STATISTICAL INVERSE MODELING AND GEOSTATISTICAL
ANALYSIS OF THE AVRA VALLEY AQUIFER

by

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STATEMENT BY AUTHOR

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ABSTRACT

Avra Valley is a deep, elongate alluvial basin in southern Arizona, which contains an extensive unconfined aquifer. This aquifer was modeled by using a statistical inverse model. The input data required by the inverse model are (1) spatially averaged log-transmissivity estimates in zones of the aquifer, (2) steady-state hydraulic head estimates at points in the aquifer, and (3) the covariance matrices of log-transmissivity and hydraulic-head estimation errors. The geostatistical interpolation technique of kriging was used to assign the spatially averaged log-transmissivities and to compute the covariance matrix of the log-transmissivity estimation errors. Estimates of the steady-state hydraulic heads were made by interpolating between known data points. Two independent determinations of the covariance matrix of the hydraulic-head estimation errors were made. The output from the inverse model is a modified set of spatially averaged log-transmissivities and the covariance matrix of their associated estimation errors. The magnitude of the estimation errors of this modified set of log-transmissivities is less than the magnitude of the estimation errors of the kriged log-transmissivities. A conditional simulation analysis was also performed to assess the magnitude of errors in the hydraulic heads predicted by the kriged log-transmissivity field and the log-transmissivity field computed by the inverse model.
INTRODUCTION

Many computer programs exist today that use numerical methods to calculate the hydraulic head distribution of an aquifer given knowledge of the aquifer parameters (transmissivity and storage coefficient), pumping rates, and boundary conditions. These programs have also been used to solve the inverse problem of ground-water hydrology for the purpose of building a model of the aquifer, i.e., as parameter estimation tools. In this latter role, the transmissivity and storage coefficient of the aquifer model are adjusted to reproduce a known hydraulic-head map for given pumping rates and boundary conditions. Calibration is generally completed for a steady-state period of the aquifer's history and then verified against another known period of the historical record (Freeze and Cherry, 1979). Steady-state calibration is a tedious procedure, which is frustrated by the fact that the solution to the inverse problem may be non-unique (Cooley, 1977, 1979; Neuman, 1973, 1975, 1980; Yakowitz and Duckstein, 1980). Such an aquifer model is purely deterministic and yields no information about the accuracy of the solution.

Stochastic aquifer modeling offers a promising alternative to ad hoc trial-and-error calibration. In contrast to a deterministic model the input of a stochastic model is considered uncertain, and hence the output must be described in probabilistic terms (Daellenbach and George, 1978).
Neuman and Yakowitz (1979) have developed a stochastic, steady-state ground-water model that will solve the inverse problem without resorting to trial-and-error calibration. Some modifications to this model have subsequently been made by Neuman (1980). The modified version of the model takes initial estimates of log-transmissivity and hydraulic head together with the covariance matrices of their estimation errors, then computes revised log-transmissivity and head estimates by minimizing a composite generalized least-squares regression criterion. The accuracy of the revised log-transmissivity and head estimates can be assessed by examining statistics computed by the model. Log-transmissivity rather than transmissivity is used by the model because the latter is a log-normally distributed quantity (Davis, 1969). The model uses a finite-element numerical scheme to solve the ground-water flow equation, and this requires discretizing the flow domain with a finite-element mesh. Thus log-transmissivities are spatially averaged over the elements or groups of elements called zones, and hydraulic heads are defined at the nodes of the mesh. The input data for the model basically comprises the initial estimates of log-transmissivity and hydraulic head, plus their estimation error covariance matrices.

This thesis will use the model of Neuman (1980) to build a stochastic ground-water model of the aquifer in Avra Valley, a deep, elongate alluvial basin in southern Arizona (Figure 1). The boundary of the study area was placed to coincide closely with the boundary of a previous model of the Avra Valley aquifer by Moosburner (1972). Some parts of the extreme north and south of the aquifer were excluded from the present modeling study because of a scarcity of data in these
Figure 1. Location and physiographic setting of Avra Valley, Pima County, Arizona, and study area boundary
areas. The geostatistical interpolation technique of kriging will be used to assign the initial estimates of spatially averaged log-transmissivity to the zones of the finite-element mesh covering the Avra Valley aquifer. Kriging has the advantage of yielding unbiased estimates with a minimum estimation error variance, as well as the covariance matrix of the estimation errors. The initial estimates of hydraulic head at the nodes of the mesh will be interpolated from a hand-drawn hydraulic-head contour map. Details of the determination of the hydraulic head estimation error covariance matrix will be discussed in a later section.

Of additional interest is the magnitude of the errors of the hydraulic heads predicted by the kriged log-transmissivity field and the revised log-transmissivity field computed by the inverse model of Neuman (1980). These errors will be assessed by calculating the variance of a large number of hydraulic head surfaces conditionally simulated from each log-transmissivity field. The objective of the simulation analysis is to evaluate the ability of the inverse model to reduce the uncertainty in the predicted hydraulic heads.
SETTING OF AVRA VALLEY

Avra Valley is an elongate north-trending alluvial basin in the Basin and Range physiographic province of south-central Arizona (Figure 1). The basin is about 30 miles long and ranges between 6 and 12 miles in width. It is bounded on the southeastern, eastern, and northeastern sides by the Sierrita, Tucson, and Torolita Mountains, respectively, and on the western side by the Roskruge, Waterman, and Silverbell Mountains. These mountains rise about 2,000 feet (ft) above the valley floor. Avra Valley is contiguous with Altar Valley to the southwest and with the Lower Santa Cruz Basin to the north. It merges with the Tucson Basin to the northeast across a narrow neck of land locally known as the Rillito Narrows.

The surface of Avra Valley slopes gently northwards at an average gradient of 20 ft/mile between the elevations of 2,500 and 1,800 ft above mean sea level. Surface gradients steepen and trend basinwards on the bajadas adjacent to the mountain flanks. Two major intermittent watercourses cross the surface of the basin (Figure 1). The Santa Cruz River flows northwesterly through the Rillito Narrows across northern Avra Valley where its channel is well defined but broad in places. Brawley Wash flows northwards from Altar Valley where it has a well-defined channel but quickly becomes braided and spreads to more than a mile in width. Farther north the braiding ceases and from this point the stream is called the Los Robles Wash before joining with the Santa Cruz River. Many small channels are incised into the bajadas.
on the valley flanks, but they become poorly defined as the surface gradient decreases toward the center of the basin, and few reach the main drainage channels.

Creosote bush is the dominant species of vegetation in Avra Valley. Riparian species such as mesquite, cottonwood, and saltcedar flourish close to the watercourses. Paloverde and varieties of cacti dominate the slightly higher elevations of the bajadas and mountain slopes (Turner, 1974).

Climate

Climatic data are available for the Arizona Sonora Desert Museum (Figure 1) in central Avra Valley (Sellers and Hill, 1974). Avra Valley is in a very arid climate zone and experiences extreme summer heat and low annual precipitation. Mean monthly temperatures range between 50°F in January and 90°F in July, and summer maxima may exceed 110°F. The average annual rainfall is 9\frac{1}{2} inches. Short-duration, high-intensity summer thunderstorms account for 40 percent of the rainfall. The winter rains are less intense and of longer duration and result from frontal systems moving inland from the Pacific Ocean. Average annual class A pan evaporation is 100 inches at The University of Arizona in Tucson, 12 miles east of the Desert Museum.

Geology

Avra Valley is an alluvial-filled graben flanked by mountains and is similar in structure to many of the valleys of the Basin and Range province. The geology of the mountains has been documented by Cooper (1960), Bikerman (1968), Bikerman and Damon (1966), Heindl
(1965), and Mayo (1968). The basin fill has been studied by Allen (n.d.), Eberly and Stanley (1978), Halpenny and Green (1965), Heidi and White (1965), and Whallon (n.d.).

Mountain Ranges

The mountain ranges are composed principally of Mesozoic and Tertiary volcanic rocks. Potassium-argon age dating of volcanic rocks from the Tucson Mountains has indicated that the igneous activity occurred during two time periods: Late Cretaceous-early Tertiary and mid-Tertiary (late Oligocene and Miocene) (Bikerman and Damon, 1966). Paleozoic sedimentary rocks crop out in many of the ranges, and the Sierrita and Silverbell Mountains are comprised partly of Precambrian granite.

Basin Fill

Avra Valley contains a Cenozoic basin fill composed mainly of alluvium, plus small amounts of evaporitic and volcanic rocks. Residual gravity surveys indicate that the basin is divided into two sub-basins by a saddle between the Roskruge and Tucson Mountains (Oppenheimer and Sumner, 1980; West, 1970). The northern sub-basin is the deepest and contains more than 9,500 ft of basin fill, whereas the southern sub-basin attains a maximum depth of about 2,500 ft (Figure 2). The stratigraphic sequence is best known in the upper 1,300 ft of the section because of the numerous water wells in the valley. Two exploratory oil wells have been drilled to depths of 3,200 and 4,600 ft in the northern Avra Valley (Eberly and Stanley, 1978).
Figure 2. Contour map of depth to bedrock in feet below land surface. -- After Oppenheimer and Sumner (1980)
Major deposition of alluvium began in the early Paleocene and continued until the late Oligocene when widespread volcanic activity commenced (the mid-Tertiary orogeny). This volcanic activity persisted until the mid-Miocene and was followed by the development of an extensive unconformity surface. Between 12 and 13 million years ago, an important regional block-faulting episode caused the deep central graben that subsequently became the depositional basin for the remainder of the Cenozoic. The stratigraphic framework of Eberly and Stanley (1978) places all formations deposited prior to the block faulting into a Unit I and all subsequent formations into a Unit II. Unit I is known only in one of the oil exploration wells, but its widespread occurrence in Avra Valley has been inferred from regional Basin and Range stratigraphy. Allen (n.d.) has correlated some of the facies in Unit II with the formations from the adjacent Tucson Basin named by Davidson (1973).

Allen (n.d.) has described three sedimentary units from water wells and shallow stratigraphic test holes in Avra Valley: (1) surficial deposits, (2) younger alluvium, and (3) older alluvium. The existence of these units is inferred from stratigraphic and geophysical well logs, but the nature of the contacts between them is not known. The surficial deposits form a thin (estimated 30 ft) sheet of buff-red, sandy silt and sandy clay that blankets most of the basin. Their hydrological significance lies in their ability to inhibit ground-water recharge. The younger alluvium is a northward-thickening sheet of heterogeneous sediment between 200 and 500 ft thick. It is characterized by 5- to 50-ft-thick, interlayered, coarse- and fine-grained beds. The
fine-grained beds are composed of silts and sandy silts, and the
course-grained beds are gravelly sands and sandy gravels. The older
alluvium is the principal unit of the stratigraphic sequence investigated
by Allen (n.d.). It is semi-consolidated, relatively homogeneous, and
comprises two distinct facies: one a coarse-grained facies of sandy
gravel and gravelly sand and the other a fine-grained facies of silt and
clay that is occasionally gypsiferous. All the sediment types described
by Allen belong to the Unit II of Eberly and Stanley (1978), and hence
their age is post-late Miocene.

Hydrogeology

Ground-water Occurrence

The upper 600 to 700 ft of alluvium in Avra Valley appears to
be hydraulically connected and forms a single unconfined aquifer.
There is evidence, however, of a possible confined aquifer in southern
Avra Valley below a depth of 1,100 ft (White, Matlock, and Schwalen,
1966), and confined aquifers at depths greater than 550 ft are known
from the Eloy district (Smith, 1940), 25 miles northwest of Marana
(Figure 1). Most wells in the basin pump water from the unconfined
aquifer and the role of the deeper confined aquifers in the ground-
water regime is not clear.

Ground water flows north then northwest through Avra Valley
into the Lower Santa Cruz Basin (Figure 3). The mountains that
border the valley are composed of rocks having relatively low per-
meabilities and hence form impermeable boundaries. The depth to water
Figure 3. Contour map of 1974 water table, Avra Valley. -- After Matlock and Morin (1976)
table in 1974 ranged between 250 and 400 feet below the land surface over most of the basin, but it was locally greater beneath some of the bajadas.

Ground-water Recharge

Three potential sources of natural ground-water recharge can be identified: (1) underflow from adjoining ground-water basins, (2) direct recharge from precipitation on the basin surface, and (3) recharge through stream channels after storm events. Man-made recharge from sewage effluent and irrigation return flows has become significant in recent years. This source of recharge will not be discussed, however, because the model of the aquifer to be built in this study will use water levels that were measured before it became significant.

Underflow from Adjoining Basins. Table 1 summarizes previous estimates of the ground-water underflow at the junctions between Avra Valley and its three adjoining alluvial basins. The estimates of Anderson (1972) and Moosburner (1972) were derived from electric-analog models of ground-water flow in the Tucson Basin and Avra Valley, respectively; those by Turner (1959) and Whallon (n.d.) were calculated using Darcy's law; and that by Fogg, Simpson, and Neuman (1979) was computed by a numerical model of the northern Tucson Basin aquifer.

Recharge from Precipitation. The bajadas are the most favorable areas for recharge from precipitation on the basin surface. This is because their steeper surface gradients promote basinward
Table 1. Estimated ground-water underflow through Avra Valley. -- in acre-feet per year

<table>
<thead>
<tr>
<th>Inflow</th>
<th>Outflow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Avra--Altar Rillito Narrows</td>
<td>Avra-Lower Santa Cruz Junction</td>
</tr>
<tr>
<td>17,500</td>
<td>17,900</td>
</tr>
<tr>
<td>9,000</td>
<td>13,000</td>
</tr>
<tr>
<td>14,700</td>
<td>22,000</td>
</tr>
<tr>
<td>16,600</td>
<td>34,700</td>
</tr>
</tbody>
</table>

a. Derived from 1940 water-level data.
b. Derived from 1957-58 water-level data.

transportation of fine sediments leaving the coarsest sediments behind as a lag deposit. These coarse sediments have a higher infiltration potential relative to the finer sediments deposited on the central basin floor. Another important factor limiting infiltration in the central basin is the large amount of evapotranspiration. A rainfall-runoff study from a small watershed in southeastern Arizona has shown that roughly a fifth of all the rainfall becomes surface runoff and the remainder is evapo-transpired from the watershed (Renard, 1970). Thus direct recharge from precipitation on the central basin floor of Avra Valley is considered to be negligible in comparison to recharge along the bajadas. Direct recharge along the boundary between the mountains and the bajadas is usually termed "mountain-front recharge."
Osterkamp (1973) has estimated the annual mountain-front recharge rates for the bajada segments in Avra Valley (Table 2). These estimates were based on correlations between recharge, precipitation, and drainage area computed by Anderson (1972) for the Tucson Basin and estimates of precipitation and drainage area in Avra Valley.

Table 2. Estimated mountain-front recharge to the Avra Valley aquifer. — in acre-feet per year. After Osterkamp (1973).

<table>
<thead>
<tr>
<th>Mountain-front Segments</th>
<th>Total Recharge Rate</th>
<th>Recharge Rate per Mile of Mountain Front</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tucson Mountains</td>
<td>1,000</td>
<td>50</td>
</tr>
<tr>
<td>Sierrita Mountains</td>
<td>1,200</td>
<td>120</td>
</tr>
<tr>
<td>Roskruge-Waterman-Silverbell Mountains</td>
<td>3,300</td>
<td>80</td>
</tr>
</tbody>
</table>

Recharge through Stream Channels. Keith and Rasmussen (1980) assert that stream-channel recharge is the main mechanism for recharging the ground-water basins of southern Arizona. There are two main reasons for this conclusion: (1) most streams in southern Arizona are losing, i.e., the water table lies below the channel bed, thus allowing some of the streamflow to percolate into the aquifer; and (2) the channel sediments are usually much coarser than the surface sediments covering the remainder of the basin, and hence have a higher infiltration potential.

Because streamflow is intermittent, recharge events cause pulselike water-level changes in wells close to the channel. Recharge
mounds are often built beneath channels within a few days of the runoff events, even when the depth to the water table is greater than 150 feet (Keith and Rasmussen, 1980). These mounds are usually short-lived, however, and to be detected the water levels in observation wells must be frequently monitored (e.g., Briggs and Werho, 1966; Renard, 1970).

The proportion of stream flow that becomes stream-channel recharge depends on many factors that are peculiar to both the runoff event and the morphology and geology of the channel. Keith and Rasmussen (1980) have concluded that most stream-channel recharge originates from streamflows generated by winter rains or the snowmelt of spring. Summer thunderstorms cause streamflows with large suspended sediment concentrations and occur when the evapotranspiration rate is very high, and hence are considered to be relatively ineffective sources of recharge. Much of the runoff that infiltrates the channel during any season may be transpired if dense stands of phreatophytes line the channel.

Roughly 45 miles of major stream channels cross the surface of Avra Valley. These channels are dry for most of the year and streamflow occurs only after summer or winter rains. The average annual discharge of the Santa Cruz River is 22,600 acre-ft for 26 years of records from the Cortaro gaging station, 5 miles southeast of the Rillito Narrows (U.S. Geological Survey, 1969). No continuous discharge records are available for the Brawley or Los Robles Washes. Their watersheds, however, are roughly a third the area of the Santa Cruz River's watershed, thus their average discharge is likely to be relatively small.
Table 3 summarizes estimates of the annual stream-channel recharge to the Avra Valley aquifer. These estimates were determined by Osterkamp (1973) from correlations between the gaged streamflows in Avra Valley and streamflow-infiltration ratios from the Tucson Basin. Because no detailed studies of stream-channel recharge have as yet been completed in Avra Valley, these figures must be considered as being only approximate. Despite the great uncertainty in the estimates of stream-channel recharge, the total amount of recharge from this source is likely to be small. Moosburner (1972) did not even require any stream-channel recharge to calibrate an electric-analog model of the Avra Valley aquifer.

Table 3. Estimated stream-channel recharge to the Avra Valley aquifer. -- in acre-feet per year. After Osterkamp (1973).

<table>
<thead>
<tr>
<th>Stream</th>
<th>Total Recharge Rate</th>
<th>Recharge Rate per Mile of Stream Channel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Santa Cruz River</td>
<td>9,000</td>
<td>450</td>
</tr>
<tr>
<td>Brawley Wash</td>
<td>2,400</td>
<td>125</td>
</tr>
<tr>
<td>Los Robles Wash</td>
<td>1,100</td>
<td>45</td>
</tr>
</tbody>
</table>

History of Ground-water Development

Cattle ranching was the major activity in Avra Valley prior to 1940. The ranchers relied on widely spaced wells pumped by windmills or low-capacity turbines for their water supply (Andrews, 1937). Crop irrigation was first practiced in the Marana area in the early 1920s. Irrigation water was imported from the adjacent Tucson Basin until 1937
when six irrigation wells were drilled to augment this supply. These wells were estimated to have pumped 10,000 acre-ft of water in 1940 (White et al., 1966). The amount of irrigated acreage increased greatly after World War II, and the pace of development reached a maximum in the early 1950s. By 1954 more than 100 wells were being pumped to irrigate about 30,000 acres of land (White et al., 1966).

Avra Valley was declared a critical ground-water area in 1954 under the Arizona Revised Statutes §§45-313C and 45-314A. The purpose of this declaration was to halt the expansion of irrigated acreage. No new wells could be drilled, but existing wells were allowed to be replaced or deepened. Since then the annual rate of ground-water pumpage has increased slowly partly due to double cropping practices (White et al., 1966).

In the early 1970s the City of Tucson began purchasing and retiring some of the Avra Valley farmlands to develop well fields to supplement Tucson's municipal water supply. In the last decade these wells pumped and transported roughly 8,000 acre-ft of water annually to Tucson (Whallon, n.d.).

During the post-World War II years the rate of ground-water pumping has far exceeded the recharge rate, and the net effect has been a marked lowering of the water table. The maximum decline since 1940 is about 150 feet in the Marana area (Figure 4).

**Previous and Current Investigations**

Avra Valley contains a large alluvial aquifer from which ground water has been pumped for many years. Andrews (1937) reported on
Figure 4. Contour map of the change in ground-water elevation between 1940 and 1978. -- After Whallon (n.d.).
the early land use and occurrence of ground water in the basin; Smith (1938, 1940) described the physiography, hydrogeology, and ground-water potential of an area covering part of northern Avra Valley and constructed a ground-water elevation map using 1910 water-level measurements; Turner (1958, 1959) assessed the ground-water potential of small areas in Avra Valley; Halpenny and Green (1965) and Heindl and White (1965) analyzed hydrogeologic data from a few test holes in the basin; White et al. (1966) synthesized many data and reported on the post-1940 impacts of ground-water development; Moosburner (1972) built an electric-analog model of the ground-water flow system; Osterkamp (1973) computed recharge rates to the aquifer by infiltration of water along stream channels and bajadas; Brown (1976) calculated a water budget for the basin in the early 1970s; Matlock and Morin (1976) assessed the post-1952 changes in the ground-water regime with an emphasis on post-1965 changes; Wicke (1978) examined the feasibility of recharging the aquifer with Santa Cruz River flood water; and Whallon (n.d.) discussed the hydrogeology of the basin. Of interest to this thesis is a finite-difference ground-water model currently being constructed by personnel of the U.S. Geological Survey in Tucson, Arizona.
STOCHASTIC INVERSE MODEL

This study is concerned with two-dimensional, steady-state flow in a heterogeneous, isotropic aquifer for which the ground-water flow equation inside a region $R$ is written

$$\nabla \cdot (T \nabla h) - q = 0$$  \hspace{0.5cm} (1)

subject to the boundary conditions:

$$h(x) = H(x) \quad \text{on } \Gamma_1$$  \hspace{0.5cm} (2)

$$- (T \nabla h) \cdot n = Q(x) \quad \text{on } \Gamma_2$$  \hspace{0.5cm} (3)

In these equations, $\Gamma$ is the boundary of $R$; $\nabla$ is the two-dimensional vector differential operator; $T$ is the aquifer transmissivity; $h$ is the hydraulic head; $q$ is the volumetric flux rate per unit area of $R$, the unit area being oriented normal to $\Gamma$ and parallel to the direction of the flow; $x$ is the position vector; $n$ is a unit vector normal to $\Gamma$ and directed away from $R$; $H$ is the prescribed head on $\Gamma_1$ (a Dirichlet boundary condition); $Q$ is the volumetric outflow rate per unit length of and normal to $\Gamma_2$ (a Neumann boundary condition); and $\Gamma_1$ and $\Gamma_2$ are segments of $\Gamma$. All notations used in this thesis are listed in Appendix A.

The Inverse Problem

If $T$, $Q$, and all boundary conditions are specified in equations (1) to (3), the boundary value problem is well posed and a stable and unique solution for hydraulic head is assured (Bear, 1979). In contrast,
the inverse problem seeks a solution for transmissivity given knowledge of \( h \), \( q \), and the boundary condition, and this problem is seldom well posed. The ill-posed nature of the inverse problem arises from two main causes. First, \( h \) and \( q \) are rarely independent input parameters; boundary fluxes, for example, are often calculated from Darcy's law, which requires knowing both the hydraulic head and transmissivity (Bear, 1979). Once a solution to the inverse problem is found, any scalar multiple of the computed transmissivity field will produce exactly the same hydraulic-head map, but with different computed flux rates. Second, the computed transmissivities are very sensitive to errors in hydraulic-head measurements (Neuman, 1973, 1980). The reason for this high sensitivity is that hydraulic head appears in the governing equation as a derivative and errors in the derivates of uncertain data may be very large.

