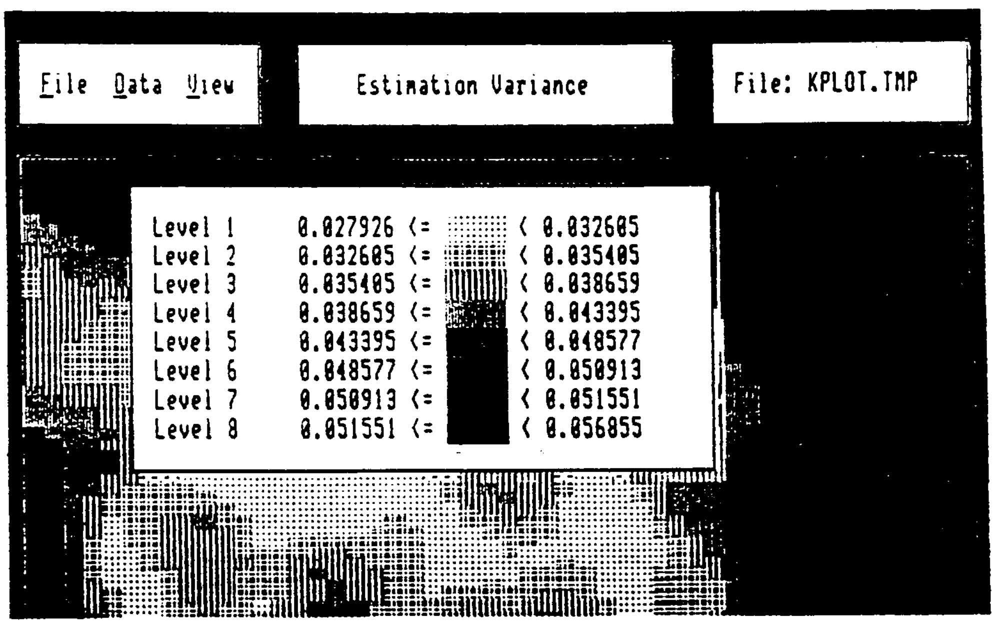
Figure **3.1.3. Example output from Manual Model Fit, Select Model(s)** program (in A) **and the Edit Variogram Model File (in B).**



Fieure 3.1.4. Contour diagram of the estimated value of the decay rate using the Ordinary (Co]Kriging and Line Contour Diagram programs is illustrated.



A



B

<u>Figure 3.1.5.</u> Contour diagram using the **Ordinary [Co]Kriging** and **Block Contour Diagram** programs. In A and B, respectively, the estimated value for the decay rate and the estimation variances are illustrated.

3.2. SALINITY IN A SOUTHWEST ARIZONA FIELD.

Description of Data

This data set contains two random functions, the electrical conductivity (EC), and the sodium adsorption ratio (SAR). The data was collected by Al-Sanabani (1982) at 101 random locations on a lm by lm grid system in a lo-ha field (soil type: Typic Haplargid). The l-2 kg samples were placed in a beaker with distilled water and a saturated paste was made. The solution was extracted from the paste and the EC of the solution measured. A more detailed description of the data and techniques used to measure the EC and SAR is given in Al-Sanabani (1982). This data set is included in the %GEODIR%\USER\DATA directory under the name, ECSAR.DAT.

Step 1: Check Distribution of Data

The hypothesis that the data were normally or lognormally distributed was tested using the Kolomogorov-Smirnov (KS) test for goodness-of-fit (Sokal and Rohlf, 1981; Rao et al., 1979). The KS test statistic was calculated and compared to the critical value at the 0.1 probability level. This level was chosen to reduce the probability of the type II error, namely the probability Of incorrectly selecting the null hypothesis (Rao et al., 1979).

For a sample size greater than 30 the critical value at the $\alpha = 0.1$ probability level can be obtained from the asymptotic expansion (Rohlf and Sokal, 1981; Rao et al., 1979):

$$KS_{crit} = 0.805/(\sqrt{n})$$

The results of the KS test indicate that the original and log-transformed data are from lognormal and normal distributions respectively, at the 0.1 probability level. Therefore a lognormal transformation will cause a data set to have a normal distribution. The KS test statistic calculated from the data sets were 0.197 and 0.065 for the original (EC) and transformed (1nEC) data, respectively. The associated critical value is 0.080 and was calculated by Eq. 1 for n = 101. Since the data are lognormally distributed, they will be transformed to a data set with a normal distribution by taking the logarithm of each datum. This new data set will be used for the geostatistical analyses.

