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Application of orthogonal polynomials to geostatistics

Ainslie Chapman

Edith Cowan University

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Application of Orthogonal Polynomials to Geostatistics

A Thesis Submitted to the
Faculty of Communications, Health and Science
Edith Cowan University
Perth, Western Australia

by Ainslie Chapman

In Partial Fulfillment of the Requirements for the Degree of
Bachelor of Science Honours (Mathematics)
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Supervisors: Associate Professor Lyn Bloom
Dr Ute Mueller
USE OF THESIS

The Use of Thesis statement is not included in this version of the thesis.
Abstract

Geostatistics is a field of study that deals with spatially dependent attributes. As information regarding these attributes is usually only available at sample locations, estimates must be made at unsampled locations. Sample data are usually measured on point support within the study region, however in reality, decisions are based on small blocks and not on points. A change-of-support model is required to obtain the theoretical distribution of block values given the sample point values. Estimates are then made for a collection of blocks, referred to as a panel. Kriging is a generic term adopted by geostatisticians for a family of estimators appropriate for spatially distributed data. The main focus of this study is the method of Disjunctive Kriging that employs the use of a family of orthogonal functions known as the Hermite polynomials.

This thesis presents comparisons of the results from Disjunctive Kriging with those from the more commonly used methods of Ordinary Kriging and Indicator Kriging. Ordinary Kriging can be used to generate estimates for each small block in the study region. Panel estimates can then be derived from the block estimates within each panel. Indicator Kriging and Disjunctive Kriging use change-of-support models to obtain estimates of functions of the attribute for the panels in the study region based on the chosen block support size. Two sets of isotropic data are analysed, one of which is approximately normally distributed and the other is positively skewed. Exhaustive data is available for both sets of data for comparative purposes.
Declaration

I certify that this thesis does not, to the best of my knowledge and belief:

(i) incorporate without acknowledgement any material previously submitted for a degree or diploma in any institution of higher education;

(ii) contain any material previously published or written by another person except where due reference is made in the text; or

(iii) contain any defamatory material.

Signature ..
Date 18-1-2002
Acknowledgements

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# Table of Contents

Abstract ............................................. 2  
Declaration ......................................... 3  
Acknowledgements .................................... 4

1. Introduction ...................................... 7  
   1.1 Background and Significance ....................... 7  
   1.2 Aims and Objectives ............................... 9  
   1.3 Thesis Outline ................................ 9  
   1.4 Software ........................................ 10  
   1.5 Notation ........................................ 10

2. Theoretical Framework ......................... 13  
   2.1 Orthogonal Polynomials ......................... 13  
      2.1.1 Legendre Polynomials ...................... 15  
      2.1.2 Chebyshev Polynomials .................... 16  
      2.1.3 Hermite Polynomials ...................... 17  
   2.2 Results from Probability Theory ............... 18  
   2.3 The Random Function Model .................... 26  
      2.3.1 Statistical Inference and Modelling ........ 28  
   2.4 Kriging ......................................... 29  
      2.4.1 Simple Kriging ............................. 31  
      2.4.2 Ordinary Kriging ........................... 31  
      2.4.3 Indicator Kriging ........................... 34  
      2.4.4 Disjunctive Kriging ......................... 41

3. Data Analysis .................................... 49  
   3.1 Moisture Data Suite ............................. 49  
      3.1.1 Statistical Description .................... 49  
      3.1.2 Spatial Description ........................ 52  
      3.1.3 Variography ................................ 56
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1.3.1 Variography of Moisture Values</td>
<td>56</td>
</tr>
<tr>
<td>3.1.3.2 Variography of Moisture Indicator Values</td>
<td>58</td>
</tr>
<tr>
<td>3.1.3.3 Variography of Block Gaussian Moisture Variable</td>
<td>61</td>
</tr>
<tr>
<td>3.1.4 Cross Validation</td>
<td>62</td>
</tr>
<tr>
<td>3.1.5 Ordinary Kriging Results</td>
<td>64</td>
</tr>
<tr>
<td>3.1.6 Indicator Kriging Results</td>
<td>68</td>
</tr>
<tr>
<td>3.1.7 Disjunctive Kriging Results</td>
<td>72</td>
</tr>
<tr>
<td>3.1.8 Comparison of Kriging Results</td>
<td>76</td>
</tr>
<tr>
<td>3.2 True Data Suite</td>
<td>79</td>
</tr>
<tr>
<td>3.2.1 Statistical Description</td>
<td>80</td>
</tr>
<tr>
<td>3.2.2 Spatial Description</td>
<td>83</td>
</tr>
<tr>
<td>3.2.3 Variography</td>
<td>87</td>
</tr>
<tr>
<td>3.2.3.1 Variography of Primary Values</td>
<td>87</td>
</tr>
<tr>
<td>3.2.3.2 Variography of Primary Indicator Values</td>
<td>89</td>
</tr>
<tr>
<td>3.2.3.3 Variography of Block Gaussian Primary Variable</td>
<td>93</td>
</tr>
<tr>
<td>3.2.4 Cross Validation</td>
<td>94</td>
</tr>
<tr>
<td>3.2.5 Ordinary Kriging Results</td>
<td>96</td>
</tr>
<tr>
<td>3.2.6 Indicator Kriging Results</td>
<td>99</td>
</tr>
<tr>
<td>3.2.7 Disjunctive Kriging Results</td>
<td>103</td>
</tr>
<tr>
<td>3.2.8 Comparison of Kriging Results</td>
<td>106</td>
</tr>
<tr>
<td>4. Discussion and Conclusions</td>
<td>109</td>
</tr>
<tr>
<td>References</td>
<td>114</td>
</tr>
<tr>
<td>Appendices</td>
<td>117</td>
</tr>
<tr>
<td>Appendix A: Moisture Indicator Directional Semivariograms</td>
<td>118</td>
</tr>
<tr>
<td>Appendix B: True Indicator Directional Semivariograms</td>
<td>120</td>
</tr>
<tr>
<td>Appendix C: GSLIB Parameter Files</td>
<td>122</td>
</tr>
</tbody>
</table>
1 Introduction

1.1 Background and Significance

Geostatistics is a term used to describe a set of methods that provide a statistical approach to estimation and decision making problems involving spatially dependent data. The practical nature of geostatistics has led to its successful application in such diverse fields as mining, petroleum, soil science, oceanography, hydrogeology, remote sensing and environmental sciences. More detail can be found in background texts such as Armstrong (1998), Chiles & Delfiner (1999), Deutsch & Journel (1998), Goovaerts (1997), Isaaks & Srivastava (1989), Journel & Huijbregts (1978) and Wackernagel (1995).

Geostatistics deals with phenomena that fluctuate in space. The knowledge of the value of a particular attribute is of little interest unless the location of measurement is known and accounted for in the data analysis. Sample data may provide some information but in most cases information regarding the entire region of interest is required. Therefore, it is necessary to make estimates at unsampled locations. This is usually done using a family of estimation algorithms for spatially dependent data, referred to by geostatisticians as kriging. Many of the commonly used kriging methods involve least-squares regression algorithms. Simple Kriging and Ordinary Kriging are examples of such methods. The final product of such analyses is often a contour map showing the estimated spatial distribution of the attribute of interest.

As geostatistical results are frequently used to help in planning and/or decision making, it is often the case that the required information is not just the estimation of an attribute over a certain region but rather a function of the attribute (Chiles & Delfiner, 1999; Rivoirard, 1994). An example of such a function is the probability of the attribute exceeding a critical threshold. There are a number of kriging methods that result in an estimator of a function of the attribute of interest. This type of estimator is a more general version of the previously outlined least-squares regression estimator.
One such method is Indicator Kriging, which is designed to estimate the probability that the attribute value is no greater than any given threshold value. The outcome of Indicator Kriging is a conditional cumulative distribution function, a distribution of local uncertainty or possible values conditional to data in the neighbourhood of the location to be estimated. This distribution of grades can also then be used to derive the average or expected value of the attribute.

Disjunctive Kriging is a kriging method that aims to estimate a function of the attribute, including, of course, the attribute itself. One of the most commonly used Disjunctive Kriging methods uses an orthogonal family of functions known as the Hermite polynomials (Chiles & Delﬁner, 1999; Rivoirard, 1994; Yates, Warrick & Myers, 1986). The use of the Hermite polynomials in this context stems from their relationship with the normal distribution and their orthogonality properties.

When making estimates in geostatistical applications, it is often desirable to map the spatial distribution on the basis of block support rather than sample support. The size of this block support refers to the minimum support upon which decisions can be made. Linear estimation of such small blocks (e.g. Block Ordinary Kriging) results in very high estimation variances. Therefore, the small block linear estimates have very low precision. A potentially serious consequence of the small block linear estimation approach is that the prediction of the content of an attribute above a cut-off based on these estimates is quite different from that based on true block values. Estimation of very large blocks will result in lower estimation variance but implies very low selectivity, which is usually an unrealistic assumption (Vann & Guibal, 1998). Non-linear estimation is the geostatistical approach to solving this problem.

Although we cannot precisely estimate small blocks by direct linear estimation, we can estimate the proportion of small blocks above a specified threshold within a large block, typically called a panel, using non-linear estimation. A change-of-support model must be incorporated in order to go from sample (point) support to (small) block support. Thus the concept of change of support is critical in practical applications of non-linear estimation. Use of such non-linear estimates allows for better decision making. (Vann & Guibal, 1998)
1.2 Aims and Objectives

The aim of this study is to investigate orthogonal polynomials and their application to geostatistics, in particular their application to Disjunctive Kriging. The theory of orthogonal polynomials is reviewed and summarised with three families of orthogonal polynomials. These are the Legendre, Chebyshev and Hermite polynomials. Particular attention however is given to the Hermite polynomials as they are used in the Disjunctive Kriging method of estimation and change-of-support modelling.

The Disjunctive Kriging algorithm, including the incorporation of the Hermite polynomials, is investigated in detail. The algorithms of the more commonly used methods of Ordinary Kriging and Indicator Kriging are also outlined as they are used to provide estimates for comparison with those obtained using Disjunctive Kriging. Change-of-support models are identified for Indicator Kriging and Disjunctive Kriging.

Two suites of data (Moisture and True) are analysed, in order to provide comparisons of the kriging methods. The Moisture data are isotropic and, although not normally distributed, are only weakly (positively) skewed. The True data are isotropic and strongly (positively) skewed. Ordinary Kriging estimates are made on blocks within the study area equal to the chosen support size. The block estimates are then converted into proportions and mean values of blocks above specified thresholds for groups of blocks, referred to as panels. The conditional probabilities generated from Indicator Kriging for the same panels are obtained and converted into proportions and mean values of blocks above the thresholds based on the discretisation of the panels into blocks of the support size. Similarly, Disjunctive Kriging is used to obtain estimates of the proportions and mean values of blocks above the specified thresholds based on blocks of support size within each panel.