The stochastic inverse model of Neuman (1980) will compute a revised transmissivity field for an aquifer given an initial estimate of this field. The computed transmissivity field will reproduce a given steady-state hydraulic-head map within known error tolerances. This model has the advantage of utilizing prior statistical information about both the hydraulic head and transmissivity fields. The objective of applying the model is to compute a transmissivity field that has less uncertainty than the initially estimated transmissivity field. This is achieved by conditioning the initially estimated transmissivity field on the steady-state hydraulic heads. Much of the following discussion describing the theory of the stochastic inverse model is derived from Neuman (1980), Neuman, Fogg, and Jacobson (1980), and Neuman and Yakowitz (1979).
Parameter Estimation Theory

Application of a finite-element numerical scheme to equation (1) yields the matrix equation

\[ A \mathbf{h} = Q \]  

where \( A \) is a \( N \times N \) square matrix, and \( \mathbf{h} \) and \( Q \) are \( N \)-component column vectors, \( N \) being the number of nodal points in the finite-element mesh. The mesh to be used is composed of a network of linear triangular elements, \( e \) (Figure 5). After applying the Galerkin method, the components of \( A \) are given by (Narashimhan, Neuman, and Witherspoon, 1978)

\[ A_{nm} = \sum_{j} \frac{T_{j}}{4\Delta_{j}} (b_{j} n m + c_{j} n m) V_{n \neq m} \]  

(5)

\[ A_{nn} = - \sum_{m \neq n} A_{nm} \]  

(6)

where the summations are taken over all elements \( j \) containing the \( n \)th node, \( n \) and \( m \) being designated by a global numbering scheme. Let the nodes of the \( j \)th element be labeled locally as \( k = 1, 2, \) and \( 3 \), (Figure 5), and let the coordinates of node \( k \) be given by \( (x_{k}, y_{k}) \), then the terms in equation (5) are

\[ b_{1} = y_{2} - y_{3} \]
\[ b_{2} = y_{3} - y_{1} \]
\[ b_{3} = y_{1} - y_{2} \]
\[ c_{1} = x_{3} - x_{2} \]
\[ c_{2} = x_{1} - x_{3} \]
\[ c_{3} = x_{2} - x_{1} \]  

(7)

and

\[ \Delta_{j} = \frac{1}{2} (b_{1} c_{2} - b_{2} c_{1}) \]  

(8)
Figure 5. Parts of a typical interior (A) and boundary (B) of a finite-element mesh
The parameter $T_j$ in equation (5) is an effective, uniform transmissivity assigned to the $j$th element, and this can be computed in different ways depending on how the transmissivity is assumed to vary inside each element. Neuman (n.d.) has concluded that if the hydraulic gradient in a two-dimensional flow field is uniform, the aquifer can be represented by an equivalent uniform porous medium whose transmissivity is the geometric mean of the measured transmissivities, provided that the latter are log-normally distributed. Statistical analyses have shown that hydraulic conductivity (and hence transmissivity) is a log-normally distributed random variable (Davis, 1969; Delhomme, 1979; Freeze, 1975). Thus, if the finite-element mesh is divided into zones within which the hydraulic gradient does not vary much, the effective transmissivity of each zone can be computed by taking the geometric mean of the measured (or interpolated) transmissivities in that zone. Let the mesh be divided into $L$ zones, $R_1$, such that each zone contains one or more triangular elements, $j$, then

$$T_j = T_{1} \cap \bigcup_{j \in R_1}$$, \hspace{1cm} 1 = 1, 2, 3, \ldots, L \hspace{1cm} (9)$$

Substitution of equations (5) and (6) into equation (4) yields

$$\sum_{m \neq n} A_{nm} (h_m - h_n) = Q_n, n = 1, 2, \ldots, N \hspace{1cm} (10)$$

where $h_k$ is the hydraulic head at the $k$th nodal point. The $n$th component of $Q, Q_n$, is the flux rate assigned to node $n$. This flux rate represents the net effect of all sources and sinks acting in the vicinity of the $n$th node, and these may be of three types: (1) lateral flux across the boundary segment, $\Gamma_n$, of the finite-element mesh (Figure 5B), (2) net
vertical recharge or discharge, including leakage, in the exclusive sub-region $S_n$ of the $n$th node, which comprises one-third of each triangular element bordering on $n$ (Figure 5), and (3) a portion of the pumping rate of each well inside the elements adjacent to $n$.

The next step in the formulation of the model is to examine the effects of data and modeling errors on equation (10). Let $h^*$ and $Q^*$ be measures or estimates of the exact (unknown) hydraulic head and flux vectors $h$ and $Q$. These vectors are related as follows:

\begin{align}
  h^* &= h + \varepsilon \\
  Q^* &= Q + \mu
\end{align}

where $\varepsilon$ and $\mu$ are $N$-dimensional error vectors. In addition to these data errors, use of the finite-element method results in a modeling error because by discretizing equation (1) the transmissivity, hydraulic head, and flux are no longer treated as continuous functions of space. This modeling error can be accommodated by adding an $N$-dimensional error vector $\eta$ to equation (4) to give

\begin{equation}
  \Delta h^* = Q + \eta
\end{equation}

Substituting equations (11) and (12) into equation (13) then yields:

\begin{equation}
  \Delta h^* - Q^* = \Delta \varepsilon - \mu + \eta
\end{equation}

Neuman (1980) has demonstrated that $\varepsilon$ can have a harmful effect on the calculation of transmissivity, but the effects of $\mu$ and $\eta$ may often be neglected, at least for nodes in the interior of the finite-element mesh. If node $n$ lies on the mesh boundary and $Q^*_n$ cannot be
accurately estimated, \( n \) can be treated as a constant-head boundary node and then \( Q^*_n \) calculated after computing the transmissivities using the inverse method. By disregarding \( \mu \) and \( \bar{n} \) and premultiplying each term by \( A^{-1} \), equation (14) simplifies to

\[
\bar{h}^* - A^{-1} Q^* = \varepsilon
\]

where \( \varepsilon \) is assumed to have a mean and covariance, respectively, of

\[
E(\varepsilon) = 0 \quad (16)
\]

\[
\text{var}(\varepsilon) = c_h^2 \text{var}_h \quad (17)
\]

Because transmissivities are assumed to be log-normally distributed, it is preferable from a statistical standpoint to work with the logarithmic transformation of \( T, Y \), where

\[
Y = \log_{10} T \quad (18)
\]

and

\[
Y^{-1} = 10^Y = T \quad (19)
\]

Equation (5) implies that

\[
A = \Delta(T) = \Delta(Y) \quad (20)
\]

where \( T \) and \( Y \) are vectors of transmissivity and log-transmissivity, respectively, for the \( L \) zones of the finite-element mesh. Thus equation (15) can be rewritten as

\[
\bar{h}^* - A^{-1}(Y) Q^* = \varepsilon \quad (21)
\]
Equations (17) and (21) can now be used to compute the transmissivity field of the aquifer. Let $\hat{Y}$ be the estimate of $Y$, the true (unknown) vector of log-transmissivities, then $\hat{Y}$ can be computed by means of the generalized nonlinear least-squares regression criterion:

$$J_1(\hat{Y}) = \frac{1}{\sigma_h^2} (h^* - \hat{h})^T \sum^{-1}_n (h^* - \hat{h})$$  \hspace{1cm} (22)

where

$$\hat{h} = A^{-1}(\hat{Y}) Q^*$$  \hspace{1cm} (23)

is the vector of computed hydraulic heads. The sum-of-squares in equation (22) could well be minimized nearly to zero, implying that the computed transmissivity vector $\hat{Y}$ will reproduce almost exactly the estimated hydraulic head vector $h^*$. Although this is an appealing prospect, the computed transmissivity field may be incongruent with transmissivities determined from aquifer tests or specific capacity measurements. To overcome this problem, prior estimates of the transmissivities are included in the model by minimizing the composite regression criterion

$$J_3(\hat{Y}) = J_1(\hat{Y}) + J_2(\hat{Y})^T \sum^{-1}_Y (Y^* - \hat{Y})$$  \hspace{1cm} (24)

where

$$J_2(\hat{Y}) = \frac{1}{\sigma_Y^2} (Y^* - \hat{Y})$$  \hspace{1cm} (25)

is a criterion of parameter plausibility. In equation (25), $Y^*$ is the vector of estimated log-transmissivities for the L zones of the finite-element mesh and is related to the vector of true (unknown) log-transmissivities $\hat{Y}$ by
\[ \mathbf{Y}^* = \mathbf{Y} + \mathbf{v} \]  
\[ \text{(26)} \]

where \( \mathbf{v} \) is an \( L \)-dimensional error vector whose mean and covariance are, respectively:

\[ E(\mathbf{v}) = \mathbf{0} \]  
\[ \text{Var}(\mathbf{v}) = \sigma^2_{\mathbf{v}} \mathbf{V}_\mathbf{v} \]  
\[ \text{(27)} \]
\[ \text{(28)} \]

Equation (24) can be rewritten as

\[ J(\hat{\mathbf{Y}}) = J_h(\hat{\mathbf{Y}}) + \frac{\sigma_h^2}{\sigma_Y^2} J_Y(\hat{\mathbf{Y}}) \]  
\[ \text{(29)} \]

where

\[ J_h(\hat{\mathbf{Y}}) = \sigma^2_h J_1(\hat{\mathbf{Y}}) \]  
\[ J_Y(\hat{\mathbf{Y}}) = \sigma^2_Y J_2(\hat{\mathbf{Y}}) \]  
\[ \text{(30)} \]
\[ \text{(31)} \]

Equation (29) is the mathematical model of Neuman (1980) and Neuman and Yakowitz (1979). Details of the solution algorithm are discussed by Neuman (1980).

In equation (29), \( \mathbf{V}_h \) and \( \mathbf{V}_Y \) are known, symmetric, and positive-definite matrices. The parameters \( \sigma_h^2 \) and \( \sigma_Y^2 \) may or may not be known. If one or both are unknown, the multiplier \( \sigma_h^2/\sigma_Y^2 \) is replaced by a non-negative scalar \( \lambda \), whose magnitude is allowed to vary so that a family of solutions of computed log-transmissivities, \( \hat{\mathbf{Y}} \), can be generated. If \( \lambda \) is very large, \( \hat{\mathbf{Y}} \) will be close to the initial log-transmissivity estimates \( \mathbf{Y}^* \) but the computed hydraulic heads, \( \hat{\mathbf{h}} \), may be incongruent with the initial head estimates, \( \mathbf{h}^* \). Minimizing equation (29) with a value of \( \lambda \) close to zero is equivalent to minimizing equation (22), which is not desirable.
The optimal value of $\lambda$, $\lambda_{\text{opt}}$, lies somewhere between these two extremes, and procedures to select this value are detailed in Neuman (1980). Some of these will be discussed later.

Estimation Error Analysis

After equation (29) has been minimized, the estimation errors of both the computed log-transmissivities and hydraulic heads can be examined by using a linearized error analysis (Schweppe, 1973, p. 368). Define

$$e_y = \hat{y} - \underline{y}$$

$$e_h = \hat{h} - \underline{h}$$

as the error vectors of log-transmissivity and hydraulic head, respectively. If $e_y$ and $e_h$ are sufficiently small, then $h$ can be approximated by the linear part of its Taylor series expansion about $\underline{y}$, which is

$$h \approx \hat{h}(\underline{y}) + Z(\underline{y} - \underline{y})$$

where $Z$ is the $N \times L$ Jacobian or sensitivity matrix

$$Z = \frac{\partial h}{\partial \underline{y}} \bigg|_{\underline{y} = \underline{y}}$$

Combining equations (11) and (34) yields

$$h^* - \hat{h}(\underline{y}) + Z\hat{y} = Z\hat{y} + \epsilon$$

By using this result together with equations (16), (17), and (26) to (28), the linear model

$$W = XY + \zeta$$

can be defined where $W$ is the $(N+L)$ column vector
\[ W = \begin{bmatrix}
  h^* - \hat{h}(\hat{Y}) + Z \hat{Y} \\
  Y^*
\end{bmatrix} \]  

(38)

\[ X = \begin{bmatrix}
  Z \\
  I
\end{bmatrix} \]  

(39)

\[ \xi = \begin{bmatrix}
  \xi \\
  \nu
\end{bmatrix} \]  

(40)

which has a mean and covariance, respectively, of

\[ E(\xi) = 0 \]  

(41)

\[ Var(\xi) = \sigma_h^2 \begin{bmatrix}
  V \xi_h & 0 \\
  0 & V \xi_Y
\end{bmatrix} \]  

(42)

The vector of true log-transmissivities, \( \underline{Y} \), and now be estimated by minimizing the linear regression criterion

\[ J_L(\hat{Y}_L) = (W - X \hat{Y}_L)^T V^{-1}(W - X \hat{Y}_L) \]  

(43)

where \( \hat{Y}_L \) represents the computed estimates of \( Y \) that correspond to the linear model of equation (37). (Note that \( \hat{Y}_L \) may differ from \( \underline{Y} \), the estimated log-transmissivities computed by minimizing equation (29).) From linear regression theory (Seber, 1977, p. 61) it follows that

\[ E(e_Y) = 0 \]  

(44)
\[ \text{and} \]
\[ \mathbb{V}(e_Y) = \sigma_h^2 (\lambda_X^T V_{\xi}^{-1} \lambda_Y)^{-1} \]
\[ = \sigma_h^2 (Z_h^T V_{\xi}^{-1} Z_h + \rho_h^2 V_{\xi}^{-1})^{-1} \]  \hspace{1cm} (45)

Equation (34) can be rewritten as
\[ \hat{h}(Y) - h = Z_e (Y - Y) \]
\[ = Z_e Y \]  \hspace{1cm} (46)

and thus follows that
\[ E(e_h) = 0 \]  \hspace{1cm} (47)

and
\[ \mathbb{V}(e_h) = E[(Z_e Y)(Z_e Y)^T] \]
\[ = E[(Z_e Y) e_Y^T Z_e] \]
\[ = Z_e \mathbb{V}(e_Y) Z_e^T \]  \hspace{1cm} (48)

In equation (45), the multiplier \( \sigma_h^2 / \sigma_Y^2 \) may be replaced by \( \lambda_{\text{opt}} \), the optimal value of \( \lambda \), and if \( \sigma_h^2 \) is unknown, its best estimate is given by (Beck and Arnold, 1977, p. 379)
\[ s^2 = [(h^* - \hat{h})^T V_h^{-1} (h^* - \hat{h})] / N \]  \hspace{1cm} (49)

where \( s^2 \) is evaluated at \( \lambda_{\text{opt}} \).

The components of the correlation matrix of the log-transmissivity estimations errors, \( \mathbb{S} \), can be computed from equation (45) by
This matrix is useful to examine the distance over which pairs of log-transmissivity estimation errors are correlated and to see if the correlation structure is directionally dependent. Log-transmissivity estimation errors generally have a marked anisotropic correlation structure (Neuman, 1980; Neuman et al., 1980). A particular value of transmissivity will uniquely determine other values of transmissivity that lie along the same streamline but will not affect the transmissivities lying off the streamline, i.e., the transmissivity field determined by the inverse model is a solution to a boundary-value problem of the Cauchy type (Neuman, 1973). This characteristic manifests itself in the sensitivity matrix of equation (35), because hydraulic heads are most sensitive to those transmissivities that lie along the same streamline. It then follows from equation (45) that the correlation between pairs of log-transmissivity estimation errors should be greatest along streamlines and least along equipotentials, the matrices $V_h$ and $V_\Theta$ do not have correlation structures that dominate the calculation of $V(e_Y)$.

Hydraulic-head Residual Analysis

The vector of the hydraulic-head weighted residuals

$$ z_h = H_h^{-1} (h^* - \hat{h}) $$  \hspace{1cm} (51)

where $H_h$ is an $N \times N$ upper triangular matrix that satisfies

$$ V_h = H_h^T H_h $$  \hspace{1cm} (52)
should ideally have a mean close to zero if the solution computed by minimizing equation (29) is optimal (Draper and Smith, 1966; Seber, 1977). The sample variance of the weighted head residuals, \( R_v \), is defined as

\[
R_v = \frac{1}{N-1} \sum_{i=1}^{N} [(z_{h^i}) - \bar{z}_h]^2
\]

(53)

where \( \bar{z}_h \) is the mean of the weighted residuals. If \( \bar{z}_h = 0 \), then

\[
R_v = s^2
\]

(54)

where \( s^2 \) is defined in equation (49).

**Required Input Data**

Essentially five pieces of input data are required before minimizing equation (29): (1) \( Y^* \), the vector of prior estimates of log-transmissivities for the \( L \) zones of the finite-element mesh; (2) \( h^* \), the vector of prior estimates of hydraulic heads for the \( N \) nodes of the mesh; (3) \( V(\varepsilon) \), the covariance matrix of the estimation errors of \( h^* \); and (5) specified boundary conditions, either constant head or constant flux.

The geostatistical interpolation technique of kriging will be used to compute the zonal log-transmissivity estimates and their corresponding estimation error covariance matrix for the mesh superimposed on the Avra Valley aquifer. Those parts of the theory of kriging that are relevant to this study will be discussed in the next chapter. The following chapter will discuss the actual preparation of the transmissivity and hydraulic-head data from Avra Valley for the inverse model.
KRIGING THEORY

Kriging is a linear interpolation technique that is based on the geostatistical theory of Matheron (1971). Geostatistics is an evolving discipline that was developed primarily for use in the mining industry, but its usefulness in other sectors of the earth sciences is becoming increasingly apparent. The object of kriging can be simply stated as follows: Given a set of values of a function at known sampling points in space (or time), determine the best estimates of the values of this function at points or regions in space (or time) where samples are lacking. To be "best," the estimator must satisfy two criteria: (1) it must be statistically unbiased and (2) the variance of the error of estimation must be minimal.

Geostatistics is a subject about which books have been written. The following general discussion is a collection of the salient points of geostatistical theory pertinent to kriging log-transmissivities. Much of the discussion is derived from the texts by David (1977) and Journel and Huijbregts (1978).

Definitions

Regionalized variable (ReV): a variable that is distributed in space (e.g., transmissivity, log-transmissivity, hydraulic head). No statistical connotation is implied by this definition.

Random variable (RV): a function that assigns a value to the result (realization) of a trial. The values an RV may assume are determined by a probability distribution (Hines and Montomgery, 1980).
Random function (RF): A particular set of values of an ReV whose components can be considered as realizations of an RV. In general, the components of an RF are dependent. Let \( Z(x) \) be an RV in space, then for every set of \( k \) points there exists a \( k \)-component random function vector

\[
\{Z(x_1), Z(x_2), \ldots, Z(x_k)\}
\]

that comprises the realizations of \( Z(x) \). The first-order moment (the expectation) of \( Z(x) \) may be a function of position and is written

\[
E[Z(x)] = m(x)
\] (55)

Three second-order moments of \( Z(x) \) are of interest: (1) the variance, (2) the covariance, and (3) the variogram. The variance of \( Z(x) \) is the second-order moment about \( m(x) \) defined as

\[
\text{Var} [Z(x)] = E\{[Z(x) - m(x)]^2\}
\] (56)

The covariance between two RVs, \( Z(x_1) \) and \( Z(x_2) \) is

\[
C(x_1, x_2) = E\{[Z(x_1) - m(x_1)][Z(x_2) - m(x_2)]\}
\] (57)

The variogram is defined as the variance of the increment \([Z(x_1) - Z(x_2)]\) and is written

\[
2\gamma(x_1, x_2) = \text{Var} [Z(x_1) - Z(x_2)]
\] (58)

The function \( \gamma(x_1, x_2) \) is called the semi-variogram.

Strict stationarity: A property possessed by an RF (or RV) when its probability density function is invariant under translation.
Second-order stationarity: a property possessed by an RF when
(1) its expectation exists and is independent of position, i.e.,
\[ E[Z(x)] = m \quad \forall x \] (59)
and (2) for each pair of RVs \( Z(x) \) and \( Z(x + s) \), where \( s \) is a displace-
ment vector, the covariance exists and depends only on \( s \), i.e.,
\[ C(s) = E[Z(x + s) \cdot Z(x)] - m^2 \quad \forall x \] (60)
Implicit in the second-order stationary assumption is the existence of the
variance, i.e.,
\[ \text{Var}[Z(x)] = E\{[Z(x) - m]^2\} \]
\[ = C(0) \quad \forall x \] (61)
and hence
\[ \gamma(s) = \frac{1}{2}E\{[Z(x + s) - Z(x)]^2\} \]
\[ = C(0) - C(s) \quad \forall x \] (62)

Intrinsic hypothesis: A hypothesis that applies to an RF whose
(1) expectation exists and is independent of position, i.e.,
\[ E[Z(x)] = m \quad \forall x \] (63)
and (2) incremental value \([Z(x + s) - Z(x)]\), where \( s \) is a displace-
ment vector, has a finite variance that is independent of position, i.e.,
\[ \text{Var} [Z(x + s) - Z(x)] = E\{[Z(x + s) - Z(x)]^2\} \]
\[ = 2\gamma(s) \] (64)
The intrinsic hypothesis is weaker than the hypothesis of second-order
stationarity because an intrinsic random function need not have a variance or a covariance. Second-order stationarity implies the intrinsic hypothesis, but the converse is not true.

**Quasi-stationary random function:** an RF for which the stationary or second-order stationary hypothesis is valid only in limited neighborhoods, the union of which composes the domain being studied. A quasi-intrinsic RF is defined in a similar way.

**Data support:** the volume \( v(x) \), centered on the point \( x \), of the sample for which a value of the RV of interest is assigned. Let \( Z(x) \) be a pointwise continuous RV in space. The averaged quantity \( Z_v(x) \) defined as

\[
Z_v(x) = \frac{1}{v(x)} \int_{v(x)} Z(y) \, dy
\]

is called the "regularization" of \( Z(x) \) over the volume \( v(x) \). If the RF \( Z(x) \) is second-order stationary, it follows that any regularized RF \( Z_v(x) \) is also second-order stationary (Journel and Huijbregts, 1978, p. 77).

The size of the supports for which a given set of data are defined are important because they affect the variance of the data set. Increasing the size of the supports implies that the data will be regularized over a larger volume. This effectively screens extreme values of the data from the calculation of the variance of the data set. Thus, the variance of the data set is inversely related to the size of the supports for which the data are defined (Journel and Huijbregts, 1978, p. 67).
Development of the Kriging Equations

Let \( Z(x) \) be a second-order stationary RF for which there are \( N \) observations (data) \( \hat{Z}_V(x_i), i=1, 2, \ldots, N, \) defined on equal supports \( V. \) Each observation \( \hat{Z}_V(x_i) \) may have an associated measurement error \( e(x_i) \) and is related to the true value of the regularized RF at \( x_i, Z_v(x_i) \) through

\[
\hat{Z}_V(x_i) = Z_v(x_i) + e(x_i)
\]  

The measurement errors \( e(x_i) \) are assumed to be (Delhomme, 1974): (1) unsystematic, i.e.,

\[
E[e(x_i)] = 0 \quad \forall x_i
\]  

(2) uncorrelated with each other, i.e.,

\[
C[e(x_i), e(x_j)] = 0 \quad \forall x_i, x_j
\]  

and (3) not correlated with the RF \( Z(x), \) i.e.,

\[
C[e(x_i), Z(x_j)] = 0 \quad \forall x_i, x_j
\]  

Kriging will be used to estimate the mean value \( Z_v(x_o) \) of the pointwise continuous RF \( Z(x) \) over the support \( V(x_o), \) where

\[
Z_v(x_o) = \frac{1}{V(x_o)} \int_{V(x_o)} Z(y) \, dy
\]  

In general, the support being kriged, \( V(x_o), \) is either larger or equal to the support for which the data are defined, \( V. \)

The kriging estimator \( Z_k(x_o) \) of \( Z_v(x_o) \) comprises a linear combination of the \( N \) observations \( \hat{Z}_V(x_i), \) i.e.,
\[ Z^*_K(x_0) = \sum_{i=1}^{N} \alpha_i \hat{Z}_V(x_i) \]  
(71)

The kriging weights, \( \alpha_i \), are calculated to ensure that \( Z^*_K(x_0) \) is an unbiased estimate of \( Z_V(x_0) \) and that the variance of the error of estimation is minimal.