Step 2: Transform the Data Set

The data set can be transformed by using the Modify an Existing Data Set option *on* the Data Set Utilities Menu. The steps necessary to use this program to add a random function called ln[EC] by taking the logarithm of the EC data are:

1. The allowable transformations can be viewed by typing Fl (Help) before selecting the variable to modify. Place the lightbar over the data set (i.e., EC) to be transformed. Type Enter.
2. Move the lightbar over one of the Unused markings and type Enter. A window will pop up in which the name for the new data set can be entered. In this case, the new data set will be called ln(EC].

3. Type in the transform equation, which for this example is:

y=log(x); (natural logarithm)

and type a F4 to start the transformation process. Once completed both the EC and ln[EC] data sets will exist in the data file.
4. To save the transformation results, type F2 and either 0 to overwrite the data file or B to save a backup copy of the old data file. If you decide you do not want to save the new data set, the type ESCAPE and you will be asked if you want to leave the program without making any changes.
5. To exit, type ESCAPE.

Step 3: Determining the Variogram

As with all kriging methods some measure of the spatial correlation structure is necessary. For disjunctive kriging the appropriate function is the auto correlation which requires a second-order stationary hypothesis (i.e., the variance must be finite).

An easy method for determining the autocorrelation from the semi-variogram is to use the following relationship

$$p(h) = 1 - \gamma(h)/\gamma(\infty)$$

which is done automatically when using the disjunctive kriging program. Using GEOPACK to determine the sample semivariogram by following the sequence given in Example 1. Next a model variogram is applied to the sample semivariogram. For this example, the automatic fitting procedure is used and yields

$$y(h) = 0.27 + 0.66[1.5h/145 - 0.5(h/145)^3]; \quad 0 < h < 145 \qquad [5]$$

$$y(h) = 0.93 = \gamma(\infty); \quad h > 145$$

and is shown in Figure 3.2.1.

This variogram model was used in the cross validation procedure listed on the Ordinary [Co]Kriging Menuwhich attempts to fit both the sample semi-variogram and the reduced mean and variance simultaneously. An acceptable model variogram is given when the reduced mean and variance are approximately 0.0 and 1.0, respectively, subject to a reasonable fit to the original sample semivariogram. Using the Cross Validation procedure on the Ordinary [Co]Kriging Menu, the reduced mean and variance of the above model can be determined and are, respectively, .0198 and 1.224.

The cross-validated model is somewhat different from the one listed above because now the fitting procedure also tries to fit the reduced mean and variance. For this case the semi-variogram model is

$$y(h) = 0.36 + 0.52[1.5h/153 - 0.5(h/153)^3]; \quad 0 < h < 153 \qquad [5]$$

$$\gamma(h) = 0.88 = \gamma(\infty); \quad h > 153$$

For the model given above, the reduced mean and variance, respectively, were 0.0241 and 1.062. One problem in using the reduced mean and variance for determining the adequacy of semivariograms is that there is no independent method for determining how close to zero and unity the reduced mean and variance should be and therefore using this technique to fit models to a variogram is somewhat subjective.

Viewing the two variograms using the Fit Models Manually option on the Variogram Menu, it appears that the neither of the models produces an adequate fit for both the sample semivariogram and reduced mean and variance. For this reason, an alternative model is chosen that falls in between the cases listed above. This model is

$$\gamma(h) = 0.30 + 0.60[1.5h/160 - 0.5(h/160)^3]; \quad 0 < h < 160 \qquad [5]$$

$$\gamma(h) = 0.90 = \gamma(\infty); \qquad h > 160$$

and has a reduced mean and variance, respectively, of 0.0203 and 1.19.

Step 4: Calculate the Hermite Coefficients

The next step in the disjunctive kriging process is to find the coefficients which define the Hermite transform function (See Theory of Geostatistics listing on the GEOPACR User's Manual, Type Fl). To obtain the Hermite coefficients it is necessary to select the Hermite Coefficients listing on the Disjunctive Kriging Menu. There are a number of questions that must be answered during the execution of this program. These questions will appear only if the Set Program Parameter program was not run prior to this selection.