1.3 Thesis Outline

Chapter 2 of the thesis presents some theoretical background of orthogonal polynomials, normal and bivariate normal distributions, the random function model and
the various methods of kriging used in this study. Chapter 3 describes the two data
suites in detail and provides the analysis and results for each suite. The formulae
developed in Chapter 2 are implemented by the GSLIB and ISATIS software pack-
ages, which were used to produce the kriging estimates. A discussion of the results
and conclusions of the study are given in Chapter 4

1.4 Software

The geostatistical and other software packages used in the analysis of the data are
listed below.

3PLOT (Kanevski et al, 1998)

GSLIB (Deutsch & Journel, 1998)

KT3D

IK3D

POSTIK

ISATIS (Bleines et al, 2000)

MICROSOFT EXCEL

MINITAB 13

VARIOWIN 2.2 (Pannatier, 1996)

1.5 Notation

The following notation is used throughout this thesis. The geostatistical notation
is the same as that used by Deutsch & Journel (1998) and Goovaerts (1997).

$A$ study region

$C(h)$ covariance function

$C(u - u_r)$ point-to-point covariance values

$\bar{C}(u_r, v(u))$ point-to-block covariance values

$\bar{C}(v(u), v(u))$ block-to-block covariance values

$C_j(h; z_k)$ covariance function of $I(u; z_k)$ at threshold $z_k$
\[\text{Cov} \{Z(u_n), Z(u_0)\} \quad \text{covariance of } Z(u_n) \text{ and } Z(u_0)\]

\[E[Z(u)] \quad \text{expected value of } Z(u)\]

\[F(u; z) \quad \text{cumulative distribution function at } u\]

\[F(u; z|\nu) \quad \text{conditional cumulative distribution function at } u\]

\[F(u_1, ..., u_N; z_1, ..., z_N) \quad \text{multivariate cumulative distribution function}\]

\[F_{X}(x) \quad \text{cumulative distribution function of } X\]

\[F_{X_1, X_2}(x_1, x_2) \quad \text{joint cumulative distribution function of } X_1 \text{ and } X_2\]

\[\|f\| \quad \text{norm of } f\]

\[(f, g) \quad \text{inner product of } f \text{ and } g\]

\[f_X(x) \quad \text{probability density function of } X\]

\[f_{X_1, X_2}(x_1, x_2) \quad \text{joint probability density function of } X_1 \text{ and } X_2\]

\[\Phi \quad \text{anamorphosis function}\]

\[G(y) \quad \text{cumulative distribution function of } Y(u)\]

\[g(y) \quad \text{probability density function of } Y(u)\]

\[\gamma(h) \quad \text{semivariogram at lag } h\]

\[\widehat{\gamma}(h) \quad \text{experimental semivariogram at lag } h\]

\[H_n \quad \text{Hermite polynomial of degree } n\]

\[I(u; z_k) \quad \text{indicator random function at } u \text{ for threshold } z_k\]

\[[I(u; z_k)]^* \quad \text{kriging estimator of } I(u; z_k)\]

\[[I(u; z_k)]_{OK}^* \quad \text{Ordinary Kriging estimator of } I(u; z_k)\]

\[[I(u; z_k)]_{SK}^* \quad \text{Simple Kriging estimator of } I(u; z_k)\]

\[i(u; z_k) \quad \text{indicator function at } u \text{ for threshold } z_k\]

\[L^2(u, b) \quad \text{space of square-integrable functions on interval } (a, b)\]

\[\lambda_o(u) \quad \text{kriging weight assigned to } z(u_n)\]

\[\lambda_o^{DK}(u) \quad \text{Disjunctive Kriging weight assigned to } z(u_n)\]

\[\lambda_o^{OK}(u) \quad \text{Ordinary Kriging weight assigned to } z(u_n)\]

\[\lambda_o^{SK}(u) \quad \text{Simple Kriging weight assigned to } z(u_n)\]

\[\lambda_{ne}(u) \quad \text{block kriging weight assigned to } z(u_n)\]

\[\lambda_{ne}^{OK}(u) \quad \text{block Ordinary Kriging weight assigned to } z(u_n)\]

\[\lambda_o(u; z_k) \quad \text{kriging weight assigned to } z(u_n) \text{ for threshold } z_k\]

\[\lambda_{O}^{OK}(u; z_k) \quad \text{Ordinary Kriging weight assigned to } z(u_n)\]

\[\lambda_{O}^{SK}(u; z_k) \quad \text{Simple Kriging weight assigned to } z(u_n)\]
\( M_v(u,z_k) \) average recovered value of attribute above \( z_k \) for \( V(u) \)
\( m(u) \) expected value of \( Z(u) \)
\( m(u_n) \) expected value of \( Z(u_n) \)
\( \mu_{OK}(u) \) Lagrange multiplier used for Ordinary Kriging
\( N(h) \) number of sample pairs separated by lag distance \( h \)
\( N(u) \) number of discretising points of block \( v(u) \)
\( n(u) \) number of sample locations in neighbourhood \( W(u) \)
\( P_n \) Legendre polynomial of degree \( n \)
\( p_n \) orthogonal polynomial of degree \( n \)
\( Q_V(u,z_k) \) quantity of attribute above \( z_k \)
\( T_n \) Chebyshev polynomial of degree \( n \)
\( T_V(u,z_k) \) proportion of \( V(u) \) above \( z_k \) value
\( \text{Var}[Z(u)] \) variance of \( Z(u) \)
\( V(u) \) panel of size \( V \) centred on \( u \)
\( v(u) \) block of size \( v \) centred on \( u \)
\( W(u) \) neighbourhood centred on \( u \)
\( w(x) \) weight function
\( X \) random variable of arbitrary distribution
\( Y(u) \) standard normal random variable at \( u \)
\( Y_v(u) \) standard normal random variable of block attribute value of \( v(u) \)
\( Z(u) \) random variable at \( u \)
\( Z(u_n) \) random variable at \( u_n \)
\( Z^*(u) \) random variable of estimated value at \( u \)
\( Z_{DK}(u) \) Disjunctive Kriging estimator of \( Z(u) \)
\( Z_{IK}(u) \) Indicator Kriging estimator of \( Z(u) \)
\( Z_{OK}(u) \) Ordinary Kriging estimator of \( Z(u) \)
\( z(u) \) actual attribute value at \( u \)
\( z(u_n) \) sample attribute value at \( u_n \)
\( z_v(u) \) block attribute value of \( v(u) \)
\( Z_v(u) \) random variable of block attribute value of \( v(u) \)
\( Z_v^*(u) \) random variable of estimated block attribute value of \( v(u) \)
\( Z_V(u) \) random variable of panel attribute value of \( V(u) \)
2 Theoretical Framework

This section aims to present an outline of the theory of orthogonal polynomials, normal and bivariate normal distributions, the random function model and the geostatistical methods of estimation used in this project.

2.1 Orthogonal Polynomials

Orthogonal systems play an important role in analysis. One reason is that many functions can be expanded in series of orthogonal functions. It is this property that leads to the use of the Hermite polynomials in Disjunctive Kriging. Important examples of orthogonal systems are orthogonal polynomials $p_n$ ($n = 0, 1, 2, ...$), where $n$ is the degree of the polynomial $p_n$. This class contains many special functions commonly encountered, e.g., Legendre, Hermite, Laguerre, Chebyshev and Jacobi polynomials (Lebedev, 1972). We will now look at one approach to the theory of orthogonal polynomials.

In order to define orthogonality we must first define the vector space we are concerned with. The space of functions defined on the interval $[a, b]$ for which

$$
\int_a^b w(x) |f(x)|^2 \, dx < \infty
$$

is denoted by $L^2_w(a, b)$ where $w$ is a weight function. This space is a vector space. The orthogonality of functions within this vector space is defined with respect to a particular inner product. An inner product on $L^2_w(a, b)$ is defined by

$$
\langle f, g \rangle = \int_a^b w(x) f(x) g(x) \, dx
$$

and the associated norm is given by

$$
\|f\|_w = \left( \int_a^b w(x) |f(x)|^2 \, dx \right)^{1/2}.
$$

Functions $f, g$ are said to be orthogonal on the interval $[a, b]$ if their inner product $\langle f, g \rangle$ is equal to zero.

An orthogonal system in the space $L^2_w(a, b)$ is a finite or infinite set of functions belonging to $L^2_w(a, b)$ that satisfy the following condition for all possible pairs of
functions \( f, g \) within the system:

\[
\langle f, g \rangle = \begin{cases} 
0, & f \neq g \\
\|f\|_2^2, & f = g
\end{cases}
\]  

(4)

A system of functions is called complete if every function in the space \( L^2_w(a, b) \) can be approximated as closely as desired by the functions of the set or by their linear combinations. An orthogonal basis for \( L^2_w(a, b) \) is a complete orthogonal system. Given a complete system for the vector space, we then develop an orthogonal basis for \( L^2_w(a, b) \).

There are many sets of functions that can be used as a basis for the vector space \( L^2_w(a, b) \) but for the purposes of this study we are interested in those bases composed of polynomials. It follows from the Weierstrass Approximation Theorem (Bartle & Sherbert, 1992) that any continuous function \( f \) on the interval \([a, b]\) can be approximated by a polynomial to any desired degree of accuracy: Given \( \varepsilon > 0 \), there exists a polynomial function \( p \), such that

\[
|f(x) - p(x)| < \varepsilon
\]

for all \( x \) in the interval \([a, b]\). This allows us to use the monomials \( \{1, x, x^2, x^3, \ldots\} \) as a basis for \( L^2_w(a, b) \). The inner product in (2) is then used to recursively construct an orthogonal basis for \( L^2_w(a, b) \) from these monomials via the Gram-Schmidt process (Lay, 1997) which consists of

1. Set \( p_0(x) = 1 \).

2. For \( n \geq 1 \) set

\[
p_{n+1}(x) = x^{n+1} - \frac{\langle x^{n+1}, p_n(x) \rangle}{\langle p_n(x), p_n(x) \rangle} p_n(x) - \ldots - \frac{\langle x^{n+1}, p_0(x) \rangle}{\langle p_0(x), p_0(x) \rangle} p_0(x).
\]

(6)

This procedure results in a family of polynomials \( p_n(n = 0, 1, 2, \ldots) \) that are pairwise orthogonal with respect to the given inner product.