For \( Z^*_K(x_0) \) to be an unbiased estimate of \( Z_V(x_0) \), the expectation of the estimation error \( \delta(x_0) \) defined as

\[ \delta(x_0) = Z^*_K(x_0) - Z_V(x_0) \]  
(72)

must be zero. To guarantee this, it is sufficient to impose the condition:

\[ \sum_{i=1}^{N} \alpha_i = 1 \]  
(73)

thus

\[ E[Z^*_K(x_0)] = E\{ \sum_{i=1}^{N} \alpha_i \hat{Z}_V(x_i) \} = m \sum_{i=1}^{N} \alpha_i \]

\[ = m \sum_{i=1}^{N} \alpha_i = m \]  
(74)

and because the RF \( Z(x) \) is assumed to be second-order stationary

\[ E[Z_V(x_0)] = m \]  
(75)

therefore

\[ E[\delta(x_0)] = 0 \]  
(76)

The variance of the estimation error is
\[
\text{Var} \left\{ \delta (x_0) \right\} = E \left\{ [Z_{R \{x_0\}} - Z_{V \{x_0\}}]^2 \right\}
\]
\[
= E \left\{ \sum_{i=1}^{N} \alpha_i (Z_{V \{x_i\}} - e(x_i)) - Z_{V \{x_0\}} \right\}^2
\]
\[
= E \left\{ \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j Z_{V \{x_i\}} Z_{V \{x_j\}} + 2 \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j Z_{V \{x_i\}} e(x_j)
\right. \\
\left. - 2 \sum_{i=1}^{N} \alpha_i Z_{V \{x_i\}} Z_{V \{x_0\}} + \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j e(x_i) e(x_j)
\right\}
\]
\[
- 2 \sum_{i=1}^{N} \alpha_i e(x_i) Z_{V \{x_0\}} + [Z_{V \{x_0\}}]^2
\]
(77)

By using the linearity of the expectation operator and the assumed properties of the measurement errors in equations (67) to (69), the second and fifth terms in equation (77) will be identically zero. The fourth term in this equation becomes

\[
\sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j E \left\{ e(x_i) e(x_j) \right\} = \sum_{i=1}^{N} \alpha_i^2 \sigma_i^2
\]
(78)

because

\[
E \left\{ e(x_i) e(x_j) \right\} = 0 \quad \forall i \neq j
\]
(79)
\[
= \sigma_i^2 \quad \forall j = i
\]
(80)

where \( \sigma_i^2 \) is the variance of the measurement error of the observation \( \hat{Z}_{V \{x_i\}} \). The three remaining terms in equation (77) can be expanded and simplified as follows:

\[
\sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j E \left\{ Z_{V \{x_i\}} Z_{V \{x_j\}} \right\} = \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j \frac{1}{2} \int \int_{V \times V} Z_{V \{x\}} Z_{V \{y\}} dy \]
\[
= \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j \tilde{C}(x_i, x_j) + m^2
\]
(81)
\[
\sum_{i=1}^{N} \alpha_i \mathbb{E}\{Z_{V}(x_i) Z_{V}(x_o)\} = \sum_{i=1}^{N} \alpha_i \frac{1}{V^2} \int_{V} dx \int_{V} Z_{V}(x) Z_{V}(y) dy
\]
\[
= \sum_{i=1}^{N} \alpha_i \bar{C}(x_i, V) + m^2
\]  

(82)

\[
\mathbb{E}\{[Z_{V}(x_o)]^2\} = \frac{1}{V^2} \int_{V} dx \int_{V} Z_{V}(x) Z_{V}(y) dy
\]
\[
= \bar{C}(V, V) + m^2
\]  

(83)

(The notation \(\bar{C}(a, b)\) denotes the mean value of the covariance function between the two supports \(a\) and \(b\).) Equation (77) can be rewritten as

\[
\text{Var}\{\delta(x_o)\} = \bar{C}(V, V) + \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j \bar{C}(x_i, x_j) - 2 \sum_{i=1}^{N} \alpha_i \bar{C}(x_i, V)
\]
\[
+ \sum_{i=1}^{N} \alpha_i^2 \sigma_i^2
\]  

(84)

An optimal set of the \(\alpha_i\) - s is obtained by minimizing equation (84) with respect to the \(\alpha_i\) - s, subject to the constraint of equation (73). This is achieved by using the technique of Lagrange multipliers. The result is a system of \((N+1)\) simultaneous equations called the "kriging system"

\[
\sum_{j=1}^{N} \alpha_j \bar{C}(x_i, x_j) + \alpha_i \sigma_i^2 - \mu = \bar{C}(x_i, V) \quad i = 1, 2, \ldots, N
\]  

(85)

\[
\sum_{j=1}^{N} \alpha_j = 1
\]

where \(\mu\) is the Lagrangian multiplier. The variance of the estimation error can be evaluated by multiplying each term in the first \(N\) of these
equations by $\alpha_i$, summing over $i = 1, 2, \ldots, N$ to obtain
\begin{equation}
\sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j \overline{C}(x_i, x_j) + \sum_{i=1}^{N} \alpha_i^2 \sigma_i^2 - \mu = \sum_{i=1}^{N} \alpha_i \overline{C}(x_i, V)
\end{equation}
(86)
and substituting this result into equation (84) to yield
\begin{equation}
\text{Var}[\delta(x_o)] = \overline{C}(V, V) - \sum_{i=1}^{N} \alpha_i \overline{C}(x_i, V) + \mu = \sigma_K^2(x_o)
\end{equation}
(87)
where $\sigma_K(x_o)$ is called the "kriging error." Note that it is not necessary to use all the data in the domain being studied to apply equation (85). In some cases, it may be preferable to limit the number of data used to evaluate the kriging system by selecting only those data in the close neighborhood of the support being kriged.

Equation (85) can be written in matrix form as
\begin{equation}
K \beta = c
\end{equation}
(88)
where $K$ is an $(N+1) \times (N+1)$ symmetrical matrix with components
\begin{align*}
K_{ij} &= C(0) + \sigma_i^2 \\
&= C(x_i, x_j) = K_{ji} \\
&= 1 \\
&= 0
\end{align*}
for $i = j = N + 1$
\begin{align*}
\forall j &= i; i = 1, 2, \ldots, N \\
\forall i &\neq j; i, j = 1, 2, \ldots, N
\end{align*}
and $\beta$ and $c$ are column vectors of order $(N+1)$ with components
\begin{align*}
\beta_i &= \alpha_i \\
&= -\mu
\end{align*}
for $i = 1, 2, \ldots, N$ and $i = N + 1$.
\[ c_i = \bar{c}(x_i, V) \quad V \quad i = 1, 2, \ldots, N \]

\[ = 1 \quad i = N + 1 \]

There is a unique solution to equation (88) if and only if \( K \) is non-singular. To ensure this, it is sufficient that the covariance function, \( C \), be positive definite and that no two data supports \( v(x_i) \) and \( v(x_j) \) coincide.

**Kriging-error Covariance Matrix Calculation**

The covariance matrix of the kriging errors can be computed after all the desired supports have been kriged. Let \( \delta^1 \) and \( \delta^2 \) be a pair of estimation errors associated with the kriged estimates of the RF \( Z(x) \) on the supports \( V^1 \) and \( V^2 \), respectively. The covariance between \( \delta^1 \) and \( \delta^2 \) is given by

\[
\text{Cov}\{\delta^1, \delta^2\} = E\{\delta^1 \delta^2\} \quad (89)
\]

because these estimation errors are unbiased (equation (76)). Equation (89) can be expanded as follows:

\[
E\{\delta^1 \delta^2\} = E\{[\sum_{i=1}^{N} \alpha_i^1 Z_V^1(x_i) + e^1(x_i)] - Z_V^1(x) \} [\sum_{j=1}^{N} \alpha_j^2 Z_V^2(x_j) + e^2(x_j)]
\]

\[
+ e^2(x_i) - Z_V^2(x) \}
\]

\[
= E\{\sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i^1 \alpha_j^2 Z_V^1(x_i) Z_V^2(x_j) + \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i^1 \alpha_j^2 Z_V^1(x_i) e^2(x_j)
\]

\[
+ \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i^1 \alpha_j^2 e^1(x_i) Z_V^2(x_j) + \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i^1 \alpha_j^2 e^1(x_i) e^2(x_j)
\]

\[
- \sum_{i=1}^{N} \alpha_i^2 Z_V^1(x_i) Z_V^2(x) - \sum_{j=1}^{N} \alpha_j^2 Z_V^2(x_j) Z_V^1(x) \}
\]
where the superscripts 1 and 2 denote the quantities associated with kriging the supports $V^1$ and $V^2$, respectively. Using the linearity of the expectation operator and equations (67) to (69) and (78), equation (90) simplifies to

\[
\text{Cov}\{\delta^1, \delta^2\} = \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i^1 \alpha_j^2 \bar{C}(x_i, x_j) - \sum_{i=1}^{N} \alpha_i^2 \bar{C}(x_i, V^2) - \sum_{j=1}^{N} \alpha_j^2 \bar{C}(x_j, V^1) + \bar{C}(V^1, V^2)
\]

(91)

The supports $V^1$ and $V^2$ used in equation (91) may or may not be disjoint. If $V^1 = V^2$, the fourth term in equation (90) is non-zero and is equal to the result in equation (78). Equation (91) will then degenerate (as expected) to equation (87). The components of the kriging-error correlation matrix, $S$, can be computed from the kriging-error covariance matrix by

\[
S_{ij} = \frac{\text{Cov}\{\delta_i, \delta_j\}}{\sigma_K(x_i) \sigma_K(x_j)} \quad V i, j = 1, 2, \ldots, M
\]

(92)

where $M$ is the number of supports that were kriged. This matrix is useful to examine the correlation structure of the kriging errors. It follows from equation (91) that the kriging-error correlation structure will be isotropic and homogeneous only if (1) the data are defined on equal supports and distributed on a regular grid, (2) all supports to be kriged are the same size and shape and are kriged using the same configuration of
data points, and (3) the semi-variogram is isotropic, i.e., it is directionally invariant.

Kriging under the Intrinsic Hypothesis

If the RF $Z(x)$ can only satisfy the intrinsic hypothesis in the domain being studied, the kriging system (equation (85)) can be rewritten in terms of the semi-variogram function $\gamma(x)$ by using the relation in equation (62) as follows:

$$
\sum_{j=1}^{N} \alpha_i \gamma(x_i, x_j) - \alpha_i \sigma_i^2 + \mu = \gamma(x_i, V) \quad i = 1, 2, \ldots, N
$$

(93)

$$
\sum_{j=1}^{N} \alpha_j = 1
$$

The variance of the kriging error becomes

$$
c_k^2(x_0) = \sum_{i=1}^{N} \alpha_i \gamma(x_i, V) - \gamma(V, V) + \mu
$$

(94)

and the covariance between the kriging errors is

$$
\text{Cov}\{\delta^1, \delta^2\} = -\sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j \gamma(x_i, x_j) + \sum_{i=1}^{N} \alpha_i^2 \gamma(x_i, V^2) + \sum_{j=1}^{N} \alpha_j^2 \gamma(x_j, V^1) - \gamma(V^1, V^2)
$$

(95)

Mechanics of Kriging

The following procedures are required in order to apply the kriging system of equations: (1) calculate the sample semi-variogram, (2) fit a model to the sample semi-variogram, (3) verify the semi-variogram model, and (4) select a kriging plan.
Sample Semi-variogram Calculation

Certain components of the kriging system are calculated with the covariance function $C$ of the RF $Z(x)$, or alternatively, if only the intrinsic hypothesis can be inferred, the semi-variogram function $\gamma$. To determine these functions it is necessary to first compute the sample semi-variogram, $\hat{\gamma}$, defined as

$$\hat{\gamma}(r) = \frac{1}{2M} \sum_{i=1}^{M} [Z_v(x_i + s) - Z_v(x_i)]^2$$

(96)

where $M$ is the number of data pairs separated by the distance $r = |s|$. Because sampling patterns are rarely regular, $\hat{\gamma}(r)$ is usually evaluated from samples lying in the interval $r \pm b/2$, where $b$ is a specified tolerance. In practice, sample semi-variograms are calculated for different direction classes of the vector $s$ to assess whether the RF $Z(x)$ is statistically anisotropic, i.e., to see if the variability is directionally dependent. Techniques for handling anisotropic RFs are discussed by Journel and Huijbregts (1978, p. 175-183).

Important features a sample semi-variogram may have are (1) a sill, (2) a range, and (3) a nugget effect (Figure 6). For large distances, a sample semi-variogram may stabilize at a constant value called the sill. Any RF whose sample semi-variogram has a sill is second-order stationary. The absence of a sill implies the mean of the RF is not constant within the domain being studied, and such an RF is said to possess "drift." For example, a parabolic sample semi-variogram results from an RF whose mean is a linear function with finite non-zero gradient. The distance at which the sill is first reached is called the range of the sample semi-variogram.
Figure 6. Characteristic features of a sample semi-variogram
By definition

\[ \gamma(0) = 0 \]  

(97)

but many sample semi-variograms appear to trend toward a finite positive value at \( r = 0 \). This discontinuity is called a nugget effect. The nugget effect is caused by measurement errors and by large micro-variations in the RF that cannot be detected with the chosen size of the sample support. In the extreme case when the components of the RF are not correlated (i.e. they are purely random), the sample semi-variogram is horizontal with a coinciding sill and nugget effect equal in value to the variance of the RF.

Sample Semi-variogram Modeling

The next step is to fit a model to the sample semi-variogram. This model then becomes the semi-variogram function of the RF \( Z(x) \). If necessary, the covariance function, \( C \), can be evaluated using equation (62), providing RF is stationary or second-order stationary.

Only certain functions qualify for use as semi-variogram models. A semi-variogram must be a conditionally positive definite function in order to ensure that the variance of any increment of the RF being studied is non-negative. Consider a linear combination, \( R \), of the RF \( Z(x) \), where

\[ R = \sum_{i=1}^{K} a_i Z(x_i) \]  

(98)

for any weights \( a_i \), and for any number of data \( K \). This linear combination is a random variable and must therefore have a non-negative variance, where
\[ \text{Var}[R] = \text{Var}[\sum_{i=1}^{K} a_i Z(x_i)] \]

\[ = \sum_{i=1}^{K} \sum_{j=1}^{K} a_i a_j C(x_i, x_j) \quad (99) \]

Thus the covariance function, \( C \), must guarantee that \( \text{Var}[R] \geq 0 \). A function that satisfies this requirement is, by definition, positive definite. Equation (99) can be rewritten in terms of the semi-variogram function by using the relation in equation (62) as follows:

\[ \text{Var}[R] = C(0) \sum_{i=1}^{K} \sum_{j=1}^{K} a_i a_j - \sum_{i=1}^{K} \sum_{j=1}^{K} a_i a_j \gamma(x_i, x_j) \quad (100) \]

If the RF \( Z(x) \) can only satisfy the intrinsic hypothesis, which implies that \( C(0) \) does not exist, \( \text{Var}[R] \) is defined only when the condition

\[ \sum_{i=1}^{K} a_i = 0 \quad (101) \]

is met, and hence

\[ \text{Var}[R] = - \sum_{i=1}^{K} \sum_{j=1}^{K} a_i a_j \gamma(x_i, x_j) \quad (102) \]

Thus, in order to guarantee that \( \text{Var}[R] \geq 0 \) in this case, the semi-variogram function, \( \gamma \), is required to be conditionally positive definite, the condition being given in equation (101).

There is a large number of potential semi-variogram functions despite the conditional positive definite requirement (see Journel and Huijbregts, 1978, p. 161-171). However, only a few of these functions are generally used. Figure 7 illustrates the most commonly used semi-variogram models.
Figure 7. Commonly used semi-variogram models
Validation of the Semi-variogram Model

The selected semi-variogram model can be verified by systematically deleting each data point one at a time, then using the remaining data to estimate the deleted datum by kriging (Delhommée, 1978; Gamblati and Volpi, 1979). The true errors $[Z^*_K(x_i) - \hat{Z}_V(x_i)]$ can be examined to see if

1. They are unbiased, i.e.,

$$\frac{1}{N} \sum_{i=1}^{N} [Z^*_K(x_i) - \hat{Z}_V(x_i)] \approx 0 \quad (103)$$

2. They are consistent with the computed kriging errors, i.e.,

$$\left(\frac{1}{N} \sum_{i=1}^{N} \frac{(Z^*_K(x_i) - \hat{Z}_V(x_i))^2}{\sigma^2_K(x_i)}\right)^{\frac{1}{2}} \approx 1 \quad (104)$$

In addition, the standard deviation of the true errors defined as

$$\sigma_T = \left\{ \frac{1}{N-1} \sum_{i=1}^{N} [Z^*_K(x_i) - \hat{Z}_V(x_i)]^2 \right\}^{\frac{1}{2}} \quad (105)$$

is a measure of the accuracy of the kriging procedure and should be relatively small when compared to the standard deviation of the actual data.

Note that $\sigma_T$ should be close to the mean value of all the kriging errors if equations (103) and (104) are valid.

Selection of a Kriging Plan

David (1976) and Journel and Huijbregts (1978, p. 344-360) discussed alternative ways of efficiently applying kriging. Of prime concern before evaluating the components of the kriging system and solving the kriging equation are (1) the accuracy of the semi-variogram model.
and (2) the calculation of the mean values $\bar{\gamma}$ or $\bar{C}$, which are required for both the kriging system and the computation of the covariance matrix of the kriging errors.

Often for distances greater than about half the average dimension of the region being studied, the number of data pairs used to calculate the sample semi-variogram is insufficient to characterize the true variability of the RF. This is a good reason to employ the quasi-stationary (or quasi-intrinsic) hypothesis and use only the data within a close neighborhood of the support being kriged to evaluate the kriging system.

The mean values $\bar{\gamma}$ or $\bar{C}$ can be computed by using either numerical integration or graphs, based on "auxiliary functions," of $\bar{\gamma}$ versus some characteristic dimension of the support(s) being examined. Numerical integration is usually preferred because it is more amenable to being written into a computer program.

Transmissivity as a Random Function

Transmissivity can be considered as a random function whose values are determined primarily by the genesis of the aquifer's host formation. It is important to realize that a particular value of transmissivity, whether determined by an aquifer test or from a specific capacity measurement, is an averaged quantity with a cylindrical support whose axis is the pumping well. The shape of the support may vary slightly if the aquifer is heterogeneous or anisotropic or is being dewatered. The size of the support is a function of many variables (pumping rate, storage coefficient, etc.), but notably it is a function of time. As pumping
progresses, the cone of depression deepens and expands radially. This causes the hydraulic properties of the aquifer to become effectively averaged over an ever-increasing neighborhood until steady-state flow is reached.

**Kriging Log-transmissivities**

It is preferable to apply kriging to the logarithmic transformation of transmissivity because it is apparently a log-normally distributed quantity (Delhomme, 1978). Let \( \hat{T}_v(x_i), i = 1, 2, \ldots, N \), be a set of \( N \) transmissivity data defined on equal supports \( v \) and let the logarithmic transformation of this set be \( \hat{Y}_v(x_i) = \log_{10}[\hat{T}_v(x)] \). After these log-transmissivities have been used to krige the \( M \) support \( V(x_j), j = 1, 2, \ldots, M \), the corresponding transmissivity estimates \( T^*_V(x_j) \) and the variance of the associated estimation errors \( \sigma^2_{T^*_V(x_j)} \) can be computed from the kriged estimates \( Y^*_V(x_j) \) and the kriging errors \( \sigma_K(x_j) \) through (Hines and Montgomery, 1980)

\[
T^*_V(x_j) = \exp [2.303 \hat{Y}_V(x_j) + 0.5(2.303 \sigma_K(x_j))^2] \quad (106)
\]

and

\[
\sigma^2_{T^*_V(x_j)} = [T^*_V(x_j)]^2\{\exp [2.303 \sigma_K(x_j)]^2 - 1\} \quad (107)
\]

The coefficient of variation, defined as

\[
CV_V = \frac{\sigma_{T^*_V(x_j)}}{T^*_V(x_j)} \quad (108)
\]

is a useful statistic to examine the relative magnitudes of the transmissivity estimates and their errors of estimation. Note that exponentiation of \( Y^*_V(x_j) \) provides the estimate,
\[ T_V' (x_j) = 10 \frac{Y_V^* (x_j)}{V} = \exp[2.303 \frac{Y_V^* (x_j)}{V}] \quad (109) \]

which is strictly only a median estimate of \( T_V^* (x_j) \). However, if the kriging errors are small, it follows from equation (106) that \( T_V' (x_j) \) will be close to \( T_V^* (x_j) \).
PREPARATION OF DATA FOR THE INVERSE MODEL

Preparation of transmissivity and hydraulic head data is required before these data may be used in the inverse model of Neuman (1980) to model the Avra Valley aquifer. The following sections describe the methods used to prepare these data.

Preparation of Transmissivity Data

Prior to using the inverse model of Neuman (1980), log-transmissivities must be assigned to zones within the aquifer and the covariance matrix of the log-transmissivity estimation errors must be calculated. For a given set of transmissivity data there are two general ways to assign the zonal log-transmissivities: (1) rely solely on the hydrologist's judgment and (2) use an interpolation technique. The first approach is subjective and may be difficult to apply if there is a large variation among the transmissivities or if the data are sparsely distributed. Using an interpolation technique is a more systematic approach, but care must be exercised because physically unreasonable transmissivities may be computed. As will be demonstrated, the interpolation technique of kriging is an efficient means of assigning the zonal log-transmissivities and of computing the covariance matrix of the log-transmissivity estimation errors.

Available Data

Transmissivity data are available from 148 sites in Avra Valley (Figure 8). These data are not evenly distributed and in some areas
Figure 8. Avra Valley transmissivity data and division into northern and southern subregions.
are scarce. Some transmissivities were calculated from aquifer tests and the remainder were predicted from specific capacity measurements.

Aquifer Test Data

The City of Tucson completed 42 aquifer tests in Avra Valley between 1965 and 1977. These tests were conducted with newly drilled and existing wells to develop a well field to augment Tucson's municipal water supply. Most tests were step-drawdown tests of 4-8 hours duration followed by a 1-2-hour period of recovery, and most were completed without any water-level measurements from observation wells.

Each aquifer test was plotted on semi-logarithmic graph paper, and the recovery data were determined to be the most reliable. The drawdown-time plots of the data from the step tests were very scattered and could not be used to compute accurate values of transmissivity. Some wells even showed evidence of developing during the step tests; turbid discharges were reported and drawdown occasionally decreased with time. However, during a recovery test the velocity of ground water entering the well casing is far less than the velocities generated by a step test, and hence the recovery data are not prone to the effects of incomplete well development.

Transmissivities were computed from the recovery data by using the Theis recovery method (Kruseman and de Ridder, 1976, p. 66), and the results are tabulated in Appendix C. The effects of partial aquifer penetration or of dewatering were not considered in the analysis.
Tranmissivity-Specific Capacity Regression Analysis

Transmissivity data can be generated by utilizing the linear relationship between transmissivity and specific capacity (Walton, 1970, p. 315). Linear regression analysis was used to equate transmissivity (the dependent variable) with specific capacity (the independent variable) and to place a confidence band on the predicted transmissivities. Because log-transmissivities are required for the inverse model, the log-transformation of the data was made prior to the regression analysis. Let \( Y_i \) and \( \log_{10}(SC_i) \), \( i = 1, 2, \ldots, N \), be \( N \) pairs of log-transmissivities and log-specific capacities derived from aquifer tests. The linear relationship

\[
Y_p = b_0 + b_1 \log_{10}(SC_o)
\]

(110)

can be determined after regressing \( Y_i \) on \( \log_{10}(SC_i) \), where \( b_0 \) and \( b_1 \) are the model coefficients and \( Y_p \) is the log-transmissivity estimate predicted from the observed log-specific capacity \( \log_{10}(SC_o) \). The variance of the error of prediction is (Hines and Montgomery, 1980, p. 373)

\[
\sigma^2_Y_p = \sigma^2_Y \left[ 1 + \frac{\sum\left(\log_{10}(SC_o) - m_{LSC}\right)^2}{SS_{LSC}} \right]
\]

(111)

where

\[
m_{LSC} = \frac{1}{N} \sum_{i=1}^{N} \log_{10}(SC_i)
\]

(112)
\[
SS_{LSC} = \sum_{i=1}^{N} \left[ \log_{10}(SC_i) - m_{LSC} \right]^2
\]  
(113)

\[
\sigma_Y^2 = \frac{1}{N-2} \sum_{i=1}^{N} \left[ Y_i - (b_0 + b_1 \log_{10}(SC_i)) \right]^2
\]  
(114)

and \( \sigma_Y \) is the standard error of estimation. The 95\% confidence interval of the estimator \( Y_p \) is

\[
Y_p \pm \sigma_Y \cdot t_{0.975,N-2}
\]

where \( t_{0.975,N-2} \) is the statistic of the t distribution for \((N-2)\) degrees of freedom such that

\[
P[|t| \leq t_{0.975,N-2}] = 0.95
\]  
(115)

A quick examination of the aquifer tests from Avra Valley revealed that the specific capacity data could not be used in a meaningful regression analysis without prior adjustment. This was because the aquifer tests were performed on two groups of wells: (1) existing agricultural wells with perforated casings, which had an average well efficiency\(^1\) of 60\%, and (2) newly drilled wells that were screened but had efficiencies as low as 20\%. The low efficiencies of the latter group of wells appears to be the result of poor well development before

\(^1\)The efficiency of a pumping well is defined as the quotient of the drawdown computed when well losses are neglected and the actual drawdown (U.S. Bureau of Reclamation, 1977).
running the aquifer tests. A lower than expected efficiency implies that the specific capacity of the well is also unusually low. It is likely that after a week or so of pumping, these inefficient wells would develop further and their efficiencies would rise to between 55% and 65%, the same efficiencies as those of wells in Avra Valley that have been pumped for many years.

The following method was developed to adjust the specific capacities of the inefficient wells so their well efficiencies became 60%:

1. Use Theis's recovery method to compute a value of transmissivity from the recovery data.
2. Examine the recovery data to determine the period when \( \frac{\partial s'}{\partial (\log_{10} t')} \) is approximately constant, where \( s' \) is the residual drawdown and \( t' = (t_p + t_r)/t_r \), where \( t_p \) is the duration of pumping and \( t_r \) is the time since pumping ceased. For the Avra Valley recovery data this period usually occurred when \( t_r \) was between 10 and 60 minutes. The early recovery data were apparently affected by water draining down the pump column after the pumping unit was shut down.
3. Select a point from the segment of the recovery data isolated in step 2, noting \( s' \) and \( t' \).
4. Use Jacob's method (Kruseman and de Ridder, 1976, p. 59) to calculate \( s'' \), the drawdown at the well-aquifer interface for a period of pumping equal to \( t_r \), a pumping rate \( Q \) equal to the time-weighted arithmetic mean of the pumping rates during the step test, and a storage coefficient \( S \). Note that \( s'' \) is relatively insensitive to the particular value of \( S \), provided that \( S \) is of the correct order of magnitude. A value of \( S \) equal to 0.1 was chosen for the Avra Valley
aquifer. Note also that Jacob's method becomes valid at the well-aquifer interface after only a few seconds of pumping for the wells in the Avra Valley aquifer.

5. Estimate \( s \), the drawdown at the well-aquifer interface at time \( t_p + t_r \), assuming that the well is still pumping, by \( s = s' + s'' \).

6. Compute the specific capacity of the well assuming a well efficiency of 60% as

\[
SC = 0.6 \frac{Q}{s}
\]

(116)

More than one data point can be selected at step 3, and steps 4-6 repeated to assess the reliability of the method.