Step 5: Create a Grid of Estimates Using Disjunctive Kriging

A total of 2500 estimates of EC and ln(EC) (using each method) were obtained on a 5 by 5 meter grid system superimposed over the field sampled by Al-Sanabani (1982). Along with each estimate a value of the kriging variance was calculated and for the disjunctive kriging method a value of the conditional probability. Bower and Wilcox (1965) gives 4.0 dS/m as a critical value of EC for many plants therefore this value (or the ln(4.0 dS/m)) was used for the critical value (i.e., Z_{cut}) in subsequent analyses. For all cases a maximum of 5 nearest neighbors within a radius equal to the range of the variogram were used in the estimation process. Next, the results were contoured to show the spatial distribution of the electrical conductivity and illustrated in Figure 3.2.2.

Step 6: Create a Grid of Conditional Probability Estimates

The disjunctive kriging estimator can also be used to determine the conditional probability that the unknown value is greater than a specified cutoff value. An example of this is given in Fig. 3.2.3 where the conditional probability that the ln[EC] is greater than ln(4.0), respectively is contoured.

From this figure one can see that the zones of high probability coincide with areas of high ln[EC]. Although the shapes of the high probability zones are similar to the shapes of the ln[EC] contours in Fig. 3.2.2, two points with the same estimated value of ln[EC] do not always produce the same conditional probability. For more information see Yates et. al. (1986)

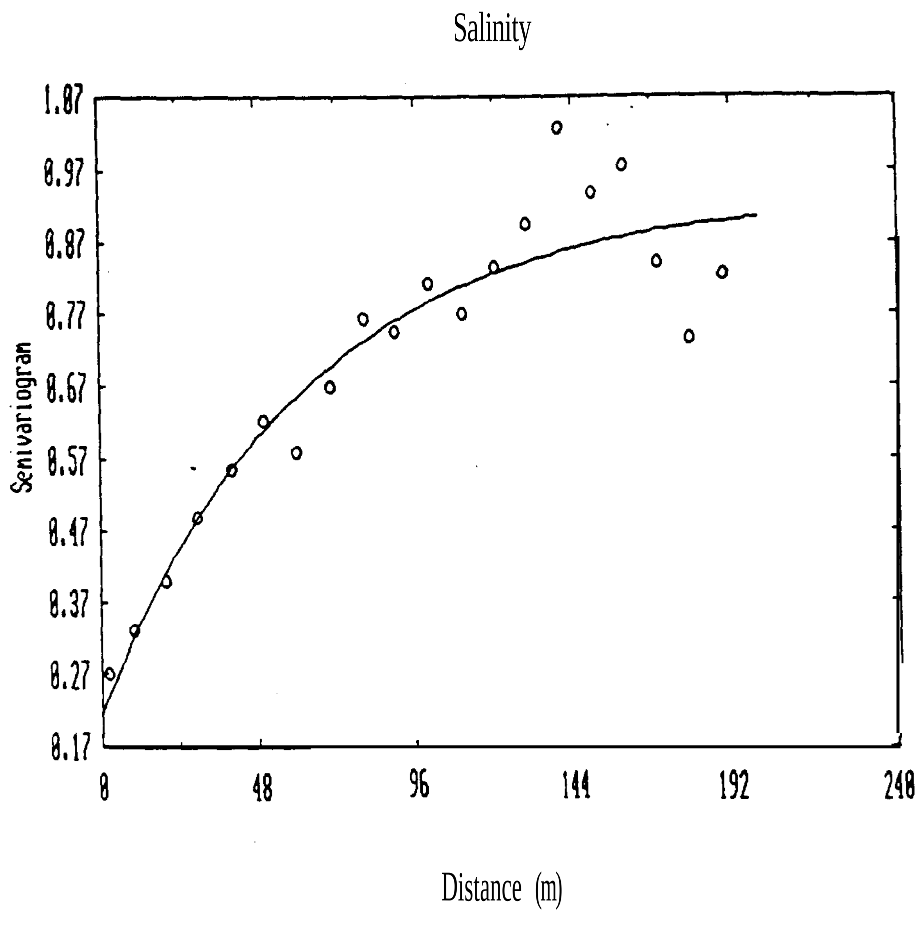


Figure 3.2.1. The semivariogram function for the natural logarithm of the electrical conductivity using the Variogram Calculation (Sample) program and the data set, ECSAR.DAT.