Since the family of orthogonal polynomials is a basis of \( L^2_w(a, b) \) we can write every function \( f \in L^2_w(a, b) \) as a linear combination of elements \( p_n \):

\[
f(x) = \sum_{n=0}^{\infty} c_n p_n(x), \quad a < x < b
\]

(7)
The coefficients \( c_n \) are determined from the orthogonality property of the orthogonal polynomials. Multiplying the series \((7)\) by the product of the weight function \( w \) and the orthogonal polynomial \( p_m \), integrating term by term over the interval \([a, b]\) and using \((4)\), we find that for each \( m = 0, 1, 2, ... \)

\[
\int_{a}^{b} w(x)f(x)p_m(x)dx = \sum_{n=0}^{\infty} c_n \int_{a}^{b} w(x)p_n(x)p_m(x)dx = c_m \| p_m \|_w^2
\]

which implies that the coefficients of the series expansion are given by

\[
c_n = \frac{1}{\| p_n \|_w^2} \int_{a}^{b} w(x)f(x)p_n(x)dx = \frac{\langle f, p_n \rangle}{\| p_n \|_w^2}, \quad n = 0, 1, 2, ...
\]

Three families of orthogonal polynomials will be discussed in the following section to illustrate the properties of orthogonal polynomials. They are the Legendre, Chebyshev and Hermite polynomials. The Legendre and Chebyshev polynomials are both defined on the interval \([-1, 1]\) but have different weight functions. The Hermite polynomials are defined on the whole of \(\mathbb{R}\). These three families of polynomials exhibit similar properties and arise from a number of mathematical approaches. As a consequence of these orthogonality properties and their particular form, the Hermite polynomials lend themselves to use in the application of Gaussian Disjunctive Kriging to be outlined later.

### 2.1.1 Legendre Polynomials

The Legendre polynomials were first encountered by the French mathematician Adrien-Marie Legendre in his work on potential theory (Apostol, 1969). They play an important role in mathematical physics, particularly in the study of boundary value problems that can be solved by the use of spherical harmonics (Lebedev, 1972). The Legendre polynomials \( P_n \) \((n = 0, 1, 2, ...)\) are defined by Rodrigues’ formula (Lebedev, 1972)

\[
P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n, \quad n = 0, 1, 2, ...
\]

for real values of the variable \( x \). The first five Legendre polynomials are

\[
P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{1}{2}(3x^2 - 1),
\]
The Legendre polynomials are orthogonal with weight \( w(x) = 1 \) on the interval \([-1, 1]\) and satisfy the following orthogonality relation:

\[
\langle P_m, P_n \rangle = \int_{-1}^{1} P_m(x)P_n(x)dx = \begin{cases} 
0, & \text{if } m \neq n \\
\frac{2}{2m+1}, & \text{if } m = n 
\end{cases}
\]  

(12)

A number of recurrence relations involving Legendre polynomials may be derived including

\[(n + 1)P_{n+1}(x) - (2n + 1)xP_n(x) + nP_{n-1}(x) = 0, \quad n = 1, 2, \ldots\]  

(13)

which connects any three Legendre polynomials with consecutive indices. This allows the recursive calculation of the Legendre polynomials once the first two are known. The Legendre polynomials also arise as a solution to the second-order differential equation

\[(1 - x^2)u'' - 2xu' + n(n + 1)u = 0\]  

(14)

where \( n \) is a positive integer.

### 2.1.2 Chebyshev Polynomials

Another commonly encountered set of orthogonal polynomials are the Chebyshev polynomials, denoted by \( T_n \) (\( n = 0, 1, 2, \ldots \)), whose main use lies in approximation theory. They were named after the Russian mathematician Pafnutii Lvovich Chebyshev and are defined by the formula (Lebedev, 1972)

\[ T_n(x) = \cos(n \arccos x), \quad x \in [-1, 1], \quad n = 0, 1, 2, \ldots \]  

(15)

The fact that they can be specified explicitly is unique to the Chebyshev polynomials. Using (15), the first five Chebyshev polynomials are

\[
\begin{align*}
T_0(x) & = 1, \\
T_1(x) & = x, \\
T_2(x) & = 2x^2 - 1, \\
T_3(x) & = 4x^3 - 3x, \\
T_4(x) & = 8x^4 - 8x^2 + 1.
\end{align*}
\]  

(16)
As with the Legendre polynomials, the Chebyshev polynomials can also be shown to satisfy an orthogonality relation. Like the Legendre polynomials, the Chebyshev polynomials are defined on the interval \([-1, 1]\) but have a different weight function given by \(w(x) = (1 - x^2)^{-1/2}\). Their orthogonality relation is specified by

\[
(T_m, T_n) = \int_{-1}^{1} (1 - x^2)^{-1/2} T_m(x) T_n(x) \, dx = \begin{cases} 
0, & m \neq n \\
\pi, & m = n = 0 \\
\pi/2, & m = n \neq 0
\end{cases}
\]  

A recurrence relation, connecting any three Chebyshev polynomials with consecutive indices, is given by

\[
T_{n+1}(x) - 2xT_n(x) + T_{n-1}(x) = 0, \quad n = 1, 2, \ldots
\]  

It can also be shown that the Chebyshev polynomials satisfy the second order differential equation

\[
(1 - x^2)u'' - xu' + n^2u = 0.
\]

### 2.1.3 Hermite Polynomials

The Hermite polynomials, denoted by \(H_n (n = 0, 1, 2, \ldots)\), were named after the French mathematician Charles Hermite. Their application lies in the area of mathematical physics in problems involving the integration of Laplace's equation and Helmholtz' equation in parabolic coordinates, in quantum mechanics regarding wave functions and in the area of geostatistics involving the method of Disjunctive Kriging and the modelling of change of support.

The Hermite polynomials are defined by (Rivoirard, 1994)

\[
H_n(x) = \frac{e^{x^2/2}}{\sqrt{n!}} \frac{d^n}{dx^n} \left( e^{-x^2/2} \right), \quad n = 0, 1, 2, \ldots
\]

for real values of the variable \(x\). The first five Hermite polynomials are

\[
\begin{align*}
H_0(x) &= 1, \\
H_1(x) &= -x, \\
H_2(x) &= \frac{1}{\sqrt{2}} \left( x^2 - 1 \right), \\
H_3(x) &= \frac{-1}{\sqrt{6}} \left( x^3 - 3x \right), \\
H_4(x) &= \frac{1}{\sqrt{24}} \left( x^4 - 6x^2 + 3 \right).
\end{align*}
\]
The Hermite polynomials are defined on $\mathbb{R}$ and are orthogonal with respect to the weight $w(x) = e^{-x^2/2}$ and satisfy

$$\langle H_m, H_n \rangle = \int_{-\infty}^{\infty} e^{-x^2/2} H_m(x) H_n(x) \, dx = \begin{cases} 0, & m \neq n \\ \sqrt{2\pi}, & m = n \end{cases} \quad (22)$$

As in the case of the Legendre and Chebyshev polynomials, the Hermite polynomials have an associated recurrence relation, connecting three Hermite polynomials with consecutive indices. This relation can be used to calculate the Hermite polynomials once the first two are known and is given by

$$H_{n+1}(x) - xH_n(x) + nH_{n-1}(x) = 0, \quad n = 1, 2, \ldots \quad (23)$$

This recurrence relation allows storage effective computation of the values of the Hermite polynomials. We also have from (20) that for each $n = 1, 2, \ldots$

$$\int H_n(x)e^{-x^2/2} \, dx = \int \frac{1}{\sqrt{n!}} \frac{d^n}{dx^n} \left( e^{-x^2/2} \right) \, dx = \frac{1}{\sqrt{n!}} \frac{d^{n-1}}{dx^{n-1}} \left( e^{-x^2/2} \right) \, dx = \frac{1}{\sqrt{n!}} e^{-x^2/2} H_{n-1}(x). \quad (24)$$

Finally, the Hermite polynomials are the solutions of the second-order differential equation

$$u'' - xu' + nu = 0. \quad (25)$$

### 2.2 Results from Probability Theory

This thesis involves the study of continuous random variables. We now define some of the properties for continuous random variables with arbitrary distribution and then for the particular case of normally distributed random variables.

A continuous random variable $X$ is characterised by its probability density function $f_X(x)$ and its cumulative distribution function $F_X(x)$ given by

$$P \{ X \leq x \} = F_X(x) = \int_{-\infty}^{x} f_X(t) \, dt. \quad (26)$$

The expected value or mean of the random variable $X$ is defined by

$$E[X] = \int_{-\infty}^{\infty} t f_X(t) \, dt \quad (27)$$
and its variance is defined by

\[ \text{Var}[X] = E[(X - E[X])^2] = E[X^2] - E[X]^2. \] (28)

The expected value of a function \( h \) of the random variable \( X \) is defined by

\[ E[h(X)] = \int_{-\infty}^{\infty} h(t) f_X(t) \, dt \] (29)

and its variance is defined as

\[ \text{Var}[h(X)] = E[(h(X) - E[h(X)])^2]. \] (30)

The joint distribution of two random variables \( X_1 \) and \( X_2 \) is characterised by their joint probability density function \( f_{X_1,X_2}(x_1,x_2) \) and their cumulative distribution function \( F_{X_1,X_2}(x_1,x_2) \) defined by

\[ P \{ X_1 \leq x_1, X_2 \leq x_2 \} = F_{X_1,X_2}(x_1,x_2) = \int_{-\infty}^{x_1} \int_{-\infty}^{x_2} f_{X_1,X_2}(t,u) \, dt \, du. \] (31)

The expected value of a function \( h \) of the random variables \( X_1 \) and \( X_2 \) is defined by

\[ E[h(X_1,X_2)] = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} h(t,u) f_{X_1,X_2}(t,u) \, dt \, du \] (32)

and its variance is given by

\[ \text{Var}[h(X_1,X_2)] = E[(h(X_1,X_2) - E[h(X_1,X_2)])^2]. \] (33)

The covariance of the random variables \( X_1 \) and \( X_2 \) is defined by

\[ \text{Cov}[X_1,X_2] = E[(X_1 - E[X_1])(X_2 - E[X_2])] = E[X_1 X_2] - E[X_1]E[X_2] \] (34)

and the covariance of the functions \( f(X_1) \) and \( h(X_2) \) is given by

\[ \text{Cov}[f(X_1), h(X_2)] = E[(f(X_1) - E[f(X_1)])(h(X_2) - E[h(X_2)])]. \] (35)