The specific capacities from 19 wells in Avra Valley were adjusted using the above procedure. This increased the number of data pairs suitable for use in the regression analysis to 37. The resulting regression equation is

\[
Y_p = 2.36 + 1.07 \log_{10}(SC_0)
\]

(117)

where specific capacity is measured in gpm/ft and transmissivity in ft²/day. The 95% confidence interval for the predicted log-transmissivity is

\[
Y_p \pm 2.03 \sigma_Y
\]

where the multiplier 2.03 is the value of \( t_{0.975,35} \) and

\[
\sigma_Y = 9.68 \times 10^{-2} \left[ 1.03 + \frac{(\log_{10}(SC_0) - 1.48)^2}{5.99} \right]^{1/2}
\]

(118)
The coefficient of determination, $R^2$, for the regression was 0.95. The data pairs, regression equation, and the 95% confidence envelope for the predicted log-transmissivities are plotted in Figure 9.

The log-transmissivities of 106 wells in Avra Valley were predicted from their log-specific capacities using equation (117). These data and the variance of the error of prediction of each log-transmissivity estimate are listed in Appendix C. The specific capacity data were taken from White et al. (1966) and Matlock and Morin (1976). Most specific capacities were derived from wells drilled by the cable-tool method and fitted with perforated casing. The specific capacities reported by White et al. (1966) were determined immediately after many of the wells were constructed. However, considering the drilling method used, these wells were probably operating close to their peak efficiencies when tested. The data of Matlock and Morin (1976) comprise pumping rates and depth-to-water measurements that were collected between 1966 and 1968. Static water levels were required to convert these data to specific capacities. These levels were estimated from water levels measured in the winter (non-pumping season) prior to the testing, which were made available by the University of Arizona Agricultural Experiment Station.

Kriging Avra Valley Log-transmissivities

The Avra Valley aquifer contains two obvious subregions with different mean values of transmissivity (Figure 8). The mean transmissivity in northern Avra Valley around the Santa Cruz River is roughly three times the mean transmissivity in southern Avra Valley.
Figure 9. Results of regressing log-transmissivity on log-specific capacity.
There is no clear reason for this difference, but the higher transmissivities in the northern subregion may be a consequence of channel-sand deposition by the Santa Cruz River. Because of the different means, transmissivity (and hence log-transmissivity) cannot be considered as a second-order stationary or intrinsic random function over the whole of Avra Valley. This is a good reason to krig the log-transmissivity fields of each subregion separately. For the kriging analysis it was necessary to place a dividing line between the two subregions, whereas, in reality, they would probably merge through a transition zone. The assumed dividing line is shown in Figure 8. The geometric means of the measured transmissivities from the northern and southern subregions are 21,500 and 7,200 ft²/day, respectively.

Sample Semi-variogram Calculation, Modeling, and Verification.

Sample semi-variograms of log-transmissivity for different direction classes in each subregion were calculated with insufficient data pairs to be considered reliable. The log-transmissivity fields of each subregion were then assumed to be isotropic for the purpose of the semi-variogram determination. A denser sampling pattern would probably invalidate this assumption because the morphology of Avra Valley implies that the sediment-size distribution in the basin is probably anisotropic.

The non-directional sample semi-variograms from both subregions are graphed in Figures 10 and 11. These were calculated using the computer code SEMIVGM, which is documented in Appendix E. Both sample semi-variograms have approximately the same nugget effect and
Figure 10. Log-transmissivity sample semi-variogram and fitted model, northern Avra Valley

\[
\gamma(r) = \begin{cases} 
0.04 + 0.03 \left[ 1.5 \left( \frac{r}{6} \right) - 0.5 \left( \frac{r}{6} \right)^3 \right] & 0 < r \leq 6 \\
0.07 & r > 6 
\end{cases}
\]
Figure 11. Log-transmissivity sample semi-variogram and fitted model, southern Avra Valley.
range, but there is a large difference in the values of their sills. The smaller sill of the northern subregion's sample semi-variogram indicates that there is less variability in the log-transmissivities from this subregion. This is further justification for kriging the subregions separately. Each sample semi-variogram was fitted with a spherical model (Figures 10 and 11). A trial-and-error procedure was used to fit the models to the sample semi-variograms, and Table 4 summarizes the results of the validation tests of the selected models.

Table 4. Log-transmissivity semi-variogram validation tests

<table>
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<th></th>
<th>Northern Subregion</th>
<th>Southern Subregion</th>
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<tbody>
<tr>
<td>Mean of true errors</td>
<td>$9.49 \times 10^{-3}$</td>
<td>$3.29 \times 10^{-3}$</td>
</tr>
<tr>
<td>True error and kriging error consistency, from Equation (104)</td>
<td>0.98</td>
<td>0.97</td>
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<tr>
<td>Standard deviation of true errors</td>
<td>$2.28 \times 10^{-1}$</td>
<td>$2.57 \times 10^{-1}$</td>
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</table>

Kriging Plan. The zonation pattern designed for the Avra Valley aquifer is illustrated in Figure 12. The maximum dimension of any zone was limited to roughly a third of the range of the semi-variograms (i.e., 2 miles). Some zones were purposely elongated, which is contrary to the assumption of statistical isotropy used when calculating the sample semi-variograms. These zones were elongated in the areas where log-transmissivity is probably statistically anisotropic, notably in the narrow central portion of the aquifer and around the
Figure 12. Zonation pattern used to krig the Avra Valley log-transmissivities.
Santa Cruz River. The shorter dimension of the elongated zones was aligned parallel to the assumed direction of fastest variation of log-transmissivity.

Figure 13 illustrates the kriging plan designed for the Avra Valley aquifer log-transmissivities. Each zone was kriged using a maximum of 25 log-transmissivity data points. These data were selected from a circular neighborhood of radius 6 miles positioned so that the centroids of the neighborhood and the zone coincided; the data lying closest to the centroid were preferentially selected. The log-transmissivity data derived from log-specific capacities had known errors of prediction, the variances of which were calculated with equation (111). These errors were then accounted for in the kriging system (see equation (85)). The log-transmissivity data derived from aquifer tests were assumed to be without error. Numerical integration was used to calculate the mean values of the semi-variogram within the zones and between the data supports and the zones. To accomplish this, each zone was approximated by a regular network of internal points: 49 for a quadrilateral and 28 for a triangle. The computer code KRIGE was used to krige the zones of the Avra Valley aquifer. This code is documented in Appendix E.

**Results of Kriging.** The kriged values of log-transmissivity and their associated kriging errors are plotted in Figures 14 and 15 and are listed in Table 5. It is important to realize that the value of log-transmissivity assigned to each zone by the kriging technique is an averaged quantity. These values may differ slightly from the known
Figure 13. Schematic of the kriging plan for the Avra Valley log-transmissivities
Figure 14: Contour map of kriged log-transmissivity, Avra Valley
Figure 15. Contour map of log-transmissivity kriging errors ($\sigma_K$), Avra Valley
Table 5. Kriged log-transmissivities and kriging errors for the zones of the Avra Valley aquifer finite-element mesh

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<th>$\sigma_k(i)$</th>
<th>Zone(i)</th>
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log-transmissivities in the immediate vicinity of each zone. However, they represent the best estimate from the available data of the effective log-transmissivity of each zone--best in the sense that the estimates are unbiased and the estimation errors are minimal. The distribution of the kriging errors shows that the zones with the most reliable log-transmissivity estimates occur in the central parts of the basin where the data are concentrated. Close to the margins of the basin where the data are scarce, however, the kriging errors are relatively large.

The corresponding transmissivities, their estimation errors, and the coefficients of variation were computed using equations (106) to (108). The transmissivities and coefficients of variation are plotted in Figures 16 and 17. There is a definite east-west trend in the kriged transmissivities from the southern third of the basin. This trend is actually the magnification of a smaller trend that is evident in the original data from this area (Figure 8). The magnification is a consequence of the kriging procedure having to select data from the central parts of the southern basin to krig the marginal zones here. Notice that the coefficients of variation are relatively high and close to unity along the southeastern margin of the basin. This indicates that there is little confidence in the kriged transmissivities from this area.

**Correlation Structure of the Kriging Errors.** Cross sections of the correlation structure for different directions in the northern and southern subregions are illustrated in Figures 18 and 19, respectively. These cross sections show that the distance over which pairs of kriging errors remain correlated varies between 3 and 6 miles. In both
Figure 16. Contour map of transmissivity derived from the kriged log-transmissivities, Avra Valley
Figure 17. Contour map of the coefficient of variation of the transmissivities derived from the kriged log-transmissivities, Avra Valley.
Figure 18. Cross sections of log-transmissivity kriging-error correlation structure, northern Avra Valley. -- For section locations, see Figure 12.
Figure 19. Cross sections of log-transmissivity kriging-error correlation structure, southern Avra Valley. -- For section locations, see Figure 12.
subregions the correlation is slightly anisotropic, and this is mainly a reflection of the irregular distribution of the transmissivity data.

Notice that the kriging error of zone 112 is slightly correlated with the kriging error of zone 117, but uncorrelated with the kriging errors of zones 114 and 115 (Figure 19A). This is an unusual correlation structure because these zones are nearly colinear, implying that the correlation would be expected to decrease monotonically with increasing distance. All zones in this cross section are kriged with many common data points, which increases the potential for kriging-error correlation over large distances. The lack of correlation between the kriging errors of zone 112 and zones 114 and 115 is caused by the second and third terms of equation (91) dominating the calculations of their covariances.

Preparation of Hydraulic-head Data

Three steps are involved in preparing hydraulic-head data for the inverse model of Neuman (1980): (1) select a steady-state period in the aquifer's history, (2) assign estimates of the hydraulic heads from this period to the nodal points of the finite-element mesh superimposed on the aquifer, and (3) determine the covariance matrix of the hydraulic-head estimation errors.

Available Steady-state Data

Prior to the late 1940s the ground-water resources of Avra Valley were essentially undeveloped (White et al., 1966), and for practical purposes the ground-water flow regime was steady state. Water levels measured in 1940 were selected to represent the hydraulic heads
of the steady-state flow regime, and a hand-drawn contour map based on these data was prepared (Figure 20). In areas where there were a few 1940 data, the contours were guided by water levels from the late 1940s and sometimes the early 1950s.

Water-level data were supplied by the U.S. Geological Survey in Tucson, Arizona, and the University of Arizona Agricultural Experiment Station. These data are listed in Appendix D, and their localizations are given in Figure 21.

Nodal Point Hydraulic-head Estimation

The hydraulic heads must be estimated as accurately as possible at the nodal points of the finite-element mesh. Slight errors in the head estimates can cause large errors in the hydraulic gradients because these gradients are usually very small. These errors, in turn, can cause large errors in the transmissivities computed by the inverse model.

In this study the heads at the nodes were estimated from the hand-drawn hydraulic-head contour map (Figure 20). Each head value was estimated by interpolating between contours. This method was used despite the misgiving by Cooley and Sinclair (1976) that a hand-drawn hydraulic-head contour map has some subjective input and is non-unique. A more systematic approach would have been to use an interpolation technique, but this was considered to be less accurate than the method used. By hand contouring the 1940 water levels, information available from later years could be integrated into the head map. This was especially true about the contours close to some of the
Figure 20. Contour map of steady-state hydraulic heads based on 1940 water-level data, Avra Valley
Figure 21. Contour map of hydraulic-head estimation-error standard deviations determined by the interpolation scheme of Yakowitz (1980, pers. comm.) with location of the 1940 water-level measurement sites.
study-area boundaries, where 1940 water-level measurements are scarce (Figure 21). An interpolation technique would not be able to successfully integrated this type of information.

Estimation-error Covariance Matrix Determination

The covariance matrix of the hydraulic-head estimation errors could not be determined accurately after the head at each node had been estimated from the hand-drawn contour map. To overcome this problem, two independent estimates of this matrix were made. The inverse model was then run twice to assess its sensitivity to each estimated covariance matrix. In both cases, the estimation errors were assumed to be uncorrelated, thus each covariance matrix was diagonal.

In the first case the variance of each estimation error was determined by an interpolation scheme recently developed by Yakowitz (1980, personal commun.). This scheme computes the estimation-error variance by using the method of cross validation after predicting the hydraulic head at each node with a non-parametric regression formula (Schuster and Yakowitz, 1979; Stone, 1974). The estimation-error variance calculated by this scheme depends on the density of data in the vicinity of the node: as the density of data increases, the estimation-error variance decreases. This is a reasonable way to compute the variances of the hydraulic-head estimation errors because the contour map from which the head at each node was estimated is most accurate where the data are plentiful. These estimation-error variances strictly pertain, however, to the nodal hydraulic-head estimates determine by the interpolation scheme of Yakowitz (1980,
personal commun.). Note that by having determined the variance of each estimation error, the parameter \( c^2_h \) in equations (17) and (29) is known and equal to unity. Figure 21 is a contour map of the estimation-error standard deviations determined by this method. This mean standard deviation at the nodal points is 6.26 ft.

For the second case the variances of the hydraulic head estimation errors were assumed to be equal but unknown. The covariance matrix was then represented by \( \sigma^2_h I \), where \( \sigma^2_h \) is a positive scalar to be determined by the inverse model and \( I \) is the identity matrix.
INVERSE MODELING OF THE AVRA VALLEY AQUIFER

The Avra Valley aquifer was modeled twice using the method of Neuman (1980). In both cases the parameter $\sigma_Y^2$ in equation (29) was set equal to unity because the covariance matrix, $V_{\nabla}$, of the log-transmissivity estimation errors had been determined by the kriging procedure. Two independent estimates of the covariance matrix of the hydraulic-head estimation errors, $V_{\xi}$, were made, and this led to the model being run twice. In the first case, the parameter $\sigma_h^2$ in equation (29) was set equal to unity because the covariance matrix had been calculated by an interpolation scheme recently developed by Yakowitz (1980, personal commun.). The optimal solution to the inverse problem was then readily determined by minimizing equation (29) once. In the second case $\sigma_h^2$ was assumed unknown, and a series of different solutions was generated. The optimal solution in this series was identified by analyzing certain statistics of the hydraulic-head weighted residuals.

Finite-element Mesh and Boundary Conditions

The finite-element mesh used to model the Avra Valley aquifer is illustrated in Figure 22. This mesh is nearly identical to the zonation pattern used to krig the log-transmissivities (Figure 12). Some zones around the Rillito Narrows and close to the southern boundary of the study area were divided into smaller elements because the hydraulic gradients were relatively large in these areas. All quadrilateral elements were routinely divided into two triangular elements.
Figure 22. Finite-element mesh and boundary conditions used to model the Avra Valley aquifer.
The boundary conditions used to model the study area are illustrated in Figure 22. Boundary types were determined from the 1940 water-level contour map (Figure 20) and from previous estimates of recharge to and discharge from the aquifer.

Impermeable boundaries were placed along most of the mountain flanks. There was little evidence of active mount-front recharge from the 1940 water-level contour map (Figure 20) or from water levels measured in 1974 (Matlock and Morin, 1976). However, the water-level data suggested that there was a small amount of recharge through a pediment on the northwest side of the Tucson Mountains (Figure 22). The recharge rate through this pediment was estimated to be 500 acre-ft/yr. This estimate was derived from the mountain-front recharge rates along the Tucson Mountains determined by Osterkamp (1973). The northern boundary of the study area was placed to coincide with a streamline and thus was another impermeable boundary of the model. Constant-head boundaries were assigned between Avra Valley and its three adjoining ground-water basins. The fluxes across these boundaries were computed after the transmissivity field had been determined by the inverse model.

Stream-channel recharge was assumed to have a negligible effect on ground-water flow in Avra Valley for modeling purposes. There was no evidence of mounding beneath the stream channels from the water-level contour map. This suggested that stream channel recharge did not have a significant impact on the ground-water flow system. The effects of ground-water pumping and possible irrigation return flows were also disregarded in the model. Pumping was neglected because a
a recent study by Fogg et al. (1979) concluded that the effects of neglecting 14,000 acre-ft/yr of pumping on a model of the Tucson Basin aquifer were insignificant. This aquifer is hydrogeologically similar to the Avra Valley aquifer. The amount of pumping in Avra Valley during 1940 is estimated to be 10,000 acre-ft (White et al., 1966). Irrigation return flows were neglected because they are likely to amount to only a small proportion of the total pumpage during 1940. The net effect of neglecting all these fluxes is to cause an unknown bias in the computed fluxes across the constant head boundaries between Avra Valley and its three adjoining ground-water basins. Neuman (1980) has demonstrated, however, that small errors in the estimates of recharge to or discharge from the aquifer have a negligible effect on the transmissivities computed by the inverse model.

Using the kriged transmissivity estimates and the above boundary conditions, the hydraulic heads at each node were computed prior to calibration by the inverse model. This head map and the 1940 water-level map are compared in Figure 23. The match between the two head maps is very poor; the hydraulic heads differ by up to 80 ft in places. A better match would have been achieved if the boundaries of the model adjacent to the mountains had been specified as constant-head rather than constant-flux boundaries. However, greater confidence can be placed in the specification of the fluxes across rather than than the heads at these boundaries. The challenge to the inverse model is then to calculate a log-transmissivity field that has less uncertainty than the kriged log-transmissivity field and that will reproduce the 1940
Figure 23. Comparison of the 1940 steady-state hydraulic heads and hydraulic heads computed by the kriged log-transmissivity field.
water-level contour map more satisfactorily than the kriged log-
transmissivities.

Case 1: \( \sigma_h^2 \) Known

Computed Transmissivity Field

Table 6 is a list of the log-transmissivities and their estimation
error standard deviations that resulted from minimizing equation (29)
when both \( \sigma_h^2 \) and \( \sigma_Y^2 \) were known. It must be remembered that a
particular value of log-transmissivity computed by the inverse model is
averaged over a zone and is not necessarily the log-transmissivity that
would be determined by a single aquifer test conducted in that zone.
A value of log-transmissivity assigned to a zone by the model is the
model's best estimate of the mean of a large number of
log-transmissivity determinations in that zone. The uncertainty
associated with each estimate is quantified by the estimation error.

The transmissivity field computed by the inverse model is con-
toured in Figure 24. This field has many of the trends evident in the
kriged transmissivity field (Figure 16) that formed part of the input
data to the model. The inverse model preserved the areas of relatively
high transmissivity in northern and southeastern Avra VAlley, and the
east-west trend of decreasing transmissivity in the southern part of the
basin is still apparent. Notice that the model has significantly altered
the magnitude of some of the kriged transmissivity estimates.

A contour map of the standard deviations of the log-
transmissivity estimation errors computed by the inverse model is illus-
trated in Figure 25. Comparing this map with the map of the
Table 6. Log-transmissivities and their estimation errors determined in Case 1 of the inverse modeling study

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Figure 24. Contour map of the transmissivity field computed by the inverse model: Case 1, $\sigma_h^2$ known
Figure 25. Contour map of the log-transmissivity estimation-error standard deviations computed by the inverse model: Case 1, $\sigma_h^2$ known.
log-transmissivity kriging errors (Figure 15) indicates that the inverse model has reduced the uncertainty in the log-transmissivity estimates in many areas. The errors are still relatively large along the boundaries of the model. This is to be expected, however, because the input log-transmissivities were most uncertain close to the boundaries. The magnitude of the reduction of the uncertainty in the log-transmissivity estimates achieved by the inverse model can be assessed by comparing the traces of the two estimation-error covariance matrices. The trace of the kriging-error covariance matrix is 2.97 and the trace of the estimation-error covariance matrix computed by the inverse model is 1.59. Thus the inverse model has significantly reduced the uncertainty in the log-transmissivity estimates.

Four cross sections of the log-transmissivity estimation-error correlation structure were prepared (Figures 26 and 27). These section lines were previously used to illustrate the correlation structure of the kriging errors (Figures 18 and 19). Comparing the log-transmissivity error correlation structures determined by the inverse model and by kriging indicates that the inverse model has slightly altered the kriging-error correlation structure. The magnitude of the correlations and the distance over which the errors remain correlated have been reduced in most sections.

Notably, there is some negative correlation between the log-transmissivity estimation errors from zones on opposite sides of southern Avra Valley (Figure 27A). These zones roughly lie along an equipotential. The negative error correlation in this case is most likely a reflection of the model conserving the mass flux rate through the
Figure 26. Cross sections of the log-transmissivity estimation-error correlation structure determined by the inverse model, northern Avra Valley. -- For section locations, see Figure 12.
Figure 27. Cross sections of the log-transmissivity estimation-error correlation structure determined by the inverse model, southern Avra Valley. -- For section locations, see Figure 12.
relatively narrow southern portion of the aquifer. To conserve the mass flux rate here, increasing the computed transmissivity on one side of the aquifer would require decreasing the computed transmissivity on the other side. This would cause the estimation errors to be negatively correlated.

The isotropic appearance of the correlation structure of the log-transmissivity estimation errors is unusual. This contrasts with the pronounced anisotropic log-transmissivity error correlation structures evident in similar studies by Neuman (1980), Neuman et al. (1980), and Neuman and Yakowitz (1979). The reason for the isotropic correlation structure in this case is that the components of the sensitivity matrix, $Z$, defined in equation (35), do not vary with direction in the vicinity of the cross sections in Figures 26 and 27, i.e., the sensitivity of hydraulic head to changes in log-transmissivity does not depend on the direction of the node from the zone. (Recall that the kriging errors had an isotropic correlation structure and the matrix $V_{\epsilon \epsilon}$ was diagonal. It then follows from equation (45) that the components of the sensitivity matrix $Z$ must be directionally invariant if the log-transmissivity estimation errors are to have an isotropic correlation structure.) The directional invariance of the sensitivity matrix $Z$ may be caused by the elongation of the Avra Valley aquifer coupled with the model's having to conserve the flux rate through the aquifer.

Computed Hydraulic Heads

The hydraulic-head surface computed by the inverse model and the 1940 steady-state water-level map are both plotted in Figure 28.
Figure 28. Comparison of the 1940 steady-state hydraulic heads and the hydraulic heads computed in Case 1 of the inverse modeling study.
Clearly the head map of the inverse model matches the steady-state water levels far more satisfactorily than the head map corresponding to the kriged log-transmissivity estimates (Figure 23).

The weighted residuals of the hydraulic heads, defined in equation (51), have a mean and variance of 0.06 ft and 1.00 ft$^2$, respectively. The small value of the mean weighted residual is consistent with regression theory (Draper and Smith, 1966). Because the mean weighted residual is close to zero, it follows from equations (49) and (54) that the variance of the weighted residuals is the best estimate of $\sigma_h^2$ provided by the model. However, $\sigma_h^2$ was known to be equal to unity prior to running the inverse model. Thus the inverse model has verified the hydraulic-head estimation errors determined by the interpolation scheme of Yakowitz (1980, personal commun.).

The mean of the standard deviations of the head estimation errors computed by the inverse model using equation (48) is 2.19 ft. This is far less than the mean standard deviation of the head estimation errors determined by the interpolation scheme of Yakowitz (1980, personal commun.), which is 6.26 ft. Thus the inverse model has significantly reduced the uncertainty in the estimated hydraulic heads.

Computed Flux Rates

The boundary flux rates computed by the inverse model are listed in Table 7. These flux rates are smaller than the previous estimates of the boundary flux rates (see Table 1). It must be remembered that some fluxes were neglected in building the model, so the computed flux rates suffer from an unknown bias. Interestingly,
Table 7. Boundary flux rates computed by the inverse model, Case 1: $\sigma_h^2$ known

<table>
<thead>
<tr>
<th>Inflow, acre-ft/yr</th>
<th>Outflow, acre-ft/yr</th>
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<tr>
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<td>Rillito Narrows</td>
</tr>
<tr>
<td>6,846</td>
<td>11,266</td>
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</table>

however, the fluxes computed by the inverse model are closest to the flux estimates of Moosburner (1972), which were derived from an electric analog model of the Avra Valley aquifer.

Case 2: $\sigma_h^2$ Unknown

Optimal Solution Determination

Determination of the optimal solution in this case first required generating a series of different solutions. These solutions were generated by replacing the multiplier $\sigma_h^2 / \sigma_Y^2$ in equation (29) with a non-negative scalar $\lambda$ and then minimizing this equation for different values of $\lambda$. Certain statistics of the hydraulic-head weighted residuals from each solution were examined to decide which solution was the optimum.

In this study, advantage can be taken of the parameter $\sigma_Y^2$ equaling unity. It then follows from equation (29) that $\lambda$ is equal to $\sigma_h^2$ at the optimal solution. The best estimate of $\sigma_h^2$ is given by the mean hydraulic-head weighted-residual sum of squares, $s^2$, defined in equation (49). Thus to pick the optimal solution simply required
plotting $s^2$ versus $\lambda$ for each solution and then selecting the solution at which $s^2$ and $\lambda$ were equal.

Figure 29 is a graph of $s^2$ and the mean hydraulic-head weighted residual, $\bar{z_h}$, versus $\lambda$. It is not clear what the sharp discontinuities at $\lambda = 18$ and $\lambda = 40$ represent. However, this graph shows that $s^2$ and $\lambda$ coincide in two places: at $\lambda = 190$ and $\lambda = 36$. Thus, there are two solutions that satisfy the optimality criterion.

Note that since the covariance matrix $\text{sym}$ in equations (17) and (29) was arbitrarily set equal to the identity matrix, $s^2$ and $\bar{z_h}$ were both calculated from the true (unweighted) hydraulic-head residuals.