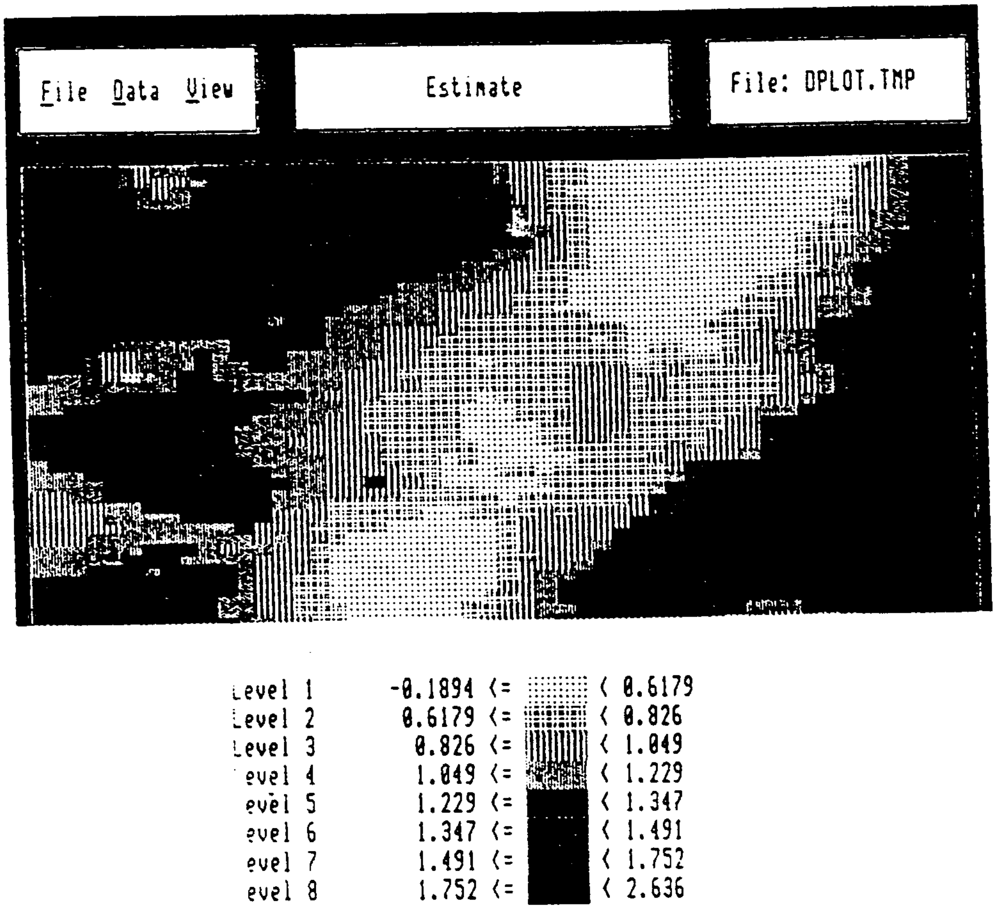


Figure 3.2.2. Contour diagram of the estimated value of the electrical conductivity using the Disjunctive [Co]Kriging and Block Contour Diagram programs.