Note that \( \text{Cov}[X_1,X_2] = \text{Cov}[X_2,X_1] \) and \( \text{Cov}[X_1,X_1] = \text{Var}[X_1] \). The correlation coefficient of \( X_1 \) and \( X_2 \) is the covariance standardised by the standard deviations of \( X_1 \) and \( X_2 \) defined by

\[ \rho_{X_1,X_2} = \text{Corr}[X_1,X_2] = \frac{\text{Cov}[X_1,X_2]}{\sqrt{\text{Var}[X_1] \text{Var}[X_2]}}. \] (36)
The conditional cumulative distribution function of $X_2$ given $X_1 = x_1$ is defined by

$$ P \{ X_2 \leq x_2 | X_1 = x_1 \} = F_{X_2} (x_2 | x_1) = \frac{\int_{-\infty}^{x_2} f_{X_1 X_2} (x_1, t) \, dt}{f_{X_1} (x_1)} $$

(37)

and the conditional probability density function of $X_2$ given $X_1 = x_1$ is defined by

$$ f_{X_2} (x_2 | x_1) = \frac{f_{X_1 X_2} (x_1, x_2)}{f_{X_1} (x_1)} $$

(38)

The conditional expectation of $X_2$ given $X_1 = x_1$ is defined by

$$ E[ X_2 | X_1 = x_1 ] = \int_{-\infty}^{\infty} t f_{X_2} (t | x_1) \, dt. $$

(39)

By Theorem 3-22 in Arnold (1990), the expected value for conditional expectation is an unconditional expectation that may be written as

$$ E[ E[ h (X_1, X_2) | X_1 ] ] = E[ h (X_1, X_2) ] $$

(40)

where $E[ h (X_1, X_2) | X_1 ]$ is itself a random variable.

The random variable $Y$ is normally distributed if its probability density function is given by

$$ f_Y (y) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(y-\mu)^2}{2\sigma^2}}, \quad y \in (-\infty, \infty), \quad \sigma > 0 $$

(41)

where $\mu$ and $\sigma^2$ are the mean and variance of $Y$. The associated cumulative distribution function is

$$ F_Y (y) = \int_{-\infty}^{y} f_Y (t) \, dt = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{y} e^{-\frac{(t-\mu)^2}{2\sigma^2}} \, dt. $$

(42)

We say that $Y$ is standard normal if it has a mean of zero and a variance equal to one, with probability density function $g(y)$ given by

$$ g(y) = \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}}, \quad y \in (-\infty, \infty) $$

(43)

and cumulative distribution function $G(y)$ given by

$$ G(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{y} e^{-\frac{t^2}{2}} \, dt. $$

(44)
Two random variables \(Y_1\) and \(Y_2\) are said to be bivariate normal if their joint probability density function is given by

\[
f_{Y_1Y_2}(y_1, y_2) = \frac{\exp\left\{ \frac{-1}{2(1-\rho^2)} \left[ \left( \frac{y_1 - \mu_{Y_1}}{\sigma_{Y_1}} \right)^2 - 2\rho \left( \frac{y_1 - \mu_{Y_1}}{\sigma_{Y_1}} \right) \left( \frac{y_2 - \mu_{Y_2}}{\sigma_{Y_2}} \right) + \left( \frac{y_2 - \mu_{Y_2}}{\sigma_{Y_2}} \right)^2 \right] \right\} \right\}}{2\pi\sigma_{Y_1}\sigma_{Y_2}\sqrt{1-\rho^2}},
\]

where \(\mu_{Y_1}\) and \(\mu_{Y_2}\) are the respective means, \(\sigma_{Y_1}^2\) and \(\sigma_{Y_2}^2\) are the respective variances, and \(\rho\) is the correlation coefficient of \(Y_1\) and \(Y_2\). The random variables \(Y_1\) and \(Y_2\) are said to be bivariate standard normal if both \(Y_1\) and \(Y_2\) have mean equal to zero and variance equal to one, and the joint probability density function is given by

\[
f_{Y_1Y_2}(y_1, y_2) = \frac{\exp\left\{ \frac{-1}{2(1-\rho^2)} \left[ y_1^2 - 2\rho y_1 y_2 + y_2^2 \right] \right\} \right\}}{2\pi\sqrt{1-\rho^2}}, \quad y_1, y_2 \in (-\infty, \infty).
\]

Since their means are zero, the covariance of the bivariate standard normal random variables \(Y_1\) and \(Y_2\) using (34) is

\[
\text{Cov}[Y_1, Y_2] = E[Y_1Y_2]
\]

and since their variances are equal to one, their correlation coefficient using (36) is

\[
\rho_{Y_1Y_2} = \text{Cov}[Y_1, Y_2] = E[Y_1Y_2].
\]

We now develop these results for random variables involving the Hermite polynomials. We define the random variable \(H_n[Y]\), \(n = 0, 1, 2, \ldots\) as a function of the standard normal variable \(Y\) with the function \(H_n\) defined by (20). Except for \(H_0[Y]\) which is constant with value one, the means of the Hermite polynomials are zero:

\[
E[H_n[Y]] = \int_{-\infty}^{\infty} H_n[y\ g(y) dy \quad \text{by (20)}
\]

\[
= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} H_n[y\ e^{-y^2/2} dy \quad \text{by (43)}
\]

\[
= \frac{1}{\sqrt{2\pi}} \left[ \int_{-\infty}^{0} H_n[y\ e^{-y^2/2} dy + \int_{0}^{\infty} H_n[y\ e^{-y^2/2} dy \right]
\]

\[
= \frac{1}{\sqrt{2\pi}} \left( \lim_{a \to -\infty} \int_{0}^{a} H_n[y\ e^{-y^2/2} dy + \lim_{b \to -\infty} \int_{b}^{0} H_n[y\ e^{-y^2/2} dy \right)
\]
\[
\frac{1}{\sqrt{2\pi}} \left( \lim_{n \to \infty} \left[ \frac{1}{\sqrt{n!}} e^{-y^2/2} H_{n-1}(y) \right]_n \right) + \lim_{b \to \infty} \left[ \frac{1}{\sqrt{n!}} e^{-y^2/2} H_{n-1}(y) \right]_b \quad \text{by (24)}
\]

\[
\frac{1}{\sqrt{2\pi}} \left( \frac{-1}{\sqrt{n!}} H_{n-1}(0) + \frac{1}{\sqrt{n!}} H_{n-1}(0) \right) = 0.
\]

Hence

\[
E[H_n[Y]] = \begin{cases} 1, & n = 0 \\ 0, & n \geq 1 \end{cases} \quad \text{(45)}
\]

The variances of the Hermite polynomials, except for \(H_0[Y]\) which is constant and therefore has variance zero, are equal to one:

\[
\text{Var}[H_n[Y]] = E[(H_n[Y] - E[H_n[Y]])^2] \quad \text{by (30)}
\]

\[
= E[(H_n[Y])^2], \quad n \neq 0 \quad \text{by (49)}
\]

\[
= \frac{\langle H_n, H_n \rangle}{\sqrt{2\pi}}, \quad n \neq 0 \quad \text{by (22) and (29)}
\]

\[
= 1, \quad n \neq 0 \quad \text{by (22).} \quad \text{(50)}
\]

The covariance of two Hermite polynomials of different orders are zero:

\[
\text{Cov}[H_m[Y], H_n[Y]] = E[(H_m[Y] - E[H_m[Y]]) (H_n[Y] - E[H_n[Y]])] \quad \text{by (35)}
\]

\[
= E[H_m[Y] H_n[Y]] \quad \text{by (49)}
\]

\[
= \int_{-\infty}^{\infty} \frac{e^{-t^2/2}}{\sqrt{2\pi}} H_m[t] H_n[t] dt \quad \text{by (29)}
\]

\[
= \frac{\langle H_m, H_n \rangle}{\sqrt{2\pi}} \quad \text{by (22).}
\]

Hence

\[
\text{Cov}[H_m[Y], H_n[Y]] = E[H_m[Y] H_n[Y]] = \begin{cases} 0, & m \neq n \\ 1, & m = n \end{cases} \quad \text{(51)}
\]

For the bivariate standard normal pair of random variables \((Y_1, Y_2)\) with correlation coefficient \(\rho_{Y_1Y_2}\), the Hermite polynomials have the following property of conditional expectation (Rivoirard, 1994):

\[
E[H_n[Y_2|Y_1]] = \left[\rho_{Y_1Y_2}\right]^n H_n[Y_1]. \quad \text{(52)}
\]
Using this result, we can write the covariance of the Hermite polynomials as

\[
\text{Cov} \left[ H_m[Y_1], H_n[Y_2] \right] = E \left[ (H_m[Y_1] - E[H_m[Y_1]]) (H_n[Y_2] - E[H_n[Y_2]]) \right] \text{ by (35)}
\]

\[
= E[H_m[Y_1] H_n[Y_2]] \text{ by (49)}
\]

\[
= E[H_m[Y_1] | H_n[Y_2]] \text{ } \text{ } \text{ } \text{ } \text{ by Bayes' Rule}
\]

\[
= [\rho_{Y_1,Y_2}]^n E[H_m[Y_1] | H_n[Y_1]] \text{ by (52)}
\]

\[
= [\rho_{Y_1,Y_2}]^n \text{ Cov} \left[ H_m[Y_1], H_n[Y_1] \right] \text{ by (51)}
\]

\[
= \text{ Cov} \left[ Y_1,Y_2 \right]^n \text{ Cov} \left[ H_m[Y_1], H_n[Y_1] \right] \text{ by (48)}
\]

\[
= \begin{cases} 
0, & m \neq n \\
\text{Cov} \left[ Y_1,Y_2 \right]^n, & m = n.
\end{cases}
\text{ by (50) and (51).}
\]

Hence

\[
\text{Cov} \left[ H_m[Y_1], H_n[Y_2] \right] = E[H_m[Y_1] H_n[Y_2]] = \begin{cases} 
0, & m \neq n \\
\text{Cov} \left[ Y_1,Y_2 \right]^n, & m = n.
\end{cases}
\text{ (53)}
\]

Therefore, the Hermite polynomials of the random variables \( Y_1 \) and \( Y_2 \) of different orders are uncorrelated and the covariance of the Hermite polynomial of degree \( n \) is the covariance of the random variables raised to the \( n \)th power.