The solution at $\lambda = 190$ is non-optimal because $s^2$ is large and roughly the same for all $\lambda > 40$. When equation (29) is minimized with a large value of $\lambda$, it follows that the composite sum of squares, $J(\hat{Y})$, will be dominated by the second term. This implies that the computed log-transmissivities will not be allowed to deviate far from the initial log-transmissivity estimates. Consequently, the computed hydraulic heads will be close to the heads calculated from the initial log-transmissivities. This means that at large values of $\lambda$ the model may be undercalibrated with respect to the hydraulic heads. A large value of $s^2$ is evidence of undercalibration. Thus by the process of elimination, the solution at $\lambda = 36$ was selected as the optimum. A supportive reason for choosing this solution as the optimum is the small value of its mean hydraulic-head weighted residual (Figure 29).

Equation (29) could well have been minimized with a value of $\lambda$ close to zero in this case. This would have forced the computed hydraulic heads to match the steady-state water levels almost exactly.
Figure 29. Graph of $s^2$ and $\bar{z}_h$ versus $\lambda$ from Case 2 of the inverse modeling study
Although achieving such a head match is appealing, the model would have been overcalibrated with respect to the hydraulic heads, i.e., the value of $s^2$ computed by the model would have been far less than the true value of $\sigma_h^2$. This implies that more confidence than was warranted would have been placed on the steady-state hydraulic-head estimates. Overcalibration is undesirable because it can cause the log-transmissivity estimation-error variances to be larger than the error variances of the initial log-transmissivity estimates (Neuman, 1980).

Results

Table 8 lists the log-transmissivities and their estimation-error standard deviations computed by the inverse model in Case 2 of the modeling study. Contour maps of the transmissivity field and the standard deviations of the log-transmissivity estimation errors are illustrated in Figures 30 and 31, respectively. The trace of the covariance matrix of the log-transmissivity estimation errors is 1.46. Examination of the correlation structures of the log-transmissivity estimation errors shows that they are very similar to their counterparts from Case 1 that have been mentioned, so these will not be discussed. Figure 32 compares the hydraulic heads computed by the inverse model in Case 2 and the 1940 steady-state water levels. The mean of the standard deviations of the hydraulic-head estimation errors is 2.13 ft. Table 9 lists the boundary fluxes computed in Case 2.

Comparison of Results from Cases 1 and 2

The transmissivity fields computed in both cases of the modeling study are very similar (cf. Figures 24 and 30). Along the southeastern
Table 8. Log-transmissivities and their estimation errors determined in Case 2 of the inverse modeling study

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<th>( [\hat{y}(e_y)_i]^{\dagger} )</th>
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<th>( \hat{y}_i )</th>
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Figure 30. Contour map of the transmissivity field computed by the inverse model: Case 2, $\sigma_h^2$ unknown
Figure 31. Contour map of the log-transmissivity estimation-error standard deviations computed by the inverse model: Case 2, $\sigma_h^2$ unknown
Figure 32. Comparison of the 1940 steady-state hydraulic heads and the hydraulic heads computed in Case 2 of the inverse modeling study.
Table 9. Boundary flux rates computed by the inverse model, Case 2: $c_h^2$ unknown

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<th>Outflow, acre-ft/yr</th>
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margin of the basin, however, the transmissivities computed in Case 2 are slightly higher.

The standard deviations of the log-transmissivity estimation errors are similar in both cases (cf. Figures 25 and 31). This similarity is also evident in the traces and the correlation structures of the covariance matrices of the log-transmissivity estimation errors from each case. The traces of the covariance matrices are 1.59 and 1.46 from Cases 1 and 2, respectively. The similarity between the correlation structures has previously been mentioned.

The match between the hydraulic-head maps computed in Cases 1 and 2 and the 1940 steady-state water levels are equally satisfactory (cf. Figures 28 and 32). The magnitude of the uncertainty in the hydraulic heads computed in both cases are similar; the mean standard deviations of the head estimation errors are 2.19 ft and 2.13 ft in Cases 1 and 2, respectively. The boundary fluxes computed by the inverse model are practically the same in both cases (cf. Tables 7 and 9).

Despite their similarity, subtle differences exist between the modeling results of Cases 1 and 2. These differences are a consequence of the different hydraulic-head estimation-error covariance
matrices used to model the aquifer in each case. The results from Case 1 are considered to be the more reliable because the head-error covariance matrix was systematically determined by the interpolation scheme of Yakowitz (1980, personal commun.). However, the use of the identity matrix to represent the head-error covariance matrix in Case 2 was not detrimental to the results of the model. Thus, each approach has proved to be a satisfactory way to model the aquifer.
CONDITIONAL SIMULATION OF HYDRAULIC HEADS

Conditional simulation is a convenient way to assess the magnitude of the errors in the hydraulic heads predicted by a particular log-transmissivity field and its estimation-error covariance matrix. Assessing these errors first requires generating a large number of possible log-transmissivity fields using Monte Carlo techniques (Schweppe, 1973). These log-transmissivity fields are generated so that: (1) their mean is the same as the log-transmissivity field being simulated and (2) the covariance matrix of the log-transmissivity residuals, defined as the difference between the simulated and mean log-transmissivity fields, is identical to the estimation-error covariance matrix of the log-transmissivity field being simulated. These conditions guarantee that each simulated log-transmissivity field is a possible representation of reality, and this is the objective of conditional simulation. The hydraulic-head distribution corresponding to each simulated log-transmissivity field is then calculated. Simple statistics of the set of simulated hydraulic-head distributions give the required information about the errors in the predicted hydraulic heads.

In this study, conditional simulation was used to examine the errors in the hydraulic heads predicted by the kriged log-transmissivity field and the log-transmissivity fields computed by the inverse model. For brevity, the results of the simulations based on the inverse model's log-transmissivity fields will be reported only for that field computed
in Case 1 of the modeling study. These results were very similar to the results of the simulations based on the field computed in Case 2. The finite-element mesh, log-transmissivity zonation pattern, and boundary conditions specified in the model were retained in the simulation analyses. Each simulated log-transmissivity field was simply a set of values of simulated log-transmissivity from every zone. Equation (4) was used to calculate the hydraulic head at all the nodes of the mesh given a simulated log-transmissivity field and the specified boundary conditions. Following the simulation of a large number of hydraulic-head distributions, the mean and variance of the simulated heads at each node were computed. The simulation analyses were performed with computer programs written by Binsariti (1980b, personal commun.).

**Theory**

For the simulation analyses, the log-transmissivity kriging errors and the log-transmissivity estimation errors computed by the inverse model are assumed to be normally distributed. The assumption of normality of the kriging errors is reasonable because these errors represent the sum of a number of error components that depend uniquely on the location of each sampling point (see equation (87)). It then follows from the Central Limit Theorem that the sum of these error components will tend to be normally distributed as the number of these components increases (Hines and Montgomery, 1980). The assumption of normality of the log-transmissivity estimation errors calculated by the inverse model is consistent with regression theory (Draper and Smith,
Let $Y$ be the particular log-transmissivity field to be simulated and let $\xi$ be the covariance matrix of its estimation errors $\xi$. The probability density function of $\xi$ is then (Schweppe, 1973)

$$
P(\xi) = \left\{ (2\pi)^{L/2} |\Sigma| \right\}^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} (\xi - \bar{m})^T \Sigma^{-1} (\xi - \bar{m}) \right\} \tag{119}
$$

where the mean of $\xi$ is

$$
E\{\xi\} = \bar{m} \tag{120}
$$

and $L$ is the number of log-transmissivity zones in the finite-element mesh. It follows from equations (44) and (76) that $\bar{m} = 0$ in this study. Thus the error vector $\xi$ has the $L$-variate distribution $N(0, \Sigma)$.

A multivariate normal generator (MVNG) can be used to simulate the log-transmissivity fields because the log-transmissivity errors are assumed to be normally distributed. Simulating a log-transmissivity field first requires generating a realization of the random variable vector $\xi_s$, which is isomorphic to $\xi$, i.e., $\xi_s$ has the same mean and second-order moment as $\xi$. The simulated log-transmissivity field $Y_s$ is then given by

$$
Y_s = Y + \xi_s \tag{121}
$$

Generating a realization of $\xi_s$ can be accomplished by first generating a realization of another random variable vector $\psi$ using a univariate normal generator such that $\psi$ has components that are distributed $N(0,1)$. The realization $\xi_s$ is then given by the MVNG

$$
\xi_s = M \psi \tag{122}
$$
where $M$ is a lower triangular matrix that satisfies
\[ MM^T = \Sigma \]  

(123)

It follows from equation (122) that
\[
E\{\xi_s\} = E\{M \psi\} \\
= ME\{\psi\} \\
= 0
\]

(124)

and thus
\[
\text{Cov} \{\xi_s\} = E\{\xi_s \xi_s^T\} \\
= E\{(M \psi) (M \psi)^T\} \\
= E\{M \psi \psi^T M^T\} \\
= ME\{\psi \psi^T\} M^T \\
= M I M^T \\
= \Sigma = \text{Cov} \{\xi\}
\]

(125)

The number of simulations required to obtain a statistically meaningful result is the final question to be addressed before the simulation analyses. In a recent study of the Tucson Basin aquifer, Binsariti (1980a) concluded that 280 simulations of the log-transmissivity field were sufficient to assure convergence of the mean and the second-order moment when the aquifer was divided into 124 zones. For the simulation study of the Avra Valley aquifer, 300 simulations were completed before conducting the statistical analyses. No checks were made to assess whether convergence of the mean and the second-order
moment had been achieved. However, 300 simulations were considered sufficient because the aquifer was divided into 122 log-transmissivity zones.

**Conditional Simulations from Kriged Log-transmissivities**

The tenth realization and the mean of the 300 realizations of hydraulic heads conditionally simulated from the kriged log-transmissivity field are contoured in Figure 33. These head maps match closely in the south of the basin, but differ consistently by about 25 ft in the north. The mean of the realizations (solid contours on Figure 33) corresponds closely with the hydraulic-head surface computed from the kriged log-transmissivity field (dashed contours on Figure 23). This implies that 300 simulations were sufficient to achieve convergence of the mean. The standard deviations of the 300 head realizations at the nodal points of the mesh are contoured in Figure 34. The greatest uncertainty in the hydraulic heads predicted by the kriged log-transmissivity field occurs in northern Avra Valley where the maximum standard deviation is 15 ft. In general, the standard deviations of the predicted heads increases with distance from the constant-head boundaries where, as expected, they are zero. The most rapid changes in the standard deviations occur adjacent to the constant-head boundaries in northern Avra Valley. The average of the standard deviations at all the nodes is 8.7 ft.

Interestingly, the greatest uncertainty in the predicted heads occurs in the north of the basin, although the largest kriging errors are in the south (Figure 15). The relatively small standard deviations
Figure 33. Comparison of the 10th realization and the mean of 300 realizations of hydraulic head conditionally simulated from the kriged log-transmissivity field.
Figure 34. Contour map of the standard deviations of the 300 hydraulic-head realizations conditionally simulated from the kriged log-transmissivity field.
of the predicted heads close to the southern constant-head boundary indicate that the hydraulic gradient here did not change much during the 300 simulations. However, the large kriging errors in the south imply that there was a large variation in the simulated log-transmissivites in this area. Consequently, the flux rates across the southern boundary changed significantly during the 300 simulations. These varying flux rates caused large fluctuations in the hydraulic gradients near the constant head boundaries in the north. The fluctuating hydraulic gradients were necessary because the mass flow rate through the aquifer had to be conserved for each simulated log-transmissivity field. The large standard deviations of the simulated hydraulic heads in the north are a result of the widely fluctuating hydraulic gradients here.

Conditional Simulations from Inverse Model Log-transmissivities

The tenth realization and the mean of the 300 realizations of the hydraulic heads conditionally simulated from the log-transmissivity field computed in Case 1 of the inverse modeling study are contoured in Figure 35. These head maps match more closely than the corresponding head maps simulated from the kriged log-transmissivity field (Figure 33). The mean of the realizations (solid contours on Figure 35) is practically identical to the hydraulic-head surface computed by the log-transmissivity field of the inverse model (dashed contours on Figure 28). This again demonstrates that 300 simulations were sufficient to achieve convergence of the mean. Figure 36 is a contour map of the standard deviations of the hydraulic heads at the nodes of the mesh for
Figure 35. Comparison of the 10th realization and the mean of 300 realizations of hydraulic head conditionally simulated from the log-transmissivity field of the inverse model.
Figure 36. Contour map of the standard deviations of the 300 hydraulic-head realizations conditionally simulated from the log-transmissivity field of the inverse model.
the 300 simulations. The trends in this contour map correlate fairly closely with the trends in the contour map of the log-transmissivity estimation-error standard deviations computed by the inverse model (Figure 25). The average standard deviation at all the nodes is 2.3 ft, which is roughly the same as the average of 2.2 ft computed by the inverse model. This is significantly less than the 8.7 ft average standard deviation of the heads predicted by the kriged log-transmissivity field. Thus, by conditioning the kriged log-transmissivities on the steady-state water levels, the inverse model has greatly reduced the uncertainty in the predicted hydraulic heads.
SUMMARY AND CONCLUSIONS

The primary objectives of this study have been to (1) construct a map of the transmissivity field of the Avra Valley aquifer that has the least amount of uncertainty, (2) quantify the uncertainty in this transmissivity field, and (3) assess the uncertainty in the hydraulic heads predicted by this transmissivity field.

Essentially three steps were involved in producing the map of the transmissivity field of the Avra Valley aquifer: (1) collecting existing transmissivity data available for the aquifer, (2) using the geostatistical interpolation technique of kriging on these data to assign spatially averaged values of log-transmissivity to the zones of a finite-element mesh covering the aquifer, (3) conditioning the kriged log-transmissivities on steady-state water levels to produce the map of the aquifer's transmissivity field. The last step was accomplished with the statistical inverse model of Neuman (1980). Each step represents a progressive refinement in the process of determining the transmissivity field of the aquifer.

Transmissivity data were derived from two sources: (1) aquifer test analyses and (2) specific capacity measurements. Most aquifer tests were of short duration, and their drawdown-time data proved to be too unreliable to calculate values of transmissivity; however, the recovery data from these tests were sufficiently accurate to determine transmissivity values. Data from many of these aquifer tests were subsequently used in a regression analysis to establish a linear relationship...
between log-transmissivity and log-specific capacity. Some specific capacities used in the regression analysis had to be adjusted because the wells from which they were determined had abnormally low efficiencies. Many log-transmissivities were then predicted from log-specific capacity measurements. Each predicted log-transmissivity had an associated error of prediction, the variance of which was determined from the regression analysis. The variance of each error of prediction was accounted for in the kriging analysis.

It was necessary to subdivide the Avra Valley aquifer into two subregions before kriging the log-transmissivities. Each subregion had a different mean value of log-transmissivity, thus the second-order stationary or intrinsic hypotheses could not be inferred to apply for the entire log-transmissivity field. Examination of the sample semi-variograms indicated that the variability of log-transmissivity in each subregion was different. This was an additional justification for kriging the subregions separately. The covariance matrices of the kriging errors from each subregion were determined following the kriging analyses. These matrices were required by the inverse model. Both matrices were combined, as were the kriged log-transmissivity fields, prior to the inverse modeling study.

The steady-state hydraulic heads of the Avra Valley aquifer, which were required by the inverse model, were represented by water levels measured in 1940. Inputting these data into the inverse model required estimating the hydraulic head at each nodal point of the finite-element mesh superimposed on the aquifer. These estimates were made by interpolating between the contours of a hand-drawn steady-state
water-level contour map. A disadvantage of this approach was that the covariance matrix of the hydraulic-head estimation errors, which was required by the inverse model, could not be accurately determined. Two independent determinations of this matrix were then made, and the inverse model was run twice to assess the sensitivity of the model to each estimate. In both cases the estimation errors were assumed to be uncorrelated, thus each covariance matrix was diagonal. In Case 1, the variance of each hydraulic-head estimation error was determined systematically by an interpolation scheme developed recently by Yakowitz (1980, personal commun.). In Case 2, the estimation-error variances were assumed to be equal but unknown and had to be determined after running the model. The results of the modeling study were very similar in both cases. This suggests that the solution determined by the inverse model of Neuman (1980) is not overly sensitive to the covariance matrix of the hydraulic-head estimation errors.

The inverse model of Neuman (1980) computed a log-transmissivity field for the Avra Valley aquifer, which had less uncertainty than the kriged log-transmissivity field. The magnitude of the reduction in the uncertainty achieved by the inverse model can be demonstrated by comparing the traces of the log-transmissivity estimation-error covariance matrices. The traces of the kriging-error covariance matrix and the covariance matrix of the log-transmissivity estimation errors determined in Case 1 of the modeling study were 2.97 and 1.59, respectively. This implies that the log-transmissivity field determined by the inverse model can be used to model the Avra Valley aquifer with greater confidence than the kriged log-transmissivity field.
A conditional simulation analysis was made to assess the magnitude of the errors in the hydraulic heads predicted by the kriged log-transmissivity field and the log-transmissivity field determined in Case 1 of the inverse modeling study. Utilization of a multivariate normal generator was possible in this analysis because the estimation errors associated with each log-transmissivity field were assumed to be normally distributed. A set of 300 possible hydraulic-head distributions was simulated from each log-transmissivity field and its estimation-error covariance matrix. The mean and variance of each set of simulated hydraulic heads were then calculated. The average standard deviations of the heads predicted by the kriged and inverse model log-transmissivity fields were 8.7 ft and 2.3 ft, respectively. This further demonstrates that the log-transmissivity field computed by the inverse model has less uncertainty than the kriged log-transmissivity field.

The following conclusions can be made about the methods used in this study:

1. Kriging is an efficient means of assigning spatially averaged values of log-transmissivity to the zones of a finite-element mesh covering an aquifer. Kriging has the advantage of yielding unbiased estimates with a minimum estimation-error variance. In addition, kriging can compute the complete covariance matrix of the log-transmissivity estimation errors. This matrix is part of the required input data for the inverse model.

2. Each kriged log-transmissivity estimate is conditioned only on the available transmissivity data. Consequently, a kriged log-transmissivity map may be judged to be hydrogeologically unrealistic,
especially in areas where the data are lacking. However, the quality of each kriged log-transmissivity estimate can be assessed by the magnitude of its kriging (estimation) error. In general, kriging errors are greatest in those areas where the data are scarce. The ability of kriging to estimate the average values of log-transmissivity for zones in an aquifer and to quantify the errors of estimation makes it a useful tool for preparing transmissivity data for the inverse model.

3. The inverse model of Neuman (1980) conditions the kriged log-transmissivity estimates on steady-state water levels by means of the ground-water flow equation. The objective of applying this model is to construct a map of the aquifer's log-transmissivity field that has less uncertainty than the map of the kriged log-transmissivity field and that will reproduce steady-state water levels within known error bounds.

4. Conditional simulation is a useful means of examining the uncertainty in the hydraulic heads predicted by a particular log-transmissivity field.

5. The methods used in this study are based on statistical theory. Motivation for the stochastic approach to aquifer modeling is provided primarily by the non-uniqueness of the solution to the inverse problem. The major advantages of the methods described in this study are that (a) they are systematic and rigorous and therefore are likely to be highly reproducible and (b) they are able to quantify the uncertainty in the computed transmissivity field and consequently in the predicted hydraulic-head distribution.
APPENDIX A

NOTATIONS

\( A \)  Finite-element conductance matrix \([L^2 T^{-1}]\); Equation (4) and (5).

\( A_{nm} \)  The component in the \( n \)th row and \( m \)th column of \( A \); Equation (5).

\( b_0, b_1 \)  Coefficients of the log-transmissivity log-specific capacity linear model; Equation (110).

\( b_1, b_2, b_3 \)  Coefficients that partially define the components of \( A[L] \); Equations (5), (7), and (8).

\( C(x_i, x_j) \)  Covariance between two random variables located at the points \( x_i \) and \( x_j \); Equation (57).

\( C(s) \)  Covariance between two random variables separated by the displacement vector \( s \); Equation (60).

\( \bar{C}(x_i, x_j) \)  Mean value of the covariance between two samples (data) that are centered on \( x_i \) and \( x_j \); Equation (81).

\( \bar{C}(x_i, V) \)  Mean value of the covariance between a sample centered on \( x_i \) and the support \( V \); Equation (82).

\( \bar{C}(V, V) \)  Mean value of the covariance within the support \( V \); Equation (83).

\( CV_V \)  Coefficient of variation of kriged transmissivity estimates; Equation (108).

\( \text{Cov}(\delta^1, \delta^2) \)  Covariance between the pair of errors \( \delta^1 \) and \( \delta^2 \) determined by kriging; Equation (91).

\( c_1, c_2, c_3 \)  Coefficients that partially define the components of \( A[L] \); Equations (5), (7), and (8).

\( E \)  Expectation operator.

\( e(x_i) \)  Measurement error of the sample \( \hat{Z}_v(x_i) \); Equation (66).

\( e_h \)  Vector of hydraulic-head estimation errors determined by inverse model \([L]\); Equation (33).
$e_Y$  Vector of log-transmissivity estimation errors determined by the inverse model; Equation (32).

$H(x)$  Hydraulic head on a prescribed constant-head boundary $[L]$; Equation (2).

$h$  Hydraulic head $[L]$; Equation (1).

$h$  Vector of true hydraulic heads $[L]$; Equation (11).

$h^*$  Vector of estimated hydraulic heads $[L]$; Equation (11).

$h$  Vector of computed hydraulic heads $[L]$; Equation (23).

$I$  Identity matrix.

$J_1(Y)$  Generalized non-linear least-squares regression criterion to compute $Y$; Equation (22).

$J_2(Y)$  Regression criterion of parameter plausibility; Equation (25).

$J(Y)$  Composite least-squares regression criterion; Equation (29).

$J_L(Y_L)$  Linear least-squares regression criterion to compute $Y_L$; Equation (43).

$K$  Left-hand-side matrix of the kriging system; Equation (88).

$M$  Lower triangular root matrix of the covariance matrix $\Sigma_w$; Equation (123).

$m(x)$  Mean value of a random function at the point $x$; Equation (55).

$m_{LSC}$  mean of observed log-specific capacities; Equation (112).

$n$  Unit vector normal to $\Gamma$.

$Q(x)$  Flux rate per unit area across a prescribed constant flux boundary $[LT^{-1}]$; Equation (3).

$Q$  Vector of true fluxes $[LT^{-1}]$; Equation (12).

$Q^*$  Vector of estimated fluxes $[LT^{-1}]$; Equation (12).

$q$  Volumetric flux rate per unit area $[LT^{-1}]$; Equation (1).
$R_x$ Variance of the hydraulic-head weighted residuals; Equation (53).

$r$ Distance between two sample pairs.

$SC$ Specific capacity $[L^2T^{-1}]$.

$SS_{LSC}$ Sum of the squared deviations of the observed log-specific capacities from $m_{LSC}$; Equation (113).

$S$ Correlation matrix of the log-transmissivity kriging errors or the log-transmissivity estimation errors determined by the inverse model; Equations (50) and (92).

$s^2$ Mean hydraulic-head residual sum of squares: Equation (49).

$s$ Displacement vector.

$T$ Transmissivity $[L^2T^{-1}]$; Equation (1).

$T^*_V$ Transmissivity determined from the kriged log-transmissivity estimate $Y^*_V$; Equation (106).

$T^*_V$ Transmissivity determined by exponentiating $Y^*_V$; Equation (109).

$V_{-h}$ Matrix whose components are scalar multiples of $V(\varepsilon)$; Equation (17).

$V_{-Y}$ Matrix whose components are scalar multiples of $V(\gamma)$; Equation (28).

$V(\varepsilon_{-h})$ Covariance matrix of $\varepsilon_{-h}$; Equation (48).

$V(\varepsilon_{-Y})$ Covariance matrix of $\varepsilon_Y$; Equation (45).

$V(\varepsilon)$ Covariance matrix of $\varepsilon$; Equation (17).

$V(\xi)$ Covariance matrix of $\xi$; Equation (42).

$V(\gamma)$ Covariance matrix of $\gamma$; Equation (28).

$Y$ Log-transmissivity; Equation (18).

$Y$ Vector of true log-transmissivities; Equation (26).

$Y^*$ Vector of estimated log-transmissivities; Equation (26).

$\hat{Y}$ Vector of computed log-transmissivities; Equation (23).
\( Y_p \) Log-transmissivity predicted from an observed log-specific capacity; Equation (110).

\( \hat{Y}_L \) Vector of computed log-transmissivities for the linearized regression problem; Equation (43).

\( Y^*_V(x_i) \) Kriged estimate of log-transmissivity for the support \( V(x_i) \).

\( Z \) Jacobian or sensitivity matrix determined in the linearized error analysis of the inverse model; Equation (35).

\( Z(x) \) A particular value of a random function at the point \( x \).

\( Z_V(x) \) A particular value of a random function that is spatially averaged within the support \( V(x) \).

\( \hat{Z}_V(x) \) Observed value of a random function at the support \( v(x) \).

\( Z^*_{K}(x) \) Kriged estimate of \( Z_V(x) \); Equation (71).

\( \alpha \) Kriging weight; Equation (71).