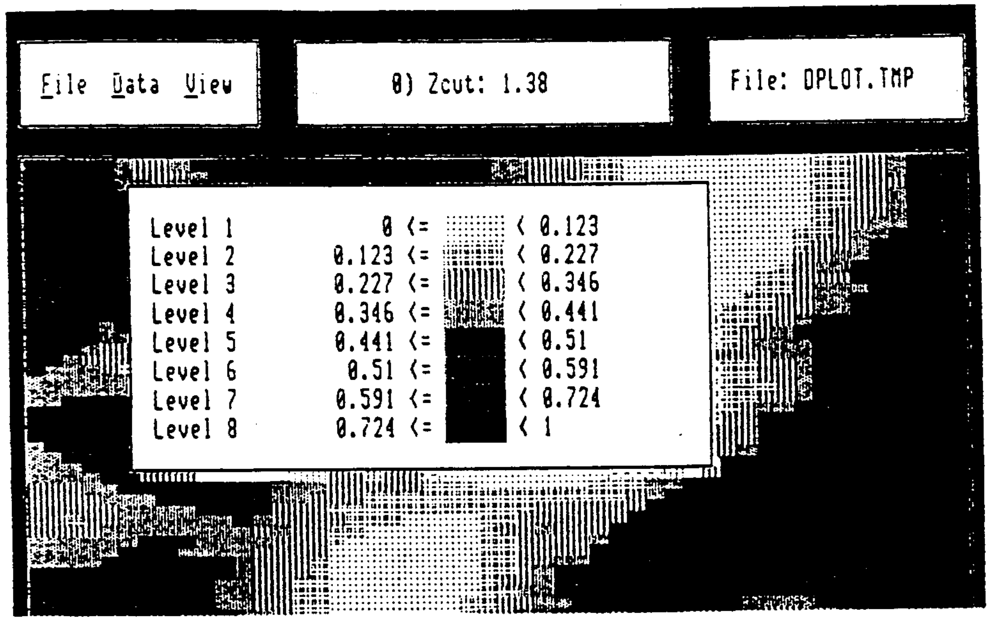


Figure 3.2.3. Contour diagram of the conditional probability that the estimated value of the electrical conductivity is greater than the natural logarithm of 4 dS/m (i.e., 1.38 log(dS/m)) using the Disjunctive [Co]Kriging and Block Contour Diagram programs. This figure shows the actual screen position of the contour levels window when displayed.

3.3. SURFACE MOISTURE, TEMPERATURE AND SOIL TEXTURE.

Description of Data

This data set contains three random functions, the surface moisture content, (θ), the surface soil temperature (T) and the sand content of the surface 1 cm. The moisture content and sand content data were collected at 71 random locations and the temperature data at 120 random locations on a lm by lm grid system in a 1 ha field at the Campbell Agricultural Center of the University of Arizona. A more detailed description of the data and techniques used to measure the EC and SAR is given in Yates and Warrick (1988). This data set is included in the Available Data Sets option (Type: F5, followed by A) and is named C912.DAT.

Step 1: Determining the Variogram

As with all kriging methods some measure of the spatial correlation structure is necessary. For cokriging a spatial correlation function is required for each random function as well a cross-correlation function for each pair of random functions to be included in the analysis. Since ordinary kriging is to be performed it is only necessary that the random functions be intrinsic (i.e., it is no longer required that the variance be finite).

GEOPACK is used to determine the sample semivariogram by following the sequence given in Example 1. Next a model variogram is applied to the sample semivariogram. For this example, the automatic fitting procedure is used and yields the following exponential models

y(h) = 0.00 + 34.2 (1 · exp[-h/8.78]); for surface moisture

γ(h) = 0.00 · 18.4 (1 · exp[-h/10.8]); for cross-semivariogram

γ(h) = 2.86 + 15.6 (1 · exp[-h/4.71]); for surface temperature

for h > 0 and are shown in Figures 3.3.1 and 3.3.2. The overall reduced mean and variance for this set of variograms is -0.0091 and 0.92, respectively.

This variogram model was used in the cross validation procedure listed on the Ordinary [Co]Kriging **Menu** which attempts to fit both the sample semi-variogram and the reduced mean and variance simultaneously. Since only one model can be cross-validated at a time the following method was used. First the semivariogram for the surface moisture was cross-validated. This was followed by cross-validating the surface temperature model. Assuming that these semi-variograms were not affected by the cross-validation of the cross-semivariogram, they were fixed during the cross-validation of the cross-semivariogram. Using this Cross Validation procedure the following variogram models

γ(h) = 0.00 + 34.0 (1 · exp[-h/8.23]); for surface moisture

y(h) = 0.00 · 18.3 (1 · exp[-h/10.3]); for cross-semivariogram

γ(h) = 4.19 + 14.3 (1 · exp[-h/5.121); for surface temperature for h > 0 were calculated. The overall reduced mean and variance for this set of variograms is -0.0068 and 0.88, respectively. Plots of the model variograms and the sample variograms are shown in the Figures. Viewing the cross-validated variogram models using the **Save** Model(s), Fit Models Manually option on the Variogram Menu indicates that either set of variogram models would be adequate representations of the spatial correlation structure.

Step 2: Create a Grid of Estimates Using CoKriging

A total of 2500 estimates of the surface moisture content were obtained on a 2 by 2 meter grid system superimposed over the CAC field site using cokriging. (the auxiliary variable was the surface temperature). Along with each estimate a value of the kriging variance was calculated. Shown in Fig. 3.3.3 is a block contour diagram of the cokriging estimates and definition of the color/pattern used in the diagram. For this example a maximum of 5 nearest neighbors of the moisture and temperature within a radius of 20 m from the estimation site was used in the estimation process. Shown in Figure 3.3.4 is the associated estimation variance for the soil moisture using the cokriging technique.