A function \( f \) of the standard normal variable \( Y \), which can be expressed in terms of Hermite polynomials, given by

\[
f (Y) = \sum_{n=0}^{\infty} f_n H_n[Y]
\]

has coefficients given by (9):

\[
f_n = \frac{\langle f, H_n[Y] \rangle}{\|H_n[Y]\|_m^2}, \quad w(y) = e^{-y^2/2}, \quad n = 0, 1, 2, \ldots
\]

From the definition of the expected value of the function of a random variable (29) we obtain

\[
E \left[ f (Y) H_n[Y] \right] = \int_{-\infty}^{\infty} f (t) H_n[t] g(t) \, dt
\]

where \( g(t) \) is defined by (43). Comparing this with the definition of the inner product (2) with \( w(y) = e^{-y^2/2} \) we obtain

\[
f_n = \frac{\langle f, H_n[Y] \rangle}{\|H_n[Y]\|_m^2} = E \left[ f (Y) H_n[Y] \right], \quad w(y) = e^{-y^2/2}, \quad n = 0, 1, 2, \ldots
\]

23
In particular, since $H_0[Y] = 1$, we obtain
\[
f_0 = E[f(Y)].
\] (58)

The variance of $f(Y)$ is given by
\[
\text{Var}[f(Y)] = E[(f(Y) - E[f(Y)])^2] = E[(f(Y))^2] - (E[f(Y)])^2
\]
\[
= E \left[ \left( \sum_{n=0}^{\infty} f_n H_n [Y] \right)^2 \right] - \left( \sum_{n=0}^{\infty} f_n E[H_n [Y]] \right)^2 \quad \text{by } (54)
\]
\[
= E \left[ \left( \sum_{n=0}^{\infty} f_n H_n [Y] \right)^2 \right] - f_0^2 \quad \text{by } (49)
\]
\[
= \sum_{n=1}^{\infty} f_n^2 E[(H_n [Y])^2]
\]
\[
= \sum_{n=1}^{\infty} f_n^2 \quad \text{by } (50).
\]

Hence
\[
\text{Var}[f(Y)] = \sum_{n=1}^{\infty} f_n^2.
\] (59)

So the variance of a function of the standard normal variable, which can be expressed in terms of the Hermite polynomials, can be written in terms of the coefficients of the Hermite expansion.

The bivariate standard normal random variables $Y_1$ and $Y_2$ with correlation coefficient $\rho_{Y_1Y_2}$ can be expressed in terms of Hermite polynomials given by
\[
\begin{align*}
f [Y_1] &= \sum_{n=0}^{\infty} f_n H_n [Y_1] \quad \text{(60)}
\end{align*}
\]
and
\[
\begin{align*}
h [Y_2] &= \sum_{n=0}^{\infty} h_n H_n [Y_2].
\end{align*}
\] (61)

The covariance between $f[Y_1]$ and $h[Y_2]$, using (35), is given by
\[
\text{Cov}[f[Y_1], h[Y_2]] = E[(f[Y_1] - E[f[Y_1]]) (h[Y_2] - E[h[Y_2]])].
\] (62)
Using the Hermite expansion of $f[Y_1]$ we can write

$$f[Y_1] - E[f[Y_1]] = \sum_{m=0}^{\infty} f_m H_m[Y_1] - E\left[\sum_{m=0}^{\infty} f_m H_m[Y_1]\right] \quad \text{by (60)}$$

$$= \sum_{m=0}^{\infty} f_m H_m[Y_1] - \sum_{m=0}^{\infty} f_m E[H_m[Y_1]]$$

$$= \sum_{m=0}^{\infty} f_m H_m[Y_1] - f_0 \quad \text{by (49)}$$

$$= \sum_{m=1}^{\infty} f_m H_m[Y_1] \quad \text{since } H_0[Y_1] = 1. \quad (63)$$

Similarly, using the Hermite expansion of $h[Y_2]$ we obtain

$$h[Y_2] - E[h[Y_2]] = \sum_{n=1}^{\infty} h_n H_n[Y_2]. \quad (64)$$

Combining (62), (63) and (64), the covariance between $f[Y_1]$ and $h[Y_2]$ is given by

$$Cov[f[Y_1], h[Y_2]] = E[(f[Y_1] - E[f[Y_1]]) (h[Y_2] - E[h[Y_2]])]$$

$$= E\left[\left(\sum_{m=1}^{\infty} f_m H_m[Y_1]\right) \left(\sum_{n=1}^{\infty} h_n H_n[Y_2]\right)\right]$$

$$= E\left[\sum_{m=1}^{\infty} \sum_{n=1}^{\infty} f_m h_n H_m[Y_1] H_n[Y_2]\right]$$

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} f_m h_n E[H_m[Y_1] H_n[Y_2]]$$

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} f_m h_n Cov[H_m[Y_1], H_n[Y_2]] \quad \text{by (53)}$$

$$= \sum_{n=1}^{\infty} f_n h_n Cov[H_n[Y_1], H_n[Y_2]] \quad \text{by (53)}$$

$$= \sum_{n=1}^{\infty} f_n h_n [Cov[Y_1, Y_2]]'' \quad \text{by (53)}.\)$$

Hence

$$Cov[f[Y_1], h[Y_2]] = \sum_{n=1}^{\infty} f_n h_n [Cov[Y_1, Y_2]]''. \quad (65)$$

In particular if $f = h$ we have

$$Cov[f[Y_1], f[Y_2]] = \sum_{n=1}^{\infty} f_n^2 [Cov[Y_1, Y_2]]'' \quad (66)$$

So the covariance of a function of the random variables can be expressed in terms of the covariance of the random variables themselves.
2.3 The Random Function Model

Geostatistics deals with the analysis of spatial data, that is data where both location and value are important. Often the problem is one of estimating an attribute \( z \) at any unsampled location \( u \) in the study region \( A \). As the attribute values at the different locations are not independent we must define a model of spatial dependence over \( A \). Any datum \( z(u_0) \) is viewed as a particular realisation of the random variable \( Z(u_0) \), and any unknown attribute value \( z(u) \) is modelled as a random variable \( Z(u) \) (Armstrong, 1998; Goovaerts, 1997; Journel & Huijbregts, 1978). The continuous random variable \( Z(u) \) is fully characterised by its cumulative distribution function given by

\[
F(u; z) = P\{Z(u) \leq z\}.
\]

We define the random function \( \{Z(u), \forall u \in A\} \), as the set of dependent random variables defined over the study region \( A \). Just as a random variable \( Z(u) \) is characterised by its cumulative distribution function, a random function is characterised by the set of all its multivariate cumulative distribution functions for any number \( N \), and choice of the \( N \) locations \( u_k, k = 1, \ldots, N \):

\[
F(u_1, \ldots, u_N; z_1, \ldots, z_N) = P\{Z(u_1) \leq z_1, \ldots, Z(u_N) \leq z_N\}.
\]

The set of all such \( N \)-variate cumulative distribution functions, for any positive integer \( N \) and for any choice of the locations \( u_k \), constitutes the joint distribution function of the random function \( Z(u) \). In practice, the joint distribution function is not known, but the first two moments of the distribution are sufficient to provide an acceptable approximate solution.

It is often assumed that the attribute under consideration is spatially homogeneous across the study region. The random function \( \{Z(u), u \in A\} \) is said to be stationary within the field \( A \) if its \( N \)-variate cumulative distribution function is invariant under any translation of the \( N \) vectors \( u_k \) for any \( N \). This means that any two vectors of random variables \( \{Z(u_1), \ldots, Z(u_N)\} \) and \( \{Z(u_1 + h), \ldots, Z(u_N + h)\} \) have the same \( N \)-variate cumulative distribution function whatever the translation.
vector \( h \):

\[
F(u_1, \ldots, u_N; z_1, \ldots, z_N) = F(u_1 + h, \ldots, u_N + h; z_1, \ldots, z_N),
\]
\( \forall u_1, \ldots, u_N \) and \( h \).

In practice, we make the assumption of second-order stationarity of the random function \( Z(u) \), which says that the expected value \( E[Z(u)] \) exists and is invariant within \( A \) (does not depend on \( u \)) and the two-point covariance exists and depends only on the separation vector \( h \):

\[
E[Z(u)] = E[Z(u + h)]
\]
\( \text{(70)} \)

\[
\text{Cov}[Z(u), Z(u + h)] = C(h)
\]
\( \text{(71)} \)

where \( C(h) \) is called the covariance function. Since the assumption of second-order stationarity does not always hold in practice, we make the weaker assumption of intrinsic stationarity, which says that the increments of the random function \( Z(u) \) are second-order stationary:

\[
E[Z(u) - Z(u + h)] = 0
\]
\( \text{(72)} \)

\[
\text{Var}[Z(u) - Z(u + h)] = 2\gamma(h)
\]
\( \text{(73)} \)

where \( 2\gamma(h) \) is called the variogram function and \( \gamma(h) \) is called the semivariogram function.

The covariance function and semivariogram of a stationary random function, if they both exist, are related by

\[
\gamma(h) = C(0) - C(h).
\]
\( \text{(74)} \)

From the definition of the correlation coefficient in (36) we define another spatial measure known as the correlogram \( \rho(h) \) by

\[
\rho(h) = \frac{\text{Cov}[Z(u), Z(u + h)]}{\sqrt{\text{Var}[Z(u)]\text{Var}[Z(u + h)]}}.
\]
\( \text{(75)} \)

The correlogram is related to the covariance function and semivariogram by

\[
\rho(h) = \frac{C(h)}{C(0)} = 1 - \frac{\gamma(h)}{C(0)}.
\]
\( \text{(76)} \)

Using (48), the covariance function and correlogram for the bivariate standard normal pair \( (Z(u), Z(u + h)) \) are equal:

\[
\rho(h) = C(h).
\]
\( \text{(77)} \)
2.3.1 Statistical Inference and Modelling

By virtue of (72) and (73), the spatial continuity of an intrinsically stationary random variable may be measured by the semivariogram, \( \gamma(h) \). It is a measure of the dissimilarity of the attribute of interest between pairs of points. The greater the value of \( \gamma(h) \), the greater the dissimilarity of the attribute of interest between the pairs of points. The semivariogram is inferred from the sample (experimental) semivariogram calculated by

\[
\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{\alpha=1}^{N(h)} [z(u_\alpha) - z(u_\alpha + h)]^2
\]

where \( z(u_\alpha) \) and \( z(u_\alpha + h) \) are the data values at locations \( u_\alpha \) and \( u_\alpha + h \) respectively and \( N(h) \) is the number of pairs of data locations separated by vector \( h \).