\( \beta \) Vector on the left-hand side of the kriging system; Equation (88).

\( \Gamma \) Boundary of flow domain.

\( \Gamma_1, \Gamma_2 \) Segments of \( \Gamma \); Equations (2) and (3).

\( \gamma(x_i, x_j) \) Value of the semi-variogram function between two random variables located at \( x_i \) and \( x_j \); Equation (58).

\( \gamma(s) \) Value of the semi-variogram function between two random variables separated by the displacement vector \( s \); Equation (62)

\( \tilde{\gamma}(r) \) Value of the sample semi-variogram between sample pairs separated by distance \( r \); Equation (96).

\( \overline{\gamma}(x_i, V) \) Mean value of the semi-variogram function between a sample centered at \( x_i \) and the support \( V \); Equation (93).

\( \overline{\gamma}(V, V) \) Mean value of the semi-variogram function within the support \( V \); Equation (93).

\( \delta(x) \) Difference between the true and kriged values of a random function at \( x \); Equation (72).

\( \varepsilon \) Difference between \( h^* \) and \( h \); Equation (11).
Composite error vector of \( \varepsilon \) and \( \eta \); Equation (4).

Error vector resulting from the finite-element numerical approximation of the ground-water flow equation; Equation (13).

\( \sigma^2_h / \sigma^2_Y \).

Lagrange multiplier; Equations (85) and (93).

Difference between \( Q^* \) and \( Q \); Equation (13).

Difference between \( Y^* \) and \( Y \); Equation (26).

Estimation error vector for any vector of log-transmissivities; Equations (119) and (120).

Simulated vector isomorphic to \( \xi \); Equation (121).

Summation sign.

Covariance matrix of \( \xi \); Equation (119).

Kriging error; Equations (87) and (94).

Standard deviation of the actual errors; Equation (105).

Variance of \( e(x_i) \); Equations (85) and (93).

Scalar multiplier of \( V_h \); Equation (17).

Scalar multiplier of \( V_Y \); Equation (29).

Variance of the estimation error of \( T_{*V} \); Equation (107).

Vector of univariate normal deviates; Equation (122).

Two-dimensional vector differential operator \( \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial x} \right) \); Equation (1).

For all.
APPENDIX B

WELL LOCATION METHODS

The methods used to locate wells are described before presenting the transmissivity and hydraulic-head data from Avra Valley in Appendices C and D, respectively. Two methods were used to locate the wells. The first method is the U.S. Geological Survey well-numbering scheme, and the following explanation of it is modified from Davis (1967, Figure 4, p. 13).

The well numbers used by the U.S. Geological Survey in Arizona accord with the Bureau of Land Management system of land subdivision. The land survey in Arizona is based on the Gila and Salt River meridian and base line, which divides the state into four quadrants. These quadrants are designated counterclockwise by the capital letters A, B, C, and D. All land north and east of the point of origin is in A quadrant, and that south and east in D quadrant. The first digit of a well number indicates the township, the second the range, and the third the section in which the well is situated. The lowercase letters a, b, c, and d after the section number indicate the well location within the section. The first letter denotes a particular 160-acre tract, the second the 40-acre tract, and the third the 10-acre tract. These letters also are assigned in a counterclockwise direction, beginning in the northeast quarter. If the location is known within a 10-acre tract, three lowercase letters are shown in the well number. In Figure [B-1], well number (D-4-5)19caa designates the well as being in the NE¼NE¼SW¼ sec. 19, T. 4 S., R 5 E. When there is more than one well in a 10-acre tract, consecutive numbers beginning with 1 are added as suffixes.

In addition to locating the wells in Appendices C and D with the above scheme, a cartesian coordinate system was also used. The reference datum for the coordinate system is in (D-16-9)19aad, which corresponds to the lower left-hand corner of the frame of Figure 1 in the text. The
Figure B-1. U.S. Geological Survey well-numbering scheme.
--From Davis (1967)
x coordinate is in miles east of the datum, and the y coordinate is in miles north of the datum.
APPENDIX C

AVRA VALLEY TRANSMISSIVITY DATA
Table C-1. Avra Valley transmissivity data from aquifer tests

<table>
<thead>
<tr>
<th>Well No. (i)</th>
<th>$X_i$ (miles)</th>
<th>$Y_i$ (miles)</th>
<th>$S_i^2$/day</th>
</tr>
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<tr>
<td>(D-11-10) 27CDC</td>
<td>9.862</td>
<td>29.684</td>
<td>17111</td>
</tr>
<tr>
<td>27DDD</td>
<td>8.221</td>
<td>28.656</td>
<td>8822</td>
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<td>(D-12-10) 12CBD</td>
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<td>(D-12-11) 33000</td>
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<td>21.680</td>
<td>850</td>
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<tr>
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APPENDIX D

AVRA VALLEY STEADY-STATE HYDRAULIC-HEAD DATA
Table D-1. Avra Valley steady-state hydraulic heads

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Table D-1. Avra Valley steady-state hydraulic heads—Continued

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Table D-1. Avra Valley steady-state hydraulic heads—Continued

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<th>$h$ (feet)</th>
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APPENDIX E

COMPUTER PROGRAMS WRITTEN IN THIS STUDY

Two computer codes are documented and listed in this appendix: (1) SEMIVGM, a program that calculates sample semi-variograms and (2) KRIGE, a program designed to assign kriged estimates to the zones of a finite element mesh. Both computer codes are written in FORTRAN IV, and they are currently set to run on the CDC Cyber 175 computer at the University of Arizona Computer Center.
Program SEMIVGM

Program SEMIVGM will calculate sample semi-variograms from data that are irregularly distributed in two-dimensional space. Sample semi-variograms can be calculated for different directions to assess whether the variability of the random function is directionally dependent. Subroutine GAMA3, which calculates the sample semi-variograms using Equation (96) in the text, is taken largely from Journel and Huijbregts (1978). A line-printer plot of all sample semi-variograms is routinely produced.

Mechanics of SEMIVGM

Data are located with a cartesian coordinate system using x and y coordinates. Pairs of data must be defined to use Equation (96) to calculate the sample semi-variograms and Figure E-1 illustrates how data pairs are determined. A pair of data occurs when two data lie at a specified distance, plus or minus a distance tolerance, and a specified direction (angle), plus or minus an angle tolerance, from each other. In Figure E-1, the datum P1 and any datum lying in the outlined neighborhood form a data pair, i.e., (P1,P2), (P1,P3), and (P1,P4) are three pairs of data. The direction for which the sample semi-variogram is calculated is specified by the variable ALP, and the angle tolerance by the variable DA. The distance r in Equation (96) is the product of a distance lag number and the length of a unit lag, PAS. Usually the distance tolerance, DP, is set equal to PAS/2.0. Equation (96) is first evaluated for a unit lag in the direction ALP, then for successive lags in the same direction until the specified maximum number of
Figure E-1. Data-pair determination for sample semi-variogram calculation
computational lags, KMAX, is reached. This procedure is then repeated for the remaining directions in which sample semi-variograms are desired.

Subroutine GAMA3 will also calculate the distance-weighted "moment center" sample semi-variogram of Kim and Knudsen (1977), \( \hat{\gamma}_{mc} \), defined as

\[
\hat{\gamma}_{mc}(r) = \frac{\sum_{i=1}^{M} r(x_i)[\hat{Z}_v(x_i + s) - \hat{Z}_v(x_i)]^2}{2 \sum_{i=1}^{M} r(x_i)}
\]  

(1)

where \( M \) is the number of data pairs separated by the distance \( r = |s| \). Although the sample semi-variogram \( \hat{\gamma}(r) \) of Equation (96) is used to determine the semi-variogram model of the random function, Kim and Knudsen (1977) explained that \( \hat{\gamma}_{mc}(r) \) is useful to see if the length of the unit lag, PAS, chosen to evaluate \( \hat{\gamma}(r) \) is correct. PAS should be varied until \( \hat{\gamma}(r) \) and \( \hat{\gamma}_{mc}(r) \) closely coincide.

User's Guide and Program Listing

The input data for SEMIVGMM are arranged into six data groups. A data group may comprise one or more data cards (records).

Only the arrays in the main program need be dimensioned. The dimensions of the arrays in the subprograms will adjust automatically if the dimensions of the arrays in the DIMENSION statement of the main program are altered. The required dimensions of the arrays are:
Variables ND, NDI, and KMAX are defined in Group 2 of the User's Guide, which follows.

<table>
<thead>
<tr>
<th>Data Group</th>
<th>Variable</th>
<th>Format</th>
<th>Card Columns</th>
<th>Description</th>
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</thead>
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<tr>
<td>1</td>
<td>HED</td>
<td>20A4</td>
<td>1-80</td>
<td>Job title--will be printed on page 1 of the output.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1 card in this group.</td>
</tr>
<tr>
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<td>ND</td>
<td>I5</td>
<td>1-5</td>
<td>Number of data points.</td>
</tr>
<tr>
<td></td>
<td>T1</td>
<td>F10.0</td>
<td>6-15</td>
<td>Scaling factor by which each coordinate is multiplied, e.g., to changed coordinates from miles to feet, set T1=5280.0. If left blank, T1=1.0 is assumed.</td>
</tr>
<tr>
<td></td>
<td>VT</td>
<td>F10.0</td>
<td>16-25</td>
<td>Data conversion factor, e.g., to change transmissivity in ft²/day to gpd/ft, set VT=7.48. If left blank, VT=1.0 is assumed.</td>
</tr>
<tr>
<td></td>
<td>LOGOPT</td>
<td>I1</td>
<td>30</td>
<td>Set to 1 if log₁₀ transformation of data is desired, otherwise leave blank. Logarithms will be taken after all data have been multiplied by VT.</td>
</tr>
<tr>
<td>Data Group</td>
<td>Variable</td>
<td>Format</td>
<td>Card Columns</td>
<td>Description</td>
</tr>
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<td>----------</td>
<td>--------</td>
<td>--------------</td>
<td>-------------</td>
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<tr>
<td>2 (con.)</td>
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<td>31-35</td>
<td>Maximum number of computational lags desired in sample semi-variogram calculation.</td>
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<td>Arc measure in degrees of angle class size (see Figure E-1). If left blank, DA=90.0/NDI is assumed.</td>
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<tr>
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<td>DP</td>
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<td>56-65</td>
<td>Length of distance class (see Figure E-1). If left blank, DP=PAS/2.0 is assumed.</td>
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<tr>
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<td>TEST</td>
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<td>66-75</td>
<td>Any data that are greater than or equal to TEST will be excluded from the sample semi-variogram calculation. If left blank, TEST=10^10 is assumed.</td>
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<tr>
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<td>I=1,2, ..., NDI. Principal directions in which sample semi-variograms are to be calculated (see Figure E-1). The first direction is specified in columns 1-5, the second in columns 6-10, etc. Use as many data cards as necessary in this group.</td>
</tr>
<tr>
<td>4</td>
<td>LABEL</td>
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<td>Titles for sample semi-variogram line printer plots. Use one card for each heading. First card corresponds to direction ALP(1), second to ALP(2), etc. NDI cards in this group.</td>
</tr>
<tr>
<td>Data Group</td>
<td>Variable</td>
<td>Format</td>
<td>Card Columns</td>
<td>Description</td>
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<td>----------</td>
<td>--------</td>
<td>--------------</td>
<td>-------------</td>
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<td>5</td>
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<td>Input format for data in Group 6. Enough format codes must be specified for 1 integer variable and 3 floating-point variables in that order. Enclose format in parentheses, e.g., (15,3F10.0). 1 card in this group.</td>
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<td></td>
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<td>Datum number.</td>
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<tr>
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<td></td>
<td>x coordinate.</td>
</tr>
<tr>
<td></td>
<td>Y(I)</td>
<td></td>
<td></td>
<td>y coordinate.</td>
</tr>
<tr>
<td></td>
<td>VR(I)</td>
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<td></td>
<td>Values of random function at the specified datum. All information about an individual datum is listed on 1 card. ND cards in this group.</td>
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</table>
PROGRAM SEMIVGM(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
DIMENSION NUM(250),X(250),Y(250),VR(250),G(500),G2(500),D(500),
NC(500),FORM(20),HED(20),ALP(10),CAN(10),SAN(10),
LABEL(200)
COMMON TEST,IOUT
DATA IES/4HYES /pN0/4HNO /
IOUT = 6
READ(5,500) HED
WRITE(6,600) HED
READ(5,510) ND,T1,VT,LOGOPT,KMAX,DA,PAS,TEST
NDIM = KMAX*NDI
IF(LOGOPT .EQ. 0) LOGOPT = NO
IF(LOGOPT .EQ. 1) LOGOPT = IES
IF(DA .EQ. 0) DA = 90.0/FLOAT(NDI)
IF(DP .EQ. 0) DP = PAS/2.0
IF(T1 .EQ. 0) T1 = 1.0
IF(VT .EQ. 0) VT = 1.0
IF(TEST .EQ. 0) TEST = 1.0E+10
READ(5,520) (ALP(I),I=1,NDI)
ID = 20*NDI
READ(5,500) (LABEL(I),I=1,ID)
READ(5,500) FORM
DO 20 I=1,ND
READ(5,FORM) NUM(I),X(I),Y(I),VR(I)
X(I) = X(I)*T1
Y(I) = Y(I)*T1
VR(I) = VR(I)*VT
IF(LOGOPT .EQ. NO) GOTO 20
G(I) = VR(I)
VR(I) = ALOG10(VR(I))
20 CONTINUE
WRITE(6,610) ND,T1,VT,LOGOPT,TEST,KMAX,PAS,DA,(ALP(I),I=1,NDI)
WRITE(6,620) (LABEL(I),I=1,ID)
WRITE(5,500) (NUM(I),I=1,ND)
DO 30 I=1,ND
READ(5,FORM) NUM(I),X(I),Y(I),VR(I)
IF(LOGOPT .EQ. IES) WRITE(6,650) NUM(I),X(I),Y(I),VR(I)
30 CONTINUE
CALL GAMA3 (VRPXPYPNDP
3(MAXPPASOPPNDIpALP,DApNC,G,G2PDPUPVPNP
1	 CAN,SAN,NDIM)
CALL PLOT (DpG,NC,KMAXpLABEL,NDIPNDIMpID)
STOP
500 FORMAT(20A4)
510 FORMAT(I5,2F10.0,3I5,F5.0,3F10.0)
520 FORMAT(10F5.0)
600 FORMAT(1H1,10X,5H*****20A4,///)
610 FORMAT(1H ,5X,41NUMBER OF DATA POINTS-------------,I4,/
1 1H ,5X,41MAP SCALE TRANSFORMATION FACTOR-------------,E11.5,/
2 1H ,5X,41DATA CONVERSION FACTOR-------------,E11.5,/
3 1H ,5X,41LOG BASE 10 TRANSFORMATION OF DATA--------,A4,/
4 1H ,5X,41HAPER LIMIT OF DATA---------------------,E11.5,/
5 1H ,5X,41NUMBER OF COMPUTATIONAL LAGS-------------,I4,/
6 1H ,5X,41LENGTH OF UNIT LAG----------------------,E11.5,/
7 1H ,5X,41NUMBER OF VARIOGRAM DIRECTIONS--------,I4,/
8 1H ,5X,41SIZE OF ANGLE CLASS (DEGREES)---------,E11.5,/
9 1H ,5X,41ANGLE DIRECTIONS FROM THE X AXIS------,/
B (1H+,46X,E11.5,/)
SUBROUTINE GAMA3 (VR,X,Y,ND,KMAX,PAS,DP,NDI,ALP,DA,NC,G,G2,D,U,V,
1
N,CAN,SAN,NDIM)

A MODIFICATION OF A ROUTINE TAKEN FROM

JOURNAL A.G. AND HUIJBREGTS CH. J.; MINING GEOSTATISTICS, ACADEMIC

..........................

SEMI-VARIOGRAM IN TWO DIMENSIONS

IRREGULAR GRID. THERE MAY BE MISSING DATA...

CALCULATION BY CLASS OF ANGLE AND DISTANCE...

.....PARAMETERS

VR(ND) DATA ARRAY
X(ND),Y(ND) X AND Y COORDINATES OF POINTS
ND NUMBER OF POINTS
KMAX MAXIMUM NUMBER OF COMPUTATION LAGS
PAS LENGTH OF BASIC LAG
DP WIDTH OF DISTANCE CLASS. IF DP=0.0,
       DP=PAS/2. IS TAKEN
NDI NUMBER OF DIRECTIONS
ALP(NDI) ANGLES DEFINING DIRECTIONS (WITH
       RESPECT TO X AXIS IN DEGREES)
DA WIDTH OF ANGLE CLASS. IF DA=0.0,
       DA=90.*NDI IS ASSUMED
NC(KMAX*NDI) NUMBER OF COUPLES/LAG/DIRECTION
G(KMAX*NDI) VARIOGRAM VALUES/LAG/DIRECTION
G2(KMAX*NDI) MOMENT CENTER VARIOGRAM/LAG/DIRECTION
D(KMAX*NDI) AVERAGE DISTANCE/LAG/DIRECTION
U AVERAGE I
V VARIANCE I OF DATA TEST
N NUMBER

.....COMMONS

IOUT LINE PRINTER UNIT NUMBER
TEST SUPERIOR BOUNDARY OF EXISTING DATA.
       IF VR.GE.TEST MISSING OR ELIMINATED DATUM

DIMENSION VR(ND),X(ND),Y(ND),G(NDIM),D(NDIM),NC(NDIM),G2(NDIM),
1       ALP(NDI),CAN(NDI),SAN(NDI)
COMMON TEST, IOUT
DATA IA"/" /

INITIALIZE

PI=3.14159265

END
DO 1 KD=1,NDI
   ALPHA=PI*ALP(KD)/180.
   CAN(KD)= COS(ALPHA)
   SAN(KD)= SIN(ALPHA)
   THETA=PI*DALPHA/180.
   CDA= COS(THETA)
   KMM=KMAX * NDI

DO 10 IK=1,KMM
   NC(IK)=0
   D(IK)=0.
   02(IK) = 0.0
   10 G(IK)=0.

IF(VR(ND).TEST)13,12,12
   N=0
   U=0.
   V=0.
   GO TO 11
13 N=1
   U=VR(ND)
   V=VR(ND)*VR(ND)
11 CONTINUE

COMPUTE SEMI-VARIOGRAM, NEW POINT

NDI=ND-1
DO 2 I=1,ND1
   VR1=VR(I)
   IF(VR1.GE.TEST)GO TO 2
   N=N+1
   U=U+VR1
   V=V+VR1*VR1
   II=I+1

NEW LAG

DO 21 J=I,ND
   IF(VR(J).GE.TEST)GO TO 21
   DX=X(J)-X(I)
   DY=Y(J)-Y(I)
   H= SQRT(DX*DX+DY*DY)
   IF(H.LT.1.E-03)GO TO 25
   K = AINT(H/PAS + 0.5) + 1.0

H1= ABS(H-(K-1)*PAS)
   IF(K.GT.KMAX.OR.H1.GT.TOL)GO TO 21

NEW DIRECTION

DO 22 KD=1,NDI
   COSD=(DX*CAN(KD)+DY*SAN(KD))/H
   IF( ABS(COSD).GE.CDA)GO TO 23

22 CONTINUE
   GO TO 21
23 IK=K+KMAX*(KD-1)
   NC(IK)=NC(IK)+1
   DIK=D(IK)+H
SUBROUTINE PLOT (D, G, N, KMAX, LABEL, NDI, NDI, M1)
DIMENSION D(NDI), G(NDI), N, M1, LABEL(M1), DOT(101),
1 SCALEX(N), SCALEY(N)
DATA BLANK, STAR, X/1H, 1H, 1H/
DO 10 I=1, NDI
1= (I-1)*2 + 1
I2= KMAX*1
I3= I1 + 1
GMAX= G(I1)
DMAX= D(I1)
DO 20 J=13, I2
1F(G(J) .EQ. 0.0) GOTO 20
1F(G(J) .GT. GMAX) GMAX= G(J)
1F(D(J) .GT. DMAX) DMAX= D(J)
CONTINUE
DELG= GMAX/50.0
DELD= DMAX/100.0
SCALEX(1)= 0.0
SCALEY(N)= 0.0
DO 30 J=2, N
SCALEX(J)= DELD*(FLOAT(10*(J-1)))
30 CONTINUE
DO 40 J=2, N
SCALEY(J-1)= GMAX — DELG*(FLOAT(J-2))
40 CONTINUE
DO 50 J=1, N
50 CONTINUE
GPLUS= SCALEY(J) + DELG/2.0
GMINUS= SCALEY(J) — DELG/2.0
DO 70 K=I1, I2
IF(G(K) .EQ. 0.0) GOTO 70
IF(G(K) .GT. GMAX) GMAX= G(K)
IF(D(K) .GT. DMAX) DMAX= D(K)
CONTINUE
IF(MOD(J-1, 5) .EQ. 0) WRITE(6, 610) SCALEY(J), DOT
IF(MOD(J-1, 5) .NE. 0) WRITE(6, 620) DOT
50 CONTINUE
RETURN
600 FORMAT(1H11, 5X, 5H*****20A4, //)
610 FORMAT(1H11, 5X, 12.5, 2X, 1H11, 101A1)
620 FORMAT(1H11, 19X, 1H11, 101A1)
630 FORMAT(1H11, 20X, 1H11, 20(5H----))
640 FORMAT(1H11, 19X, 5(E11.5, 9X), E11.5)
650 FORMAT(1H, 29X, 5(E11.5, 9X), /)
660 FORMAT(1HO, 10X, 46H PLOTTING CODES: * = GREATER THAN 30 DATA PAIRS,
1 /1HO, 26X, 25HX = 30 OR LESS DATA PAIRS)
END
Program KRIGE

Program KRIGE is designed to (1) assign kriged estimates to the zones of an irregular, two-dimensional finite-element mesh, which may comprise either quadrilaterals or triangles, and (2) compute the covariance matrix of the kriging errors. The program has four user options because kriging is potentially an expensive procedure and it is important to check that all input data are correct. These options are: (1) data checking only, with no kriging being attempted; (2) jackknifing the field data, whereby each datum is systematically deleted and then kriged using the remaining data; (3) kriging the zones of the finite-element mesh; and (4) evaluation of the kriging-error covariance matrix. Options 2 and 3 operate independently; however, option 4 is contingent on the successful execution of option 3. The jackknifing option (option 2) is useful to assess the accuracy of the semi-variogram model selected for the kriging analysis.

It is the opinion of the author that the criticisms about kriging being a prohibitively expensive exercise and requiring large amounts of computer time are unwarranted. However, computation of the kriging-error covariance matrix can require a relatively larger amount of computer time. For example, kriging the 46 zones of the northern Avra Valley subregion using the kriging plan discussed in the text required about 7 seconds of C.P.U. time on the CDC Cyber 175 computer at The University of Arizona. However, calculating the kriging-error covariance matrix in this case required about 160 seconds of C.P.U. time.
Mechanics of KRIGE

Program KRIGE uses the "moving-neighborhood" method to determine which data will be used to krig each zone. Potentially, all the data in the domain being studied could be used to krig a zone; however, case studies have shown that those data closest to the centroid of each zone are usually assigned the largest kriging weights (David, 1976; Kim and Knudsen, 1977). This is a good reason to limit the number of data used to evaluate the kriging system. With the moving-neighborhood method, only those data that lie in a circular neighborhood around each zone are considered when the kriging system for that zone is being evaluated. Each circular neighborhood is positioned such that its center coincides with the centroid of its corresponding zone. The data lying in each neighborhood are then ranked according to their distance from the zone's centroid. Those data that lie closest to the centroid, up to a specified maximum number, are subsequently used to evaluate the kriging system. Kriging using the moving-neighborhood method must be employed when only the intrinsic hypothesis can be inferred in the domain being studied.

Program KRIGE is currently written to use a spherical semi-variogram model. If a different semi-variogram model is required, subroutine GAMMA must be rewritten. Instructions for rewriting this subroutine are included in the listing of the program.

Up to eight semi-variogram parameters are allowed in the program at present. Usually only two or three semi-variogram parameters are necessary; however, more parameters may be required if a
composite (or "nested") semi-variogram model is to be used (see Journel and Huijbregts, 1978, Chap. 3). Geometric anisotropy of the semi-variogram model, if present, is accounted for by making a general transformation of the coordinates (Journel and Huijbregts, 1978, p. 129).

The kriging system is written in terms of a "pseudocovariance" rather than in terms of the covariance (Equation (86)) or the semi-variogram (Equation (93)). The pseudocovariance, \( C'(s) \), is defined by Journel and Huijbregts (1978, p. 306) as

\[ C'(s) = A - \gamma(s) \]

where \( A \) is any positive real number that is at least as great as the largest value of the semi-variogram function between two points in the domain being studied. Writing the kriging system in terms of the pseudocovariance forces the matrix \( \mathbf{K} \) in Equation (88) to be positive definite. This allows certain efficient numerical schemes to be used when solving for the kriging weights. Writing the kriging system in terms of the pseudocovariance is an efficient means of applying kriging when the intrinsic hypothesis must be inferred.

The mean values of the semi-variogram within the zones and between the data points and the zones are evaluated using numerical integration. To accomplish this, each zone is approximated by a regular network of points.