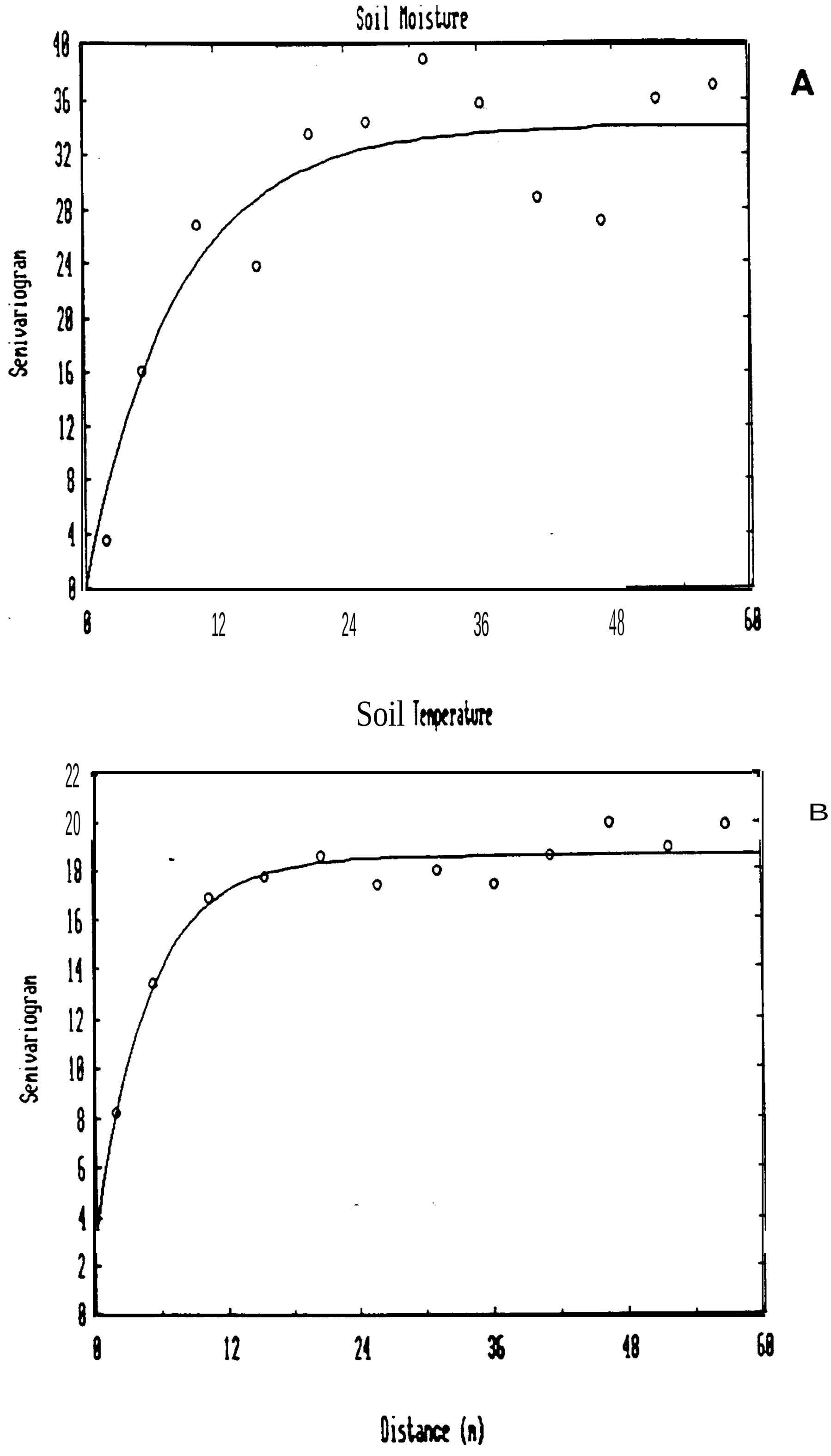


Figure 3.3.1. The semivariogram function for the surface moisture content (in A) and the surface soil temperature (in B) using the Variogram Calculation (Sample) program and the data set, C912.DAT.