The experimental semivariogram provides a set of experimental values \( \hat{\gamma}(h) \) for a finite number of lags, \( h_k, k = 1, ..., K \) and directions. A model (continuous function) must be fitted to these experimental values so as to deduce semivariogram values for any possible lag \( h \) required and to smooth out sample fluctuations. Not all functions can be valid semivariogram models. A permissible function must be conditionally negative definite to ensure the non-negativity of the variance (Goovaerts, 1997). To ensure the permissibility of a semivariogram model and thereby avoid having to test the permissibility of a semivariogram model after its construction, a common practice consists of using only linear combinations of basic models that are known to be permissible (Goovaerts, 1997).

The basic semivariogram models used in this study, which are frequently used basic models, are the nugget effect, spherical and exponential models. These models are all bounded, and therefore a sill is actually or practically reached at a distance \( a \) referred to as the range. The nugget effect reaches its sill as soon as the lag spacing is greater than zero and the spherical model reaches its sill at distance \( a \). The exponential model reaches its sill asymptotically and the distance \( a \) at which 95\% of the sill is reached is known as the practical range. If the semivariogram is dependent on distance only it is called isotropic, otherwise it is said to be anisotropic. The three basic models given in their isotropic form (dependent on distance \( h = |h| \)) with sill standardised to one are:
1. Nugget effect model

\[ g(h) = \begin{cases} 
0, & h = 0 \\
1, & h > 0 
\end{cases} \]

2. Spherical model

\[ g(h) = \begin{cases} 
1.5 \frac{h}{a} - 0.5 \left( \frac{h}{a} \right)^3, & 0 \leq h \leq a \\
1, & h > a 
\end{cases} \]

3. Exponential model

\[ g(h) = 1 - \exp \left( -\frac{3h}{a} \right), \quad h \geq 0 \]

Attributes often exhibit patterns of spatial variability with changing direction which is known as anisotropy. Anisotropy may be detected if experimental semivariograms are calculated separately in different directions. If the directional semivariograms have the same shape and sill but the range varies smoothly, the anisotropy is said to be geometric. If the directional semivariograms have different sills the anisotropy is said to be zonal. If anisotropy is evident in the experimental semivariograms, then an anisotropic semivariogram model must be fitted (Armstrong, 1998; Goovaerts, 1997). Modelling anisotropy calls for functions that depend on the vector \( h \) rather than on the distance \( h = |h| \) only.

### 2.4 Kriging

The specification of a model of spatial dependence enables the estimation of attribute values at unsampled locations. A family of least-squares linear regression algorithms known as kriging algorithms can be used to facilitate estimation of the continuous attribute of interest. This project focuses on methods accounting for data related solely to the continuous attribute being measured, though it should be mentioned that there are kriging algorithms for incorporating secondary information (Goovaerts, 1997).

Kriging is the name coined by the French mathematician Matheron, in recognition of South African mining engineer Danie Krige, for his pioneering work using linear regression methods for resource estimation (Krige, 1951). The term kriging is commonly used to describe the family of generalised least-squares regression
algorithms resulting in estimators of the form

\[ Z^*(u) = \sum_{\alpha=1}^{n(u)} \lambda_\alpha Z(u_\alpha) \]  

(79)

where \( Z^*(u) \) is the random variable of the estimated value, \( Z(u_\alpha) \) is the random variable at the sample location \( u_\alpha \), \( \lambda_\alpha \) is the weight assigned to the sample value at location \( u_\alpha \) and \( n(u) \) is the number of sample data within a given neighbourhood \( W(u) \) centred on \( u \). The number of data involved in the estimation as well as their weights may change from one location to another as only the \( n(u) \) data closest to the location \( u \) being estimated are retained.

The basic linear kriging estimator \( Z^*(u) \) is defined as

\[ Z^*(u) = m(u) + \sum_{\alpha=1}^{n(u)} \lambda_\alpha (Z(u_\alpha) - m(u_\alpha)) \]  

(80)

where \( m(u) \) and \( m(u_\alpha) \) are the expected values of the random variables \( Z(u) \) and \( Z(u_\alpha) \) respectively. Linear kriging methods use the modelled spatial correlation function, estimated from the sample data, to assign weights.

Kriging is a best linear unbiased estimation (BLUE) method. An estimator is unbiased if

\[ E[Z^*(u) - Z(u)] = 0. \]  

(81)

The estimation or error variance is defined as

\[ \sigma_B^2(u) = Var[Z^*(u) - Z(u)]. \]  

(82)

The kriging estimator is "best" in the sense that it has minimum estimation variance, that is, the expected squared difference between the estimate \( Z^*(u) \) and the true value \( Z(u) \) denoted by

\[ E[(Z^*(u) - Z(u))^2] \]  

(83)

is the minimum over all possible linear estimators.
2.4.1 Simple Kriging

Simple Kriging will be used within the method of Disjunctive Kriging to be outlined later. In Simple Kriging, the mean is assumed to be known and constant throughout the study region:

$$m(u) = m, \text{ known for all } u \in A.$$  \hspace{1cm} (84)

Using (80) and (84) the Simple Kriging estimator is given by

$$Z_{SK}^*(u) = m + \sum_{\alpha=1}^{n(u)} \lambda_{\alpha}^{SK}(u)[Z(u_\alpha) - m]$$  \hspace{1cm} (85)

$$= \sum_{\alpha=1}^{n(u)} \lambda_{\alpha}^{SK}(u)Z(u_\alpha) + \left[1 - \sum_{\alpha=1}^{n(u)} \lambda_{\alpha}^{SK}(u)\right]m.$$

The Simple Kriging estimator is already unbiased since the error mean is equal to zero. The $n(u)$ optimal weights $\lambda_{\alpha}^{SK}(u)$ are determined so as to minimise the error variance, which translates into solving the following system of $n(u)$ equations:

$$\sum_{\beta=1}^{n(u)} \lambda_{\beta}^{SK}(u)C(u_\alpha - u_\beta) = C(u_\alpha - u), \hspace{1cm} \alpha = 1, ..., n(u).$$  \hspace{1cm} (86)

The Simple Kriging variance is given by

$$\sigma_{SK}^2(u) = Var [Z_{SK}^*(u) - Z(u)] = C(0) - \sum_{\alpha=1}^{n(u)} \lambda_{\alpha}^{OK}(u)C(u_\alpha - u).$$  \hspace{1cm} (87)

2.4.2 Ordinary Kriging

The assumption of a known and constant mean throughout the study region is very strong and in most instances not valid. Instead of Simple Kriging, Ordinary Kriging is often used. Ordinary Kriging accounts for local variation of the mean by limiting the domain of stationarity of the mean to the local neighbourhood $W(u)$ centered on the location $u$ being estimated:

$$m(u') = \text{constant but unknown for } u' \in W(u).$$  \hspace{1cm} (88)

The linear estimator (80) is then a linear combination of the $n(u)$ random variables $Z(u_\alpha)$ and is given by

$$Z^*(u) = \sum_{\alpha=1}^{n(u)} \lambda_{\alpha}(u)Z(u_\alpha) + \left[1 - \sum_{\alpha=1}^{n(u)} \lambda_{\alpha}(u)\right]m(u).$$  \hspace{1cm} (89)
The unknown local mean \( m(u) \) is filtered from the linear estimator by forcing the kriging weights to sum to one. The Ordinary Kriging estimator \( Z_{OK}(u) \) is then written as a linear combination of only the \( n(u) \) random variables \( Z(u_n) \):

\[
Z_{OK}(u) = \sum_{a=1}^{n(u)} \lambda_{a}^{OK}(u)Z(u_n) \quad \text{with} \quad \sum_{a=1}^{n(u)} \lambda_{a}^{OK}(u) = 1. \tag{90}
\]

The \( n(u) \) weights \( \lambda_{a}^{OK}(u) \) are determined so as to minimise the error variance subject to the condition that the sum of the kriging weights equals one. This translates into solving the following system of \( n(u) + 1 \) equations:

\[
\begin{align*}
\sum_{\beta=1}^{n(u)} \lambda_{\beta}^{OK}(u)C(u_\alpha - u_\beta) + \mu_{OK}(u) &= C(u_\alpha - u), \quad \alpha = 1, ..., n(u) \\
\sum_{\beta=1}^{n(u)} \lambda_{\beta}^{OK}(u) &= 1
\end{align*}
\]  

where the \( \lambda_{a}^{OK} \) are the Ordinary Kriging weights and \( \mu_{OK}(u) \) is the Lagrange multiplier associated with the condition that the sum of the weights be one. Using (74), the Ordinary Kriging system may also be expressed in terms of the semivariogram by

\[
\begin{align*}
\sum_{\beta=1}^{n(u)} \lambda_{\beta}^{OK}(u)\gamma(u_\alpha - u_\beta) - \mu_{OK}(u) &= \gamma(u_\alpha - u), \quad \alpha = 1, ..., n(u) \\
\sum_{\beta=1}^{n(u)} \lambda_{\beta}^{OK}(u) &= 1
\end{align*}
\]  

Ordinary Kriging provides not only a least-squares estimate of the attribute but also the associated error variance. The minimum error variance of Ordinary Kriging is given by

\[
\sigma_{E_{OK}}^2(u) = \text{Var} [Z_{OK}(u) - Z(u)] = C(0) - \sum_{a=1}^{n(u)} \lambda_{a}^{OK}(u)C(u_n - u) - \mu_{OK}(u). \tag{93}
\]

The error variance is dependent on both the covariance model and the data configuration but is independent of the data values. As the location \( u \) being estimated gets further away from data locations \( u_n \), both the covariance term \( C(u_n - u) \) and the kriging weight \( \lambda_{a}^{OK}(u) \) decrease and hence the kriging variance increases.

**Block Ordinary Kriging**

The development of the Ordinary Kriging method thus far has been confined to the goal of point estimation. Often the target value is an estimate of the average.
value of the attribute over a block of specific dimensions. The linearity of the Ordinary Kriging algorithm allows direct estimation of linear averages of the attribute \( z(u) \). The target of the block estimation is the average value of the attribute \( z(u) \) over a block \( v(u) \) centred on \( u \) with the block value \( z_o(u) \) defined as

\[
z_o(u) = \frac{1}{v} \int_{v(u)} z(u') du' \approx \frac{1}{N(u)} \sum_{i=1}^{N(u)} z(u'_i)
\]  

where \( v(u) \) is a block of measure \( v \) centred at \( u \) discretised by the \( N(u) \) points \( u'_i \) within the block.