The kriging weights are solved for by using the IMSL Edition 8 subroutine LEQT1F (International Mathematical and Statistical Library, 1980). This subroutine uses the Crout algorithm to perform Gaussian
elimination. Subroutine LEQT1F is called once in each of the sub-
routines JAKNYF and ZNKRGE of program KRIGE. If necessary, a dif-
ferent subroutine could be written to replace LEQT1F if this IMSL
subroutine is not available.

User's Guide and Program Listing

The input data for KRIGE are arranged into 10 data groups. A
data group may comprise one or more data cards (records).

The arrays used in KRIGE are dimensioned in four common
statements and one DIMENSION statement. If any of the arrays that
are dimensioned in the COMMON statements of the main program unit
require redimensioning, they must also be redimensioned in the sub-
routines that contain the same COMMON statements. However, the
dimensions of the arrays that are listed in the DIMENSION statement of
the main program unit need only be altered in this program unit; the
dimension of these arrays in the subroutines will adjust automatically.

The required dimensions of the arrays are:

P -- see Group 2 of the User's Guide below
NUM(ND)
X(ND)
Y(ND)
Z(ND)
VAR(ND)
DIST(ND)
IHOL(ND)
XND(NUMNP)
YND(NUMNP)
ND1(NZONE)
ND2(NZONE)
ND3(NZONE)
ND4(NZONE)
XC(NZONE)
YC(NZONE)
NDATA(NZONE,NPTS)
The variables ND, NUMNP, NZONE, NPTS, NPZONE, and MBW are all defined in various data groups of the User's Guide listed below.

<table>
<thead>
<tr>
<th>Data Group</th>
<th>Variable</th>
<th>Format</th>
<th>Card Columns</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>IOPT1</td>
<td>I1</td>
<td>1</td>
<td>Data-checking option. Leave blank if data check only is required. Otherwise set equal to 1.</td>
</tr>
<tr>
<td></td>
<td>HEAD</td>
<td>19A4</td>
<td>5-80</td>
<td>Job title--will be printed on page 1 of the output.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1 card in this group</td>
</tr>
<tr>
<td>2</td>
<td>P(1)</td>
<td>8F10.0</td>
<td>1-80</td>
<td>I=1,2, .. ,8. Possible semi-variogram parameters. The program is currently written for a spherical semi-variogram model, and only P(1) to P(3) need be assigned non-zero values as follows: P(1)=nugget effect, P(2)=sill - nugget, P(3)=range. P1 is specified in columns 1-10, P(2) in columns 11-20, etc., and P(8) in columns 71-80.</td>
</tr>
<tr>
<td>Data Group</td>
<td>Variable</td>
<td>Format</td>
<td>Card Columns</td>
<td>Description</td>
</tr>
<tr>
<td>------------</td>
<td>----------</td>
<td>--------</td>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>2</td>
<td>PSEUDO</td>
<td>F10.0</td>
<td>1-10</td>
<td>&quot;Pseudocovariance&quot; parameter. Must be at least as great as the largest value of the semi-variogram function between two points in the domain being studied. If left blank PSEUDO = P(1) + P(2) is assumed. This will cause the kriging system for the spherical semi-variogram model to be written in terms of the covariance function.</td>
</tr>
<tr>
<td></td>
<td>(con.)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>ANG</td>
<td>F10.0</td>
<td>11-20</td>
<td>Angle of anisotropy in degrees. This is the angle between the x-axis and the major axis of the anistropy ellipse (Figure E-2).</td>
</tr>
<tr>
<td></td>
<td>AFR</td>
<td>F10.0</td>
<td>21-30</td>
<td>Anistropy factor (Figure E-2). If left blank, AFR = 1.0 is assumed, i.e., the semi-variogram model is assumed to be isotropic. If AFR &gt; 1, the semi variogram model must correspond to the model in the direction of the major axis of the anistropy ellipse (Journel and Huijbregts, 1978, p. 179).</td>
</tr>
<tr>
<td>3</td>
<td>NUMNP</td>
<td>I5</td>
<td>1-5</td>
<td>Number of nodal points in the finite-element mesh.</td>
</tr>
<tr>
<td></td>
<td>NZONE</td>
<td>I5</td>
<td>6-10</td>
<td>Number of zones in the finite-element mesh.</td>
</tr>
<tr>
<td></td>
<td>T1</td>
<td>F10.0</td>
<td>11-20</td>
<td>x-coordinate displacement. All x-coordinates will be displaced by T1. This permits the coordinates of all the data in Groups 4 and 6 to be aligned with the coordinates of another map, for example.</td>
</tr>
</tbody>
</table>
AFR = \frac{a}{b}

Figure E-2. Anisotropy ellipse of semi-variogram model
<table>
<thead>
<tr>
<th>Data Group</th>
<th>Variable</th>
<th>Format</th>
<th>Card Columns</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 (con.)</td>
<td>T2</td>
<td>F10.0</td>
<td>21-30</td>
<td>y-coordinate displacement. Same explanation as for T1 except for the y-coordinate.</td>
</tr>
<tr>
<td></td>
<td>T3</td>
<td>F10.0</td>
<td>31-40</td>
<td>Scaling factor by which each displaced coordinate is multiplied, e.g., all x-coordinates in Groups 4 and 6 will be transformed as (x+T1)*T3 and all y-coordinates as (y+T2)*T3. This parameter allows map scales to be changed. If left blank, T3=1.0 is assumed.</td>
</tr>
</tbody>
</table>

This data group contains the finite-element mesh nodes and their coordinates. Figure E-3 illustrates a typical finite-element mesh that may be used by program KRIGE. Nodes may be numbered in any order, starting from node 1 and ending in node NUMNP. It is more efficient, however, to consecutively number the nodes from one edge of the mesh to the other.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Format</th>
<th>Card Columns</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>I5</td>
<td>1-5</td>
<td>Node number.</td>
</tr>
<tr>
<td>XND(N)</td>
<td>F10.0</td>
<td>6-15</td>
<td>x-coordinate of node N.</td>
</tr>
<tr>
<td>YND(N)</td>
<td>F10.0</td>
<td>16-25</td>
<td>y-coordinate of node N.</td>
</tr>
</tbody>
</table>

In general, one data card is required for each node of the finite-element mesh. However, if there is a sequence of consecutively numbered, evenly spaced nodes, as, for example, nodes 5 to 9 in Figure E-3A, only the first and last nodes in
Figure E-3. Typical finite-element mesh (A) and zone of a finite-element mesh (B) which may be used by program KRIGE
This data group contains the information about the zones of the finite-element mesh. Each zone requires a number. Zones may be numbered in any fashion starting from zone 1 and ending in zone NZONE. It is more efficient, however, to number the zones consecutively from one edge of the mesh to the other. The numbers of the nodes at the corners of each zone must be specified. Corner node numbers are designated in a counterclockwise order (see Figure E-3B).

<table>
<thead>
<tr>
<th>Data Group</th>
<th>Variable</th>
<th>Format</th>
<th>Card Columns</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 (con.)</td>
<td></td>
<td></td>
<td></td>
<td>that sequence need be specified. The intermediate nodes in the sequence will be automatically generated. The data cards in Group 4 must be ranked according to node number, node 1 being first and node NUMNP being last.</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td></td>
<td></td>
<td>This data group contains the information about the zones of the finite-element mesh. Each zone requires a number. Zones may be numbered in any fashion starting from zone 1 and ending in zone NZONE. It is more efficient, however, to number the zones consecutively from one edge of the mesh to the other. The numbers of the nodes at the corners of each zone must be specified. Corner node numbers are designated in a counterclockwise order (see Figure E-3B).</td>
</tr>
</tbody>
</table>

- **N** I5 1-5 Zone number.
- **ND1(N)** I5 6-10 Number of first corner node.
- **ND2(N)** I5 11-15 Number of second corner node.
- **ND3(N)** I5 16-20 Number of third corner node.
- **ND4(N)** I5 21-25 Number of fourth corner node. If zone N is a triangle, ND4(N) must be zero.
<table>
<thead>
<tr>
<th>Data Group</th>
<th>Variable</th>
<th>Format</th>
<th>Card Columns</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 (con.)</td>
<td></td>
<td></td>
<td></td>
<td>consecutively numbered nodes, as, for example, zones 1 to 3 or zones 5 to 8 in Figure E-3A, only the first and last zones and their respective corner nodes need be specified. The corner nodes of these zones must be specified in the same relative order, e.g., in Figure E-3A, if node 10 is ND1(5), then node 13 must be ND1(8). The intermediate zones in the sequence will be automatically generated. Every triangular zone must be specified. The data cards in Group 5 must be ranked according to zone number: zone 1 being first and zone NZONE being last.</td>
</tr>
<tr>
<td>6</td>
<td>ND</td>
<td>I5</td>
<td>1-5</td>
<td>Number of data points.</td>
</tr>
<tr>
<td></td>
<td>DCF</td>
<td>F10.0</td>
<td>6-15</td>
<td>Data conversion factor; e.g., to convert transmissivity in ft²/day to gpd/ft, set DCF = 7.48. If left blank, DCF = 1.0 is assumed.</td>
</tr>
<tr>
<td></td>
<td>LOGOPT</td>
<td>I1</td>
<td>20</td>
<td>Set to 1 if ( \log_{10} ) transformation of data is desired, otherwise leave blank. Logarithms will be taken after all data have been multiplied by DCF.</td>
</tr>
<tr>
<td></td>
<td>FORM</td>
<td>15A4</td>
<td>21-80</td>
<td>Input format for data in Group 7. Enough format codes must be specified for one integer variable and four floating-point variables in that order. Enclose format in parentheses, e.g., (15,3F10.0,F15.0).</td>
</tr>
</tbody>
</table>

1 card in this group
<table>
<thead>
<tr>
<th>Data Group</th>
<th>Variable</th>
<th>Format</th>
<th>Card Columns</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>NUM(I)</td>
<td></td>
<td></td>
<td>Datum number.</td>
</tr>
<tr>
<td></td>
<td>X(I)</td>
<td></td>
<td></td>
<td>x-coordinate.</td>
</tr>
<tr>
<td></td>
<td>Y(I)</td>
<td></td>
<td></td>
<td>y-coordinate.</td>
</tr>
<tr>
<td></td>
<td>Z(I)</td>
<td></td>
<td></td>
<td>Value of random function at specified datum.</td>
</tr>
<tr>
<td></td>
<td>VAR(I)</td>
<td></td>
<td></td>
<td>Variance of error of measurement, sampling, or prediction of Z(I).</td>
</tr>
</tbody>
</table>

All information about an individual datum is listed on one card.

**ND cards in this group**

If IOPT1=0 in Group 1, skip Groups 8 and 9 and proceed directly to Group 10.

---

<table>
<thead>
<tr>
<th>Data Group</th>
<th>Variable</th>
<th>Format</th>
<th>Card Columns</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>IOPT2</td>
<td>I1</td>
<td>1</td>
<td>Set equal to 1 if jack-knifing is required. If jackknifing is not required, set IOPT2=0 and proceed to Group 9.</td>
</tr>
<tr>
<td></td>
<td>ICHK1</td>
<td>I5</td>
<td>6-10</td>
<td>Set equal to 1 if a check of the kriging system during jackknifing is required. This will cause many pages of output to be produced. The numbers of data points used to jackknife</td>
</tr>
<tr>
<td>Data Group</td>
<td>Variable</td>
<td>Format</td>
<td>Card Columns</td>
<td>Description</td>
</tr>
<tr>
<td>------------</td>
<td>----------</td>
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<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>8 (con.)</td>
<td></td>
<td></td>
<td></td>
<td>each datum, the right-hand vector of the kriging system (written in terms of the pseudocovariance), and the kriging weights will be printed for each datum if ICHK1=1. If no check of the kriging system is required, set ICHK1=0.</td>
</tr>
<tr>
<td>NPTS</td>
<td>I5</td>
<td>11-15</td>
<td></td>
<td>The maximum number of data points that will be used to evaluate the kriging system. These data will be found in the circular neighborhood around each deleted datum.</td>
</tr>
<tr>
<td>RMAX</td>
<td>F10.0</td>
<td>16-25</td>
<td></td>
<td>Radius of circular neighborhood within which the data used to evaluate the kriging system will be found.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1 data card in this group</td>
</tr>
<tr>
<td>9</td>
<td></td>
<td></td>
<td></td>
<td>This group contains the information required to execute the zone-kriging option and to compute the kriging-error covariance matrix.</td>
</tr>
<tr>
<td>IOPT3</td>
<td>I1</td>
<td>1</td>
<td></td>
<td>Set equal to 1 if the zones of the finite-element mesh are to be kriged. If kriging is not desired, set IOPT3=0 and proceed to Group 10.</td>
</tr>
<tr>
<td>ICHK2</td>
<td>I1</td>
<td>10</td>
<td></td>
<td>Set equal to 1 if a check of the kriging system of each zone is required. This will cause many pages of output to be produced. The numbers of data points used to krig each zone, the right-hand side vector of the kriging system (written in terms of the pseudocovariance),</td>
</tr>
<tr>
<td>Data Group</td>
<td>Variable</td>
<td>Format</td>
<td>Card Columns</td>
<td>Description</td>
</tr>
<tr>
<td>------------</td>
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</tr>
<tr>
<td>9 (con.)</td>
<td></td>
<td></td>
<td></td>
<td>and the kriging weights for each zone will be printed if ICHK2=1. If no check of the kriging system is required, set ICHK2=0.</td>
</tr>
</tbody>
</table>

**NPTS** | I5 | 11-15 | The maximum number of data points that will be used to evaluate the kriging system. These data will be found in the circular neighborhood around each zone. If left blank and IOPT2 =1 in Group 8, then the value NPTS set in Group 8 will be assumed. |

**NPZONE** | I5 | 16-20 | Number of points used to approximate a quadrilateral zone for numerical integration. This number must be the square of an integer, e.g., 9, 36, 64, etc. The number of points used to approximate a triangle will be $\sqrt{NPZONE}*(\sqrt{NPZONE} + 1)/2$. |

**RMAX** | F10.0 | 21-30 | Radius of circular neighborhood within which the data used to evaluate the kriging system will be found. If left blank and IOPT2=1 in Group 8, then the value of RMAX set in Group 8 is assumed. |

**IPNCH1** | I1 | 35 | Set equal to 1 if the results of kriging the zones are to be punched on cards, one card per zone. The punched output will include the zone number, its centroid coordinates, the kriged estimate, and the kriging error ($\sigma_K$). If no punched output is desired, set IPNCH1=0. |
<table>
<thead>
<tr>
<th>Data Group</th>
<th>Variable</th>
<th>Format</th>
<th>Card Columns</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>9 (con.)</td>
<td>IOPT4</td>
<td>I1</td>
<td>40</td>
<td>Set equal to 1 if the kriging-error covariance matrix is to be evaluated. If this is not desired, set IOPT4=0 and proceed to Group 10.</td>
</tr>
<tr>
<td>MBW</td>
<td>I5</td>
<td></td>
<td>41-45</td>
<td>Reduced band width of the kriging-error covariance matrix. MBW must never be larger than NZONE. If MBW is accidentally set greater than NZONE, MBW=NZONE is assumed. The correlation between kriging errors generally becomes negligible when the centroids of their corresponding zones are separated by greater than about twice the range of the semi-variogram model. Thus evaluating the covariance between the kriging errors of zones that lie far apart may be wasteful in terms of computer time. MBW can be used to prevent the calculation of the covariance between the kriging errors of zones separated by large distances. The kriging errors of two zones whose numbers (N in Group 5) differ by more than MBW are assumed to be uncorrelated. Choice of MBW is dependent on how the zones of the finite-element mesh are numbered.</td>
</tr>
<tr>
<td>IPNCH2</td>
<td>I1</td>
<td></td>
<td>50</td>
<td>Set equal to 1 if the kriging-error covariance matrix is to be punched on cards. Because this matrix is symmetric, only the upper triangle will be punched. This will be punched in band-symmetric storage mode. Set IPNCH2=2 if the upper triangle of the</td>
</tr>
<tr>
<td>Data Group</td>
<td>Variable</td>
<td>Format</td>
<td>Card Columns</td>
<td>Description</td>
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<tr>
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</tr>
<tr>
<td>9 (con.)</td>
<td></td>
<td></td>
<td></td>
<td>kriging-error covariance is to be written to a permanent file. In this case, TAPE1 must be cataloged as a permanent file. The upper triangle of the covariance matrix will be written to TAPE1, again in band-symmetric storage mode, using the format code 5E16.8.</td>
</tr>
</tbody>
</table>

1 card in this group

| 10        | END      | A3     | 5-7          | This group is used to terminate the job. If another job is to be run, proceed to Group 1 and begin coding again. Otherwise punch "END" in columns 5-7. |

1 card in this group
PROGRAM KRIGE(INPUTP0UTP1JTPPUNCH,TAPE5=INPUTpTAPE6=OUTPUTp
1 TAPE7=PUNCH,TAPE1)
COMMON /GRP1/ P(8),PSEUD9
COMMON /GRP2/ NUM(175),X(175),Y(175),Z(175),VAR(175),DIST(175),
1 IHOL(175)
COMMON /GRP3/ XND(200),YND(200),ND1(200),ND2(200),ND3(200),
1 ND4(200),XC(200),YC(200)
COMMON /GRP4/ MBW,NPZ0NE,NDATA(200,25),RLAMDA(200,25),
1 XLOC(200,64),YLOC(200,64),CVR(200,100)
DIMENSION HEAD(19),FORM(15),A(26,26),B(26,1),WKAREA(26),BTEMP(25),
1 INDX(25),SIDE2(8,2),SIDE4(8,2)
DATA IES/4H YES/,NO/4H NO/,END/4HEND /
100 READ(5,500) IOPT1,HEAD
IF(HEAD(1) .EQ. END) GOTO 220
CALL DATE(DAT)
WRITE(6,600) HEAD,DAT
IF(IOPT1 .EQ. 0) WRITE(6,601)
READ(5,510) (P(I),I=1,8),PSEU00p4NG,AFR
IF(AFR .EQ. 0.0) AFR = 1.0
IF(PSEUDO .EQ. 0.0) PSEUDO = P(1) + P(2)
ANG = ANG*0.017453292
COSA = COS(ANG)
SINA = SIN(ANG)
A1 = COSA**2 + AFR*(SINA**2)
A2 = SINA**2 + AFR*COSA**2
A3 = SINA*COSA*(1.0 - AFR)
A4 = SINA**2 + (SINA**2)/AFR
A5 = SINA*COSA*(1.0 - 1.0/AFR)
READ(5,520) NUMNP,NZONE,T1,T2,T3
IF(T3 .EQ. 0.0) T3 = 1.0
WRITE(6,620) T1,T2,T3,NMNP,NZONE
ID = 0
110 ID1 = ID
READ(5,530) ID,XND(ID),YND(ID)
IF(ID .LE. ID1) GOTO 170
IF(ID .GT. ID. NUMNP) GOTO 180
XND(ID) = (XND(ID) + T1)*T3
YND(ID) = (YND(ID) + T2)*T3
IF(ID .EQ. ID1+1 .AND. ID .EQ. NUMNP) GOTO 120
IF(ID .EQ. ID1+1) GOTO 110
DELX = (XND(ID) - XND(ID1))/FLOAT(ID - ID1)
DELY = (YND(ID) - YND(ID1))/FLOAT(ID - ID1)
IF(ID .EQ. ID1+1) GOTO 110
DO 10 I=ID2,ID3
XND(I) = XND(ID1) + DELX*FLOAT(I - ID1)
YND(I) = YND(ID1) + DELY*FLOAT(I - ID1)
10 CONTINUE
IF(ID .EQ. NUMNP) GOTO 120
GOTO 110
120 ID = 0
130 ID1 = ID
READ(5,540) ID,ND1(ID),ND2(ID),ND3(ID),ND4(ID)
IF(ID .LE. ID1) GOTO 190
IF(ID .GT. ID1+1 .AND. ND4(ID) .EQ. 0) GOTO 200
IF(ID .GT. NZONE) GOTO 210
IF(ID .EQ. ID1+1 .AND. ID .EQ. NZONE) GOTO 140
IF(ID .EQ. ID1+1) GOTO 130
ID2 = ID1 + 1
ID3 = ID - 1
DO 20 I=ID2, ID3
   ND1(I) = ND1(ID1) + I - ID1
   ND2(I) = ND2(ID1) + I - ID1
   ND3(I) = ND3(ID1) + I - ID1
   ND4(I) = ND4(ID1) + I - ID1
20 CONTINUE
IF(ID .EQ. NZONE) GOTO 140
GOTO 130
140 DO 30 I=1, NZONE
   N1 = ND1(I)
   N2 = ND2(I)
   N3 = ND3(I)
   N4 = ND4(I)
   XC(I) = (XND(N1) + XND(N2) + XND(N3))/3.0
   YC(I) = (YND(N1) + YND(N2) + YND(N3))/3.0
   IF(N4 .EQ. 0) GOTO 30
   CX = (XND(N1) + XND(N3) + XND(N4))/3.0
   CY = (YND(N1) + YND(N3) + YND(N4))/3.0
   AT1 = (XND(N1)*YND(N3) - YND(N1)*XND(N3))/2.0
   AT2 = (XND(N2)*YND(N3) - YND(N2)*XND(N3))/2.0
   XC(I) = (XC(I)*AT1 + CX*AT2)/(AT1 + AT2)
   YC(I) = (YC(I)*AT1 + CY*AT2)/(AT1 + AT2)
30 CONTINUE
DO 40 I=1, NUMNP
   WRITE(6,630) I, XND(I), YND(I)
   XTEMP = XND(I)
   XND(I) = A1*XTEMP + A3*YND(I)
   YND(I) = A3*XTEMP + A2*YND(I)
40 CONTINUE
WRITE(6,640)
DO 50 I=1, NZONE
   IF(N4(I) .EQ. 0) GOTO 150
   WRITE(6,650) I, N1(I), N2(I), N3(I), N4(I), XC(I), YC(I)
   GOTO 50
150 WRITE(6,651) I, ND1(I), N2(I), N3(I), XC(I), YC(I)
50 CONTINUE
READ(5,550) ND, DCF, LOGOPT, FORM
IF(DCF .EQ. 0.0) DCF = 1.0
IF(LOGOPT .EQ. 0) LOGOPT = NO
IF(LOGOPT .EQ. 1) LOGOPT = IES
WRITE(6,660) ND, DCF, LOGOPT
DO 60 I=1, ND
   READ(5, FORM) NUM(I), X(I), Y(I), Z(I), VAR(I)
   X(I) = (X(I) + T1)*T3
   Y(I) = (Y(I) + T1)*T3
   Z(I) = Z(I)*DCF
   IF(LOGOPT .EQ. IES) Z(I) = ALOG10(Z(I))
   WRITE(6,670) NUM(I), X(I), Y(I), Z(I), VAR(I)
   XTEMP = X(I)
   X(I) = A1*XTEMP + A3*Y(I)
   Y(I) = A3*XTEMP + A2*Y(I)
60 CONTINUE
KRASH = 0
II = NO - 1
DO 70 I=1, II
   I2 = I + 1
70 CONTINUE
DO 80 J=I2,ND
   IF(X(I) .NE. X(J) .OR. Y(I) .NE. Y(J)) GOTO 80
   KRASH = KRASH + 1
   IF(KRASH .EQ. 1) WRITE(6,680)
   WRITE(6,681) NUM(I),NUM(J)
80 CONTINUE
70 CONTINUE
   IF(KRASH .GT. 0) GOTO 220
   IF(IOPT1 .EQ. 0) GOTO 100
   READ(5,560) IOPT2,ICHK1,NPTS,RMAX
   IF(IOPT2 .EQ. 0) GOTO 160
   NDIM = NPTS + 1
   N1 = NPTS
   R1 = RMAX
   CALL JAKNYF (ND,NPTS,NDIM,RMAX,ICMK1,A,B,WKAREA,8TEMPIPINDX)
160 READ(5,570) IOPT3,ICMK2,NPTS,NPZONE,RMAX,IPNCH1,IOPT4,RB,E,IPNCH2
   IF(IOPT3 .EQ. 0) GOTO 100
   IF(NPZ .EQ. 0) NPTS = N1
   NDIM = NPTS + 1
   NPS = IFIXI(SQRT(FLOAT(NPZONE) + 0.1))
   NPTR = NPS*(NPS + 1)**2 + 0.1
   CALL ZNKRGE (A4,A5,A6,ICMK2,NDIM,NPTS,NPZONE,RMAX,A,8,8TEMA,INDX)
   IF(IOPT4 .EQ. 0) GOTO 100
   CALL COVAR (NPZONE,NPTS,NPZ,IPNCH2)
   GOTO 100
170 WRITE(6,631) ID
   GOTO 220
180 WRITE(6,632) ID
   GOTO 220
190 WRITE(6,652)  ID
   GOTO 220
200 WRITE(6,653) ID
   GOTO 220
210 WRITE(6,654) ID
220 STOP
500 FORMAT(I1,3X,19A4)
510 FORMAT(8F10.0)
520 FORMAT(2I5,3F10.0)
530 FORMAT(I5,2F10.0)
540 FORMAT(5I5)
550 FORMAT(I5,F10.0,I5,15A4)
560 FORMAT(I1,4X,2I5,F10.0)
570 FORMAT(I1,4X,3I5,F10.0,4I5)
580 FORMAT(I1H,5X,5H****,19A4,20X,A10,///)
601 FORMAT(I1H,10X,4H***DATA CHECK ONLY — PROGRAM WILL NOT EXECUTE,
1 ////)
610 FORMAT(I1H,5X,20HVARIOMATIC PARAMETERS,,
1 8(IH,10X,2H2P(.I1,27H)----------------------,E11.5,\//),
2 1H,10X,30H"PSEUDO"--------------------------------- ,E11.5,/
3 1H,10X,30HANGLE OF ANISOTROPY------------------ ,E11.5,/
4 1H,10X,30HANISOTROPY FACTOR--------------------- ,E11.5,///)
620 FORMAT(I1H,5X,36HCOORDINATE TRANSFORMATION PARAMETERS,,
1 1H,10X,30HCOORDINATE DISPLACEMENT------ ,E11.5,/
2 1H,10X,30HCOORDINATE DISPLACEMENT------ ,E11.5,/
3 1H,10X,30HSCALING FACTOR------------------ ,E11.5,///)
4 1H,5X,28HZNATION PATTERN INFORMATION,,
5 1H,10X,30HNUMBER OF NODAL POINTS---------- ,I4,\/
SUBROUTINE JAKNYF (ND,NPTS,NDIM,RMAX,ICHK1,A,B,WKAREA,BTEMP,INDX)
COMMON /GRP1/ P(8),PSEUDO
COMMON /GRP2/ NUM(175),X(175),Y(175),Z(175),VAR(175),DIST(175),
            IHOL(175)
DIMENSION A(NDIM,NDIM),B(NDIM,1),WKAREA(NDIM),BTEMP(NPTS),
            INDX(NPTS)
CALL SECOND(TM1)
WRITE(6,600) NPTS,RMAX
NKRG = 0
DIFSUM = 0.0
DIFSQ = 0.0
RMSE = 0.0
IF(ICHK1 .EQ. 1) GOTO 100
WRITE(6,610)
WRITE(6,620)
100 DO 10 I=1,ND
   10 IT = 0
   DO 20 J=1,ND
      IF(J .EQ. I) GOTO 20
      DX = X(J) - X(I)
      DY = Y(J) - Y(I)
      DIS = SQRT(DX**2 + DY**2)
      IF(DIS .GT. RMAX) GOTO 20
      IT = IT + 1
      DIST(I) = DIS
      IHOL(I) = J
      IF(IT .EQ. I) GOTO 20
   CALL DSORT (I)
   20 CONTINUE
I2 = MINO(I1,NPTS)
IF(I2 .LT. 3) GOTO 140
I3 = I2 + 1
DD 30 J=1,I2
J1 = IHOL(J)
J2 = J + 1
INDX(J) = NUM(J1)
A(J,J) = PSEUDO
IF(J .EQ. I2) GOTO 110
DD 40 K=J2,I2
K1 = IHOL(K)
DX = X(K1) - X(J1)
DY = Y(K1) - Y(J1)
CALL GAMMA (DX, DY, GH)
A(J,K) = PSEUDO - GH
A(K,J) = A(J,K)
40 CONTINUE
110 A(J,I3) = 1.0
A(I3,J) = 1.0
CALL GAMMA (DIST(J), 0.0, GH)
B(J) = PSEUDO - GH
BTEMP(J) = B(J, 1)
30 CONTINUE
A(I3,I3) = 0.0
B(I3, 1) = 1.0
IF(ICHK1 .EQ. 0) GOTO 120
WRITE(6,640) I2, (INDX(J), J=1,I2)
WRITE(6,650) (B(J,1), J=1,I3)
123 CALL LEQT1F (A, I3, I3, NDIM, B, 5, WKAREA, IER)
B(I3, 1) = -B(I3, 1)
IF(ICHK1 .EQ. 0) GOTO 130
WRITE(6,660) (B(J,1), J=1,I2)
WRITE(6,670) B(I3, 1)
WRITE(6,610)
130 ZK = 0.0
VZK = 0.0
DD 60 J=1,I2
J1 = IHOL(J)
ZK = ZK + B(J,1)*Z(J1)
VZK = VZK + B(J,1)*(PSEUDO - BTEMP(J))
60 CONTINUE
DIFF = ZK - Z(I)
DIFSUM = DIFSUM + DIFF
VZK = VZK + B(I3,1)
DIFSQ = DIFSQ + DIFF**2
RMSE = RMSE + (DIFF**2)/VZK
VZK = VZK**0.5
WRITE(6,680) NUM(I), Z(I), ZK, DIFF, VZK
140 IF(ICHK1 .EQ. 1) WRITE(6,610)
WRITE(6,690) NUM(I)
150 CONTINUE
NKRG = ND - NKRG
IF(NKRG .EQ. 0) GOTO 150
DIFMN = DIFSUM/FLOAT(NKRG)
VDIF = (DIFSQ - (DIFMN**2)*FLOAT(NKRG))/(FLOAT(NKRG) - 1.0)
RMSE = SQRT(RMSE/FLOAT(NKRG))
CALL SECOND(TM2)
TM2 = TM2 - TM1
WRITE(6,695) DIFMN,VDIF,RMSE,TM2
RETURN