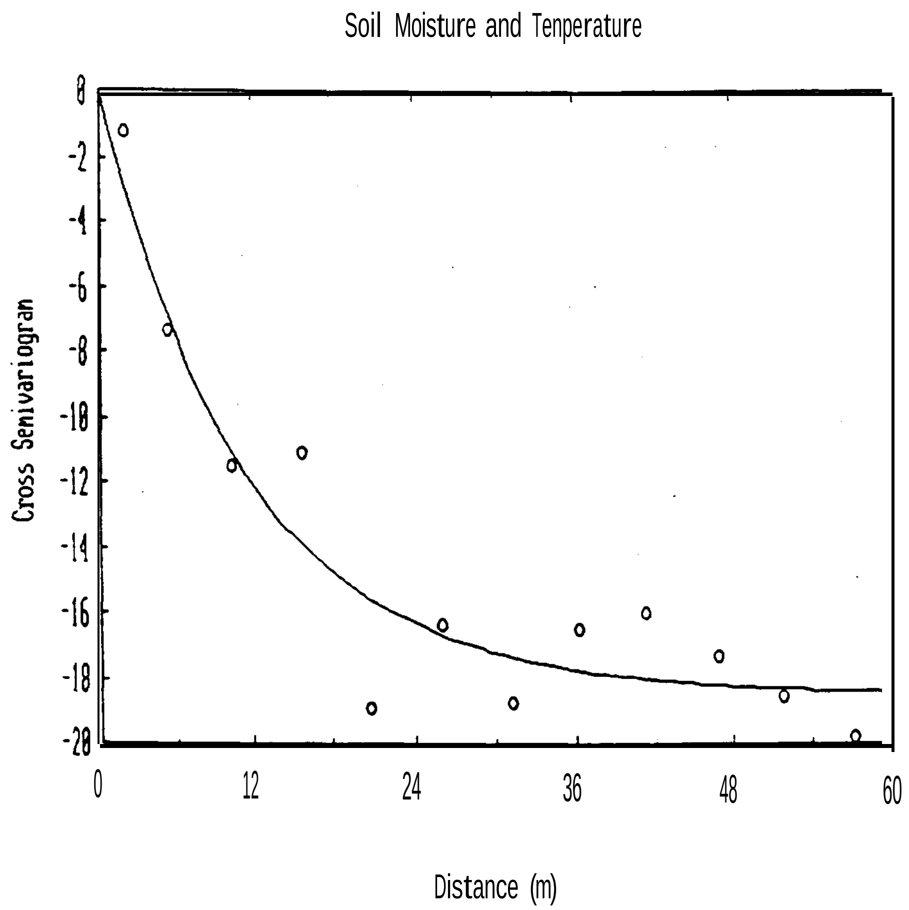


Figure 3.3.2. The cross-semivariogram function for the surface moisture content and the surface soil temperature using the Variogram Calculation (Sample) program and the data set, C912.DAT.