We denote the block random variable for \( v(u) \) by \( Z_o(u) \) and the corresponding block estimator random variable by \( Z'_o(u) \). The \( N(u) \) point values \( z(u'_i) \) are estimated by means of

\[
Z'_o(u_i) = \sum_{a=1}^{n(u)} \lambda^O(u_a) Z(u_a)
\]

using the point kriging system of type (91) and then averaged into an estimate for the block value \( z_o(u) \) given by

\[
Z'_o(u) = \frac{1}{N(u)} \sum_{i=1}^{N(u)} Z'_o(u'_i).
\]  

If the point kriging is performed with the same \( n(u) \) data for all \( N(u) \) point estimates, the point kriging system can be averaged into a single block kriging system. The block kriging estimator can then be written as

\[
Z'_o(u) = \sum_{a=1}^{n(u)} \lambda^O(u_a) Z(u_a)
\]  

where \( \lambda^O(u) \) is the block kriging weight assigned to \( z(u_a) \). The block Ordinary Kriging system is given by

\[
\left\{ \begin{array}{l}
\sum_{\beta=1}^{n(u)} \lambda^O(v(u)) C(u_a - u_\beta) + \mu^O(u_a) = Cov(u_a, v(u)), \quad a = 1, \ldots, n(u) \\
\sum_{\beta=1}^{n(u)} \lambda^O(v(u)) = 1 
\end{array} \right.
\]

This system is identical to the point Ordinary Kriging system of (91) except that the point-to-point covariance values \( C(u_a - u_\beta) \) have been replaced by point-to-block covariance values \( \overline{C}(u_a, v(u)) \) defined as

\[
\overline{C}(u_a, v(u)) = \frac{1}{|v|} \int_{v(u)} C(u_a - u') du'.
\]
This covariance is approximated by the arithmetic average of the point support covariances defined between location \( u_o \) and the \( N(u) \) points \( u'_i \) discretising the block \( u(u) \):

\[
\overline{C}(u_o, v(u)) \approx \frac{1}{N(u)} \sum_{i=1}^{N(u)} C(u_o - u'_i). \tag{100}
\]

Provided that the same \( n(u) \) data are used for all \( N(u) \) point kriging systems and for the block kriging system, each block kriging weight is the average of the \( N(u) \) point kriging weights:

\[
\lambda_{aK}^{OK}(u) = \frac{1}{N(u)} \sum_{i=1}^{N(u)} \lambda_{a_i}^{OK}(u'_i). \tag{101}
\]

Thus the block kriging system yields an estimate identical to that obtained by averaging the \( N(u) \) point estimates \( z_{aK}^{OK}(u'_i) \):

\[
z_{vOK}^{OK}(u) = \frac{1}{N(u)} \sum_{i=1}^{N(u)} z_{vK}^{OK}(u'_i). \tag{102}
\]

The Block Ordinary Kriging variance is obtained by replacing point-to-point covariance values \( C(u - u_o) \) by point-to-block covariance values \( \overline{C}(u_o, v(u)) \) in the equation for point Ordinary Kriging kriging variance (93):

\[
\sigma_{vEOK}^2(u) = Var[Z_{vOK}^*(u) - Z(u)] = \overline{C}(v(u), v(u)) - \sum_{a=1}^{n(u)} \lambda_{aK}^{OK}(u) \overline{C}(u_o, v(u)) - \mu_{OK}(u)
\]

where the within block covariance is given by

\[
\overline{C}(v(u), v(u)) = \frac{1}{(N(u))^2} \sum_{i=1}^{N(u)} \sum_{j=1}^{N(u)} C(u'_i - u'_j). \tag{104}
\]

### 2.4.3 Indicator Kriging

Linear kriging methods are designed for the estimation of the attribute itself. To this end, kriging methods of the form (79) are appropriate. Sometimes we need to estimate, not the attribute itself, but one or more functions of the attribute. This is where alternative methods, including Indicator Kriging and Disjunctive Kriging, are used. Indicator Kriging and Disjunctive Kriging are referred to as nonlinear
kriging algorithms, but are actually linear kriging algorithms applied to specific nonlinear transforms of the original data.

Indicator Kriging interprets the conditional cumulative distribution function $F(u; z_k)(n)$ as the conditional expectation of an indicator random variable $I(u; z_k)$ given the sample data $z(u_1), z(u_2), ..., z(u_n)$:

$$F(u; z_k)(n) = E[I(u; z_k)|z(u_1), z(u_2), ..., z(u_n)]$$

where the indicator random function is given by

$$I(u; z_k) = \begin{cases} 
1, & Z(u) \leq z_k \\
0, & Z(u) > z_k 
\end{cases}$$

The least squares estimate of the indicator $i(u; z_k)$ is also the least squares estimate of its conditional estimation. Thus the conditional cumulative distribution function value $F(u; z_k)(n)$ can be obtained by kriging the unknown indicator random function $I(u; z_k)$ using indicator transforms of the neighbouring information. The method of Indicator Kriging does not assume any particular shape or analytical expression for the conditional distribution $F(u; z_k)(n)$. The conditional cumulative distribution function $F(u; z_k)(n)$ is modelled through a set of $K$ threshold values $z_k$ discretising the range of $z$:

$$F(u; z_k(n)) = P\{Z(u) \leq z_k(n)\}, \quad k = 1, ..., K.$$ 

The $K$ conditional cumulative distribution function values are then interpolated within each class $(z_k, z_{k+1})$ and extrapolated beyond the two extreme threshold values $z_1$ and $z_K$.

The indicator approach begins with a selection of the number of thresholds and their values. Typically, the threshold values are chosen such that the range of $z$-values is split into classes of approximately equal frequency. Critical $z$-values are identified as thresholds so that the conditional cumulative distribution function at these values will not have to be interpolated or extrapolated later. More threshold values are chosen within the part of the distribution that is of greatest interest. The rule of thumb is that at least five thresholds should be chosen in order to provide
a reasonable discretisation of the local distribution but the number of thresholds should not exceed fifteen to alleviate computation and inference efforts.

Once the $K$ thresholds have been chosen, each datum $z(u_n)$ is coded into a vector of $K$ cumulative probabilities of the type

$$P\{Z(u) \leq z_k|\text{specific local information at } u\} \quad k = 1, ..., K. \quad (108)$$

This discrete cumulative distribution function represents the local information about the $z$-value at $u$ prior to any correction or updating based on neighbouring data. Since there is no uncertainty about $z(u_n)$ the local prior probabilities are step-functions $i(u; z_k)$ defined as

$$i(u; z_k) = \begin{cases} 1, & z(u) \leq z_k, \\ 0, & z(u) > z_k \end{cases} \quad k = 1, ..., K. \quad (109)$$

The objective is to evaluate at any location $u$ the set of $K$ conditional cumulative distribution function values or posterior probabilities defined by

$$F(u; z_k|(n)) = P\{Z(u) \leq z_k|Z(u_1) = z(u_1), Z(u_2) = z(u_2), ..., Z(u_n) = z(u_n)\}, \quad k = 1, ..., K \quad (110)$$

where $u_1, u_2, ..., u_n$ are the data locations in the search neighbourhood $W(u)$. The point kriging estimate of $i(u; z_k)$ is used as a model for the conditional cumulative distribution function value of $z(u)$ at the particular threshold value $z_k$:

$$[F(u; z_k|(n))]^* = [i(u; z_k)]^*_\text{krig}. \quad (111)$$

Each conditional cumulative distribution function value is derived as a linear combination of neighbouring indicator data, using a linear kriging algorithm such as Simple Kriging or Ordinary Kriging. This requires the solution of $K$ kriging systems, one for each threshold value $z_k$, at any location $u$.

In order to estimate the indicator value $i(u; z_k)$, the linear estimator of (80) can be expressed in terms of indicator random variables as

$$[I(u; z_k)]^* = E[I(u; z_k)] + \sum_{\alpha=1}^{n(u)} \lambda_\alpha(u; z_k) [I(u_\alpha; z_k) - E[I(u_\alpha; z_k)]] \quad (112)$$
where \( \lambda_n(u; z_k) \) is the weight assigned to \( i(u_n; z_k) \) interpreted as a realisation of the indicator random function \( I(u_n; z_k) \). Two forms of Indicator Kriging are distinguished, depending on whether or not the indicator mean is considered constant within the study area.

Simple Indicator Kriging considers the indicator mean known and constant throughout the study area:

\[
E[I(u; z_k)] = F(z_k), \quad \text{known for all } u. \tag{113}
\]

The Indicator Kriging estimator (112) becomes

\[
[F(u; z_k|(n))]_{IK} = [I(u; z_k)]_{IK} = \sum_{\alpha=1}^{n(u)} \lambda_{\alpha}^{SK}(u; z_k) I(u_\alpha; z_k) + \lambda_{i=1}^{SK}(u; z_k) F(z_k)
\]

where the weight of the mean is defined as

\[
\lambda_{i=1}^{SK}(u; z_k) = 1 - \sum_{\alpha=1}^{n(u)} \lambda_{\alpha}^{SK}(u; z_k). \tag{115}
\]

The Simple Indicator Kriging weights are provided by a kriging system of the form (86) where the covariance function \( C(h) \) has been replaced by the covariance function of \( I(u; z_k) \) denoted \( C_I(h; z_k) \):

\[
\sum_{\beta=1}^{n(u)} \lambda_{\alpha}^{SK}(u; z_k) C_I(u_\alpha - u_\beta; z_k) = C_I(u_k - u; z_k), \quad \alpha = 1, ..., n(u). \tag{116}
\]

Ordinary Indicator Kriging allows one to account for local fluctuations of the indicator mean by limiting the domain of stationarity of that mean to a local neighbourhood \( W(u) \):

\[
E[I(u'; z_k)] = \text{constant but unknown}, \quad u' \in W(u). \tag{117}
\]

The Indicator Kriging estimator of (112) becomes

\[
[F(u; z_k|(n))]_{IK} = [I(u; z_k)]_{IK} = \sum_{\alpha=1}^{n(u)} \lambda_{\alpha}^{OK}(u; z_k) I(u_\alpha; z_k) \tag{118}
\]

where the Ordinary Indicator Kriging weights are given by a kriging system of the form (91) with \( C(h) \) replaced by \( C_I(h; z_k) \):

\[
\begin{align*}
\sum_{\beta=1}^{n(u)} \lambda_{\alpha}^{OK}(u; z_k) C_I(u_\alpha - u_\beta; z_k) + \mu_{OK}(u; z_k) &= C_I(u_k - u; z_k), \quad \alpha = 1, ..., n(u) \\
\sum_{\beta=1}^{n(u)} \lambda_{\alpha}^{OK}(u; z_k) &= 1
\end{align*}
\tag{119}
\]
Correcting for Order Relation Deviations

At any location \( u \), each estimated posterior probability \( [F(u; z_k(n))]^* \) must lie in the interval \([0, 1] \) and the series of such \( K \) estimates must be a non-decreasing function of the threshold value \( z_k \):

\[
[F(u; z_k(n))]^* \in [0, 1] \tag{120}
\]

\[
[F(u; z_k(n))]^* \leq [F(u; z_k(n))]^* \quad \forall z_{k'} > z_k. \tag{121}
\]

The common practice is to correct for order relation deviations after the estimation of the \( [F(u; z_k(n))]^* \) probabilities. To do so, the original series of conditional cumulative distribution function values \( \{[F(u; z_k(n))]^*, k = 1, ..., K \} \) must be corrected to a new set of posterior probabilities \( \{[F(u; z_k(n))]^", k = 1, ..., K \} \) honouring the two order relations (120) and (121). A common algorithm implemented for this purpose, including in both the GSLIB and ISATIS software packages, consists of averaging the results of an upward and downward correction of conditional cumulative distribution function values (Bleines et al, 2000; Deutsch & Journel, 1998; Goovaerts, 1997).