150 FORMAT(1H1,5X,36H*****JACK-KNIFING OF FIELD DATA*****,,///,///,1H ,
         10X,5X,50HMAX. NO. OF DATA USED TO KRIGE DELETED DATUM----- ,I
24,/,1H ,10X,50H RANGE OF SEARCH FROM DELETED DATUM FOR DATA----- ,
3 E11.5,///,///)
610 FORMAT(1H ,7X,1HI,10X,4HZ(I),12X,1H KRIGED Z(I),8X,1HK(Z(I)) - Z,
         3H(I),9X,7HKRIGING,10X,8HNO. DATA,1H ,77X,5HERROR,12X,
2 6HPOINTS)
620 FORMAT(/1H0)
630 FORMAT(1H0,125(1H—))
640 FORMAT(1H0,1H ,5X,32H STATISTICS OF THE KRIGING ERRORS,,//,
1 1H ,10X,34H MEAN OF K(Z(I)) - Z(I)---------- ,E11.5//
2 1H ,10X,34H VARIANCE OF K(Z(I)) - Z(I)---------- ,E11.5//,
3 1H ,10X,34H REDUCED MEAN SQUARE ERROR---------- ,E11.5///,/
4 1H ,5X,47H APPROX. CPU TIME IN SECONDS REQUIRED TO JACK,
5 20H-KNIFE FIELD DATA = ,F9.2)
END

SUBROUTINE ZNKRGE (A4,A5,A6,ICHK2,INPCH1,NDIM,NPS,NPTS,NPTR,
        NZONE,RMAX,A,B,BTEMP,INDEXSIDE4,WKAREA),
1 COMMON /GRP1/ P(8),PSEUDO
COMMON /GRP2/ NUM(175),X(175),Y(175),Z(175),VAR(175),DIST(175),
1       IHOL(175)
COMMON /GRP3/ NDIM(200),YND(200),ZND(200),ND(200),ND1(200),
1       ND2(200),ND3(200),ND4(200),X(200),Y(200)
COMMON /GRP4/ MBW,NPZONE,NDATA(200,25),RLAMDA(200,25),
1       XLOC(200,64),YLOC(200,64),CVR(200,100)
DIMENSION A(NDIM,NDIM),B(NDIM,1),WKAREA(NDIM),BTEMP(NPTS),
1 INDEX(NPTS)
CALL SECOND(TM1)
WRITE(6,600) NPTS,NPZONE,NPTR,RMAX
IF(ICHK2 .EQ. 1) GOTO 100
WRITE(6,610)
WRITE(6,620)
100 R2 = RMAX**2
DO 10 I=1,NZONE
   II = 0
   DO 20 J=1,ND
      DX = X(J) - XC(I)
      DY = Y(J) - YC(I)
      DIS = DX**2 + DY**2
      IF(DIS > R2) GOTO 20
      II = II + 1
   DIST(I1) = DIS
   IHOL(II) = J
   20 CONTINUE
   WRITE(6,630) R2
   WRITE(6,640) II,NDIM
IF(I1 .EQ. 1) GOTO 20
CALL DSORT(I1)
20 CONTINUE
XTEMP = XC(I)
XC(I) = A4*XTEMP + A6*YC(I)
YC(I) = A6*XTEMP + A5*YC(I)
I2 = MINO(I1,NPTS)
I3 = I2 + 1
DO 30 J=1,I2
NDATA(I,J) = IHOL(J)
30 CONTINUE
IF(NPTS .GT. I2) NDATAI,I3) = 0
IF(I2 .LT. 3) GOTO 140
DO 40 J=1,I2
J1 = IHOL(J)
J2 = J + 1
INDX(J) = NUM(J1)
A(J,J) = PSEUDO + VAR(J1)
IF(J .EQ. I2) GOTO 110
DO 50 K=J2,I2
K1 = IHOL(K)
OX = X(K1) — X(J1)
DY = Y(K1) — Y(J1)
CALL GAMMA(DX,DY,GH)
A(J,K) = PSEUDO — GH
A(K,J) = A(J,K)
50 CONTINUE
A(I3,1) = 1.0
A(I3,J) = 1.0
CALL PTVAR(I,NDATI,1,NPTR,X(J1),Y(J1),SIDE2,SIDE4,PBVR)
B(J,1) = PSEUDO — PBVR
BTEMP(J) = B(J,1)
40 CONTINUE
B(I3,1) = 0.0
IF(ICHK2 .EQ. 0) GOTO 120
WRITE(6,640) I2,(INDX(J),J=1,I2)
WRITE(6,650) (B(J,1),J=1,12)
120 CALL LEGTIF(A,I3,NDIM,B,5,WKAREA,IER)
B(I3,1) = —B(I3,1)
IF(ICHK2 .EQ. 0) GOTO 130
WRITE(6,660) (B(J,1),J=1,12)
WRITE(6,670) B(I3,1)
WRITE(6,610)
130 DO 60 J=1,I2
KLAMDA(I,J) = B(J,1)
60 CONTINUE
ZK = 0.0
VZK = 0.0
UG 70 J=1,I2
J1 = IHOL(J)
ZK = ZK + B(J,1)*Z(J1)
VZK = VZK + B(J,1)*(PSEUDO — BTEMP(J))
70 CONTINUE
CALL BKVAR(I,NU4(I),NPTR,BVAR)
CVR(I,1) = VZK — BVAR + B(I3,1)
VZK = SQRT(CVR(I,1))
WRITE(6,690) I,XC(I),YC(I),ZK,VZK,BVAR,I2
IF(IPNCH1 .EQ. 1) PUNCH(7,700) I,XC(I),YC(I),ZK,VZK
IF(ICHK2 .EQ. 1) WRITE(6,630)
GOTO 10
140 IF (ICHK2 .EQ. 1) WRITE(6,610)
   WRITE(6,680) IXC(I), YC(I)
   IF (ICHK2 .EQ. 1) WRITE(6,630)
   XLOC(I,1) = 0.0
   CVR(I,1) = 0.0
10 CONTINUE
   CALL SECOND(TM2)
   TM2 = TM2 - TM1
   WRITE(6,695) TM2
   RETURN
600 FORMAT(1H1,5X,48H*****KRIGING OF ZONES — KRIGED ESTIMATES ARE SPA,
   1 33HTIALLY AVERAGED IN EACH ZONE****,///,1H,
   2 10X,50HMAX. NO. OF DATA USED TO KRIGE EACH ZONE—————,
   3 8H———,I4/1H,
   4 10X,51HNO. OF INTERNAL PTS. USED TO APPROX. A QUADRILATERA,
   5 7H———,I4/1H,49X,19HTRIANGLE—————,I4/1H,10X,
   6 55HRANGE OF SEARCH FROM ZONE CENTROID FOR DATA—————,
   7 /3HM—,E11.5///)
610 FORMAT(1H1H,5X,4HZONE,7X,20HCENTROID COORDINATES,10X,7HKRIGING,13X,
   1 7HKRIGING,11X,12HAVE. VARIQ.,9X,8HNO. DATA,1/H,47X,
   2 5HVALUE,15X,5HERR3R,14X,7HIN ZONE,13X,6HPOIN5,1/H,20X,
   3 1HX,10X,1HY)
620 FORMAT(//1H)
630 FORMAT(1H0,125(1H-))
640 FORMAT(1H0,5X,41HTHE FOLLOWING,I4,25H DATA POINTS WERE USED TO,
   1 22H KRIGE THE NEXT ZONE: /1H0,(/1H*,5X,25I5))
650 FORMAT(1H0,5X,41HTHE RIGHT HAND SIDE VECTOR OF THE KRIGING,
   1 8H SYSTEM: /1H0,(/1H*,5X,10E12.5))
660 FORMAT(1H0,5X,20HTHE KRIGING WEIGHTS: /1H0,(/1H*,5X,10E12.5))
670 FORMAT(1H0,5X,26HTHE LAGRANGIAN MULTIPLIER: /1X,E12.5))
680 FORMAT(1H0,18X,34HZONE NOT KRIGED — FEWERS THAN 3 ,
   1 21HDATA IN NEIGHBROOD)
690 FORMAT(1H0,18X,34HZONE NOT KRIGED — FEWERS THAN 3 ,
   1 21HDATA IN NEIGHBROOD)
695 FORMAT(///,1H0,5X,43HAPPROX. C.P.U. TIME IN SECONDS REQUIRED TO ,
   1 18HKRIGE ALL ZONES = ,F9.2)
700 FORMAT(15,2F10.3,2E15.6)
END
CV2 = 0.0
DO 40 L=1,NPTS
  IF(NDATA(J,L) .EQ. 0) GOTO 200
  L1 = NDATA(J,L)
  DX = X(L1) - X(K1)
  DY = Y(L1) - Y(K1)
  CALL GAMMA (DX, DY, GH)
  CV2 = CV2 + GH*RLAMDA(J,L)
40 CONTINUE
CV1 = CV1 + CV2*RLAMDA(I,K)
30 CONTINUE

CV3 = 0.0
DO 50 K=1,NPTS
  IF(NDATA(I,K) .EQ. 0) GOTO 230
  K1 = NDATA(I,K)
  CV4 = 0.0
  DO 60 L=1,NPZONE
    DX = X(K1) - XLOC(J,L)
    DY = Y(K1) - YLOC(J,L)
    CALL GAMMA (DX, DY, GH)
    CV4 = CV4 + GH
  60 CONTINUE
  CV3 = CV3 + RLAMDA(I,K)*CV4/FLOAT(NPZONE)
  GOTO 50
220 CONTINUE

CV5 = 0.0
DO 70 K=1,NPTS
  IF(NDATA(J,K) .EQ. 0) GOTO 250
  K1 = NDATA(J,K)
  CV6 = 0.0
  DO 80 L=1,NPZONE
    DX = X(K1) - XLOC(I,L)
    DY = Y(K1) - YLOC(I,L)
    CALL GAMMA (DX, DY, GH)
    CV6 = CV6 + GH
  80 CONTINUE
  CV5 = CV5 + RLAMDA(J,K)*CV6/FLOAT(NPZONE)
  GOTO 70
240 CONTINUE

CV7 = 0.0
N1 = NPZONE
N2 = NPZONE
DO 90 K=1,NPZONE
  IF(XLOC(I,K) .EQ. 0.0) GOTO 260
  DO 100 L=1,NPZONE
    DX = XLOC(I,L) - XLOC(J,L)
    DY = YLOC(I,L) - YLOC(J,L)
    CALL GAMMA (DX, DY, GH)
    CV7 = CV7 + GH
  100 CONTINUE
90 CONTINUE

IF(XLOC(J,N3+1) .EQ. 0.0) N2 = N3
GOTO 270
N1 = N3
IF(XLOC(J,N3+1) .EQ. 0.0) N2 = N3
CV7 = CV7/FLOAT(N1*N2)
CVR(I,J-I+1) = -CV1 + CV3 + CV5 - CV7
GOTO 20
20 CONTINUE
270

CONTINUE
10 CONTINUE
DO 110 I=1,NZONE
   I1 = I + 1
   DO 120 J=1,I
      IF(J .GT. I-MBW) XLOC(J,1) = CVR(J,J-I+1)
      IF(J .LE. I-MBW) XLOC(J,1) = 0.0
120 CONTINUE
WRITE(6,610) Ip(XLOC(J,1),J=1,I)
110 CONTINUE
WRITE(6,620)
DO 130 I=1,NZONE
   IF(I .EQ. 1) GOTO 300
   I1 = I + 1
   I2 = I - 1
   DO 140 J=1,I2
      IF(J .LE. I-MBW) GOTO 290
      IF(CVR(I,J) .EQ. 0.0 .0R. CVR(J,1) .EQ. 0.0) GOTO 290
      XLOC(J,1) = CVR(J,I)/SQRT(CVR(I,1)*CVR(J,1))
      GOTO 140
290 XL0C(J,1) = 0.0
140 CONTINUE
300 XL0C(I,1) = 1.0
WRITE(6,610) Ip(XLOC(J,1),J=1,I)
130 CONTINUE
CALL SECOND (TM2)
TM2 = TM2 - TM1
WRITE(6,630) TM2
IF(IPNCH2 .EQ. 0) GOTO 310
DO 150 I=1,MBW
   IF(IPNCH2 .EQ. 1) PUNCH(7,700) (CVR(J,I),J=1,NZONE)
   IF(IPNCH2 .EQ. 2) WRITE(1,710) (CVR(J,I),J=1,NZONE)
150 CONTINUE
310 RETURN
600 FORMAT(1H1,9X,48H*****THE LOWER TRIANGLE OF THE COVARIANCE MATRIX,)
   1 40H OF THE KRIGING (ESTIMATION) ERRORS*****,/////)
610 FORMAT(1H1,9X,42H*****THE LOWER TRIANGLE OF THE CORRELATION,)
   1 47H MATRIX OF THE KRIGING (ESTIMATION) ERRORS*****,/////)
620 FORMAT(1H1,9X,42H*****THE LOWER TRIANGLE OF THE CORRELATION,)
   1 49H CALCULATE THE KRIGING-ERROR COVARIANCE MATRIX = ,F9.2)
700 FORMAT(8E10.4)
710 FORMAT(5E16.8)
END

SUBROUTINE DSORT (ID)
C
C****THIS SUBROUTINE HAS BEEN MODIFIED FROM
C
C KIM, Y.C., AND H.P. KNUDSEN, 1977, GEOSTATISTICAL
C ORE RESERVE ESTIMATION FOR A ROLL-FRONT TYPE
C URANIUM DEPOSIT (PRACTITIONER'S GUIDE): DEPT.
C OF MINING AND GEOLOGICAL ENGINEERING, THE
SUBROUTINE GAMMA (DX, DY, GH)

C****THIS SUBROUTINE CALCULATES THE VALUE OF THE SEMI-VARIOGRAM FUNCTION
BETWEEN TWO POINTS. THE PARAMETER LIST OF THIS SUBROUTINE CONTAINS
THREE ARGUMENTS:

DX -- THE DIFFERENCE BETWEEN THE X-COORDINATES OF THE TWO POINTS
FOR WHICH THE SEMI-VARIOGRAM FUNCTION IS BEING CALCULATED

DY -- THE DIFFERENCE BETWEEN THE Y-COORDINATES OF THE TWO POINTS
FOR WHICH THE SEMI-VARIOGRAM FUNCTION IS BEING CALCULATED

GH -- THE VALUE OF THE SEMI-VARIOGRAM FUNCTION THAT IS RETURNED
TO THE PROGRAM UNIT WHICH CALLED SUBROUTINE GAMMA

DX AND DY ARE INPUT ARGUMENTS, AND ARE USED TO CALCULATE THE
DISTANCE "D" BETWEEN THE TWO POINTS (SEE LINE 3 BELOW).

SUBROUTINE GAMMA IS CURRENTLY WRITTEN FOR A SPHERICAL SEMI-
VARIogram MODEL, SO IT MUST BE REWRITTEN IF A DIFFERENT SEMI-
VARIogram MODEL IS REQUIRED. IF THIS SUBROUTINE IS TO BE REWRITTEN,
THE DISTANCE "D" MUST FIRST BE CALCULATED FROM DX AND DY, THEN
THE VALUE OF THE SEMI-VARIOGRAM, GH, IS CALCULATED. A MAXIMUM
OF 8 SEMI-VARIOGRAM PARAMETERS IS CURRENTLY ALLOWED. THESE ARE
STORED IN THE ARRAY "P", WHICH IS PASSED IN THE COMMON STATEMENT.
REMEMBER:

*****BY DEFINITION, GAMMA(0) = 0.0
*****BY DEFINITION, GAMMA(0) = 0.0
*****BY DEFINITION, GAMMA(0) = 0.0, EVEN IF THE SEMI-VARIOGRAM
MODEL HAS A NUGGET EFFECT.

*******************************************************************************
COMMON /GRP1/ P(8), PSEUD0
IF (DX .EQ. 0.0 .AND. DY .EQ. 0.0) GOTO 40
D = SQRT(DX**2 + DY**2)
20 IF (D .GT. P(3)) GOTO 30
GH = P(1) + P(2)*(1.5*D/P(3) - 0.5*(D/P(3))**3)
GOTO 50
30 GH = P(1) + P(2)
GOTO 50
40 GH = 0.0
50 RETURN
END

SUBROUTINE PTBVAR (ID, N4, NPS, NPTR, X, Y, SIDE2, SIDE4, PBVR)
COMMON /GRP4/ MBW, NPSZONE, NDATA(200,25), RDLAMA(200,25),
1 XLOC(200,64), YLOC(200,64), CVR(200,100)
CALL PTLOC (ID, NPS, NPTR, SIDE2, SIDE4)
PBVR = 0.0
N = NPZONE
IF (N4 .EQ. 0) N = NPS
DO 10 I = 1, N
DX = X - XLOC(ID, I)
DY = Y - YLOC(ID, I)
CALL GAMMA (DX, DY, GH)
PBVR = PBVR + GH
10 CONTINUE
PBVR = PBVR/FLOAT(N)
RETURN
END

SUBROUTINE PTLOC (ID, NPS, NPTR, SIDE2, SIDE4)
COMMON /GRP3/ XND(200), YND(200), ND1(200), ND2(200), ND3(200),
1 ND4(200), XC(200), YC(200)
COMMON /GRP4/ MBW, NPSZONE, NDATA(200,25), RDLAMA(200,25),
1 XLOC(200,64), YLOC(200,64), CVR(200,100)
DIMENSION SIDE2(NPS, 2), SIDE4(NPS, 2)
RNPS = FLOAT(NPS + 1)
N1 = ND1(ID)
N2 = ND2(ID)
N3 = ND3(ID)
N4 = ND4(ID)
DX2 = (XND(N3) - XND(N2))/RNPS
DY2 = (YND(N3) - YND(N2))/RNPS
IF (N4 .EQ. 0) GOTO 100
DX4 = (XND(N4) - XND(N1))/RNPS
DY4 = (YND(N4) - YND(N1))/RNPS
GOTO 110
100 DX4 = (XND(N3) - XND(N1))/RNPS
DY4 = (YND(N3) - YND(N1))/RNPS
110 DO 10 I = 1, RNPS
RI = FLOAT(I)
SIDE2(I, 1) = XND(N2) + DX2*RI
SIDE2(I, 2) = YND(N2) + DY2*RI
SIDE4(I, 1) = XND(N1) + DX4*RI
SIDE4(I, 2) = YND(N1) + DY4*RI
10 CONTINUE
CONTINUE
IPS = NPS
JPS = 0
DO 20 I=1,NPS
   RIPS = FLOAT(IPS + 1)
   DX1 = (SIDE4(I,1) - SIDE2(I,1))/RIPS
   DY1 = (SIDE4(I,2) - SIDE2(I,2))/RIPS
   DO 30 J=1,IPS
      RJ = FLOAT(J)
      XLOC(ID,J+JPS) = SIDE2(I,1) + DX1*RJ
      YLOC(ID,J+JPS) = SIDE2(I,2) + DY1*RJ
   CONTINUE
30 CONTINUE
   JPS = JPS + IPS
   IF(N4 .EQ. 0) IPS = IPS - 1
CONTINUE
20 CONTINUE
IF(N4 .NE. 0) GOTO 120
XLOC(ID,NPTR+1) = 0.0
120 RETURN
END

SUBROUTINE BLKVAR (ID,N4,NPTR,BVAR)
COMMON /GRP4/ MBW, NPZONE, NDATA(200,25), RLM0A(200,25),
XLOC(200,64), YLOC(200,64), CVR(200,100)
1
BVAR = 0.0
N = NPZONE
IF(N4 .EQ. 0) N = NPTR
DO 10 I=1,N
   DO 20 J=1,N
      IF(J .EQ. I) GOTO 20
      DX = XLOC(ID,J) - XLOC(ID,I)
      DY = YLOC(ID,J) - YLOC(ID,I)
      CALL GAMMA (DX, DY, GH)
      BVAR = BVAR + GH
20 CONTINUE
10 CONTINUE
BVAR = BVAR/FLOAT(N*(N - 1))
RETURN
END
REFERENCES


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