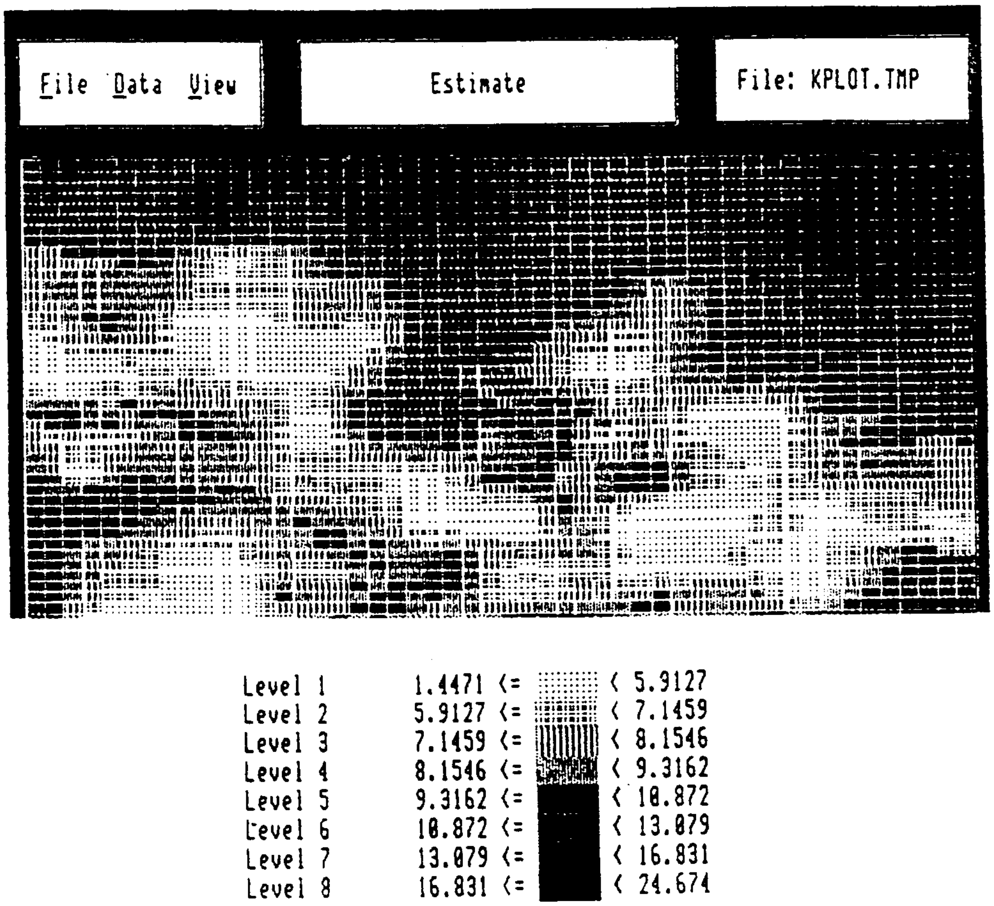


Figure 3.3.3. Contour diagram of the estimated value of the electrical conductivity using the Ordinary [Co]Kriging and Block Contour Diagram programs.

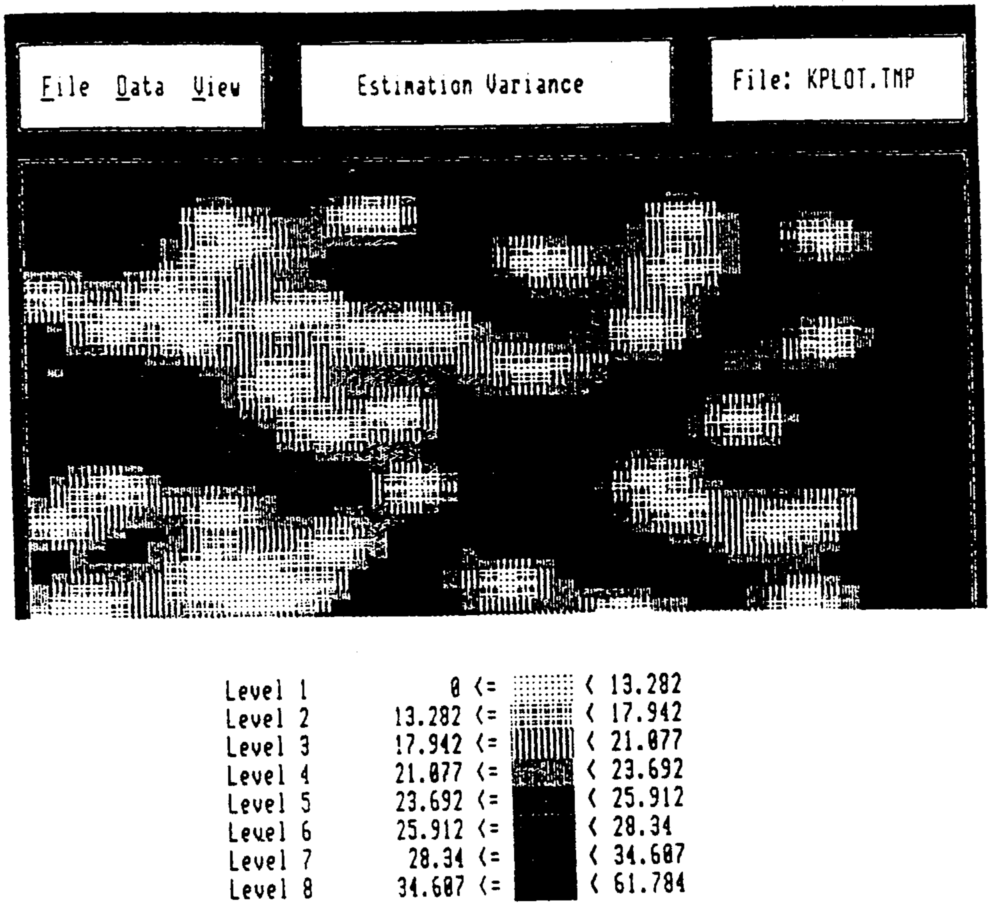


Figure 3.3.4. Contour diagram of the estimation variance for electrical conductivity using the Ordinary [Co]Kriging and Block Contour Diagram programs.

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