Change of Support in Indicator Kriging

Indicator Kriging estimates of \( I(u; z_k) \) have thus far been confined to the goal of point estimation using point data, referred to as point support. As mentioned previously, the target may be an estimate over a block of given dimensions. In terms of Indicator Kriging this refers to modelling the block conditional cumulative distribution function \( F_v(u; z_k(n)) \) using the block indicator variable \( i_v(u; z_k) \) defined as

\[
i_v(u; z_k) = \begin{cases} 
1, & z_v(u) \leq z_k \\
0, & z_v(u) > z_k 
\end{cases} \tag{122}
\]

As block data do not exist, the block conditional cumulative distribution function must be modelled from the known point data. The indicator variable \( i(u; z) \) is a non-linear transform of the original variable \( z(u) \) and therefore the block indicator \( i_v(u; z_k) \) is not a linear average of the point indicators \( i(u; z_k) \). As a consequence, we cannot derive the block conditional cumulative distribution function by averaging a series of point estimates. To overcome this problem, we seek to make
estimates for a large block V(u) centred on u, referred to as a panel, by deriving an estimate at the centre of the panel of the proportion of blocks in the panel above a given threshold on the basis of the distribution of the N(u) smaller blocks v(u_i) of size v within the panel. Making an estimate based on the distribution of blocks within the region is known as block support, and v is called the support size, which is the minimum block size on which a decision may be based. A model is required for the change from point support to block support.

The traditional approach to the change of support in Indicator Kriging has been to apply a variance correction factor on a global basis to the point Indicator Kriging estimates. The most widely used technique for achieving this in practical applications of Indicator Kriging is affine correction, a simple factoring of the point variance to estimate the theoretical block variance (Glacken & Blackney, 1988). An affine transformation is used to reduce the variance of a distribution without changing its mean. Specifically the method transforms a value y of the point distribution into a value y' of the block distribution using the following linear formula:

\[ y' = \sqrt{f}(y - m) + m \]  

(123)

where the mean of both distributions is m, the variance of the original distribution is \( \sigma^2 \) and the variance of the transformed distribution will be \( f \sigma^2 \) (Isaaks & Srivastava, 1989; Journel & Huijbregts, 1978). This method presupposes that we have a variance correction factor \( f \) in mind.

The variance correction factor \( f \) can be estimated based on assumptions about how the distribution of values changes as their support changes. Krige's Relationship (Isaaks & Srivastava, 1989) is defined by

\[ \sigma^2(u, A) = \sigma^2(u, v(u)) + \sigma^2(v(u), A) \]  

(124)

where \( \sigma^2(v_1, v_2) \) is the variability of a region \( v_1 \) within a region \( v_2 \) and \( u \) refers to an arbitrary point in the block \( v(u) \). Equation (124) states that the total variance of points within a study region is equal to the sum of the variances of point values within blocks and the variance of block values within the study region. Using
Krige's Relationship the variance adjustment factor, from point support to block support, is the ratio of the block variance to the point variance:

\[ f = \frac{\sigma^2(v(u), A)}{\sigma^2(u, A)} = 1 - \frac{\sigma^2(u, v(u))}{\sigma^2(u, A)}. \tag{125} \]

The value of \( \sigma^2(u, v(u)) \) is estimated by the average value of the variogram model for the block \( v(u) \) obtained by discretising the block \( v(u) \) into several points and calculating the average variogram value \( \bar{\gamma}(v(u), v(u)) \) between all possible pairs of points. In practice, the semivariogram model of the raw variable is fitted with a sill equal to the variance of the sample values, and the sill of the variogram model for the study region \( A \) is the estimate of \( \sigma^2(u, A) \). This ensures that both \( \sigma^2(u, v(u)) \) and \( \sigma^2(u, A) \) are estimated from the same semivariogram model. In this project, the value of \( \bar{\gamma}(v(u), v(u)) \) is obtained from the Gaussian Anamorphosis Modelling process implemented in the ISATIS program.

Point kriging estimates \([I(u; z_k)]^*\) are made at the centre of the panels \( V(u) \) and then corrected to the panel estimate of the proportion of blocks in the panel below a threshold \( z'_k \). The threshold value \( z_k \) for the point distribution is adjusted to that of the block distribution \( z'_k \) using (123) and (125) whilst the associated probability remains the same:

\[
\left[ \frac{1}{N(v)} \sum_{i=1}^{N(v)} I_v(u_i; z'_{k}) \right]^* = [I(u; z_k)]^*, \quad z'_k = \sqrt{f(z_k - m)} + m \tag{126} \]

where \( I_v(u_i; z'_{k}) \) is the indicator random variable of \( i_v(u_i; z'_k) \) defined in (122).

Estimating Panel Tonnage and Mean Attribute Value above a Threshold

For the purposes of comparison of the different kriging methods in this project, it was decided to focus on estimates of the tonnage and average attribute value of each panel in the study region for specified thresholds. The panel tonnage \( T_V(u; z_k) \) for a threshold \( z_k \) is the proportion of the blocks within that panel that have an attribute value greater than the specified threshold (Rivoirard, 1994):

\[ T_V(u; z_k) = 1 - \frac{1}{N(v)} \sum_{i=1}^{N(v)} I_v(u_i; z_k). \tag{127} \]
The average value $M_V(u; z_k)$ of the attribute above a threshold $z_k$ for a panel is given by (Rivoirard, 1994)

$$M_V(u; z_k) = \frac{Q_V(u; z_k)}{T_V(u; z_k)} \quad (128)$$

where $Q_V(u; z_k)$ is the quantity of attribute in a panel above a threshold $z_k$ defined by (Rivoirard, 1994)

$$Q_V(u; z_k) = \frac{1}{N(v)} \sum_{i=1}^{N(v)} Z_v(u_i) [1 - I_n(u_i; z_k)]. \quad (129)$$

### 2.4.4 Disjunctive Kriging

The Disjunctive Kriging estimator is a kriging estimator of the form

$$[f [Z(u)]]^* = \sum_{\alpha=1}^{n(u)} \lambda_\alpha [Z(u_\alpha)] Z(u_\alpha) \quad (130)$$

where $\lambda_\alpha [Z(u_\alpha)]$ denotes a kriging weight that depends on $Z(u_\alpha)$. It must be noted that the particular case $f[Z(u)] = Z(u)$ means that Disjunctive Kriging can be used for estimating the variable $Z(u)$ itself. The method of Disjunctive Kriging involves decomposing the function to be estimated into a sum of uncorrelated components that can then be kriged separately, hence the term disjunctive.

### Gaussian Disjunctive Kriging

There are a number of different models available for use in Disjunctive Kriging. One of these is Gaussian Disjunctive Kriging (Chiles & Delfiner, 1999; Rivoirard, 1994) where the function to be estimated is expanded in terms of Hermite polynomials. Gaussian Disjunctive Kriging presupposes that the variable $Z(u)$ is univariate normal and that the variables $(Z(u), Z(u + h))$ are bivariate normal. In practice the variable studied, $Z(u)$, is rarely normally distributed and so a transformation is required to convert $Z(u)$ to a standard normal (Gaussian) random variable $Y(u)$. The function $\Phi$ that relates $Z(u)$ and $Y(u)$ is called the anamorphosis function and we have $Z(u) = \Phi [Y(u)]$ where $\Phi$ is the function that associates with each value $z$ of $Z(u)$ the value $y$ of $Y(u)$ such that the respective cumulative probabilities are equal:

$$P \{Z(u) \leq z\} = P \{Y(u) \leq y\}. \quad (131)$$
The transformed pairs \((Y(u), Y(u + h))\) are assumed to be bivariate standard normal. The anamorphosis function can then be expanded in terms of the Hermite polynomials \(H_j [Y(u)]\) by

\[
Z(u) = \Phi [Y(u)] = \sum_{j=0}^{\infty} \phi_j H_j [Y(u)]
\]

where the coefficients \(\phi_j\) of the expansion are given by (9)

\[
\phi_j = \frac{\langle \Phi, H_j \rangle}{\| H_j \|_w^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-y^2/2} \Phi (y) H_j (y) dy, \quad j = 0, 1, 2, ...
\]

(133)

In practice, the anamorphosis function is determined from the histogram of the raw variable. In this case the coefficients are calculated as follows:

\[
\phi_j = \begin{cases} 
\sum_i p_i z_i, & j = 0 \\
\sum_{i=2}^j (z_{i-1} - z_i) \frac{1}{\sqrt{\pi}} H_{n-1} (y_i) g (y_i), & j \neq 0
\end{cases}
\]

(134)

where \(p_i = P \{ z_i < Z(u) < z_{i+1} \} \).

Gaussian Disjunctive Kriging can be used to estimate any function that can be expressed as a series of Hermite polynomials. A function of the attribute written in terms of the anamorphosis function can be expressed as a series of Hermite polynomials, namely

\[
f [Z(u)] = f [\Phi [Y(u)]] = \sum_{j=0}^{\infty} f_j H_j [Y(u)]
\]

(135)

where the \(f_j\)'s are the coefficients determined using (9):

\[
f_j = \frac{\langle f \circ \Phi, H_j \rangle}{\| H_j \|_w^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-y^2/2} f [\Phi (y)] H_j (y) dy, \quad j = 0, 1, 2, ...
\]

(136)

As there is no spatial correlation between Hermite polynomials of different order (53), the polynomials of (135) have only to be kriged separately to give the Disjunctive Kriging estimator of the unknown \(f [Z(u)]\). Simple Kriging is used to krig the polynomials as the mean of the Hermite polynomials is known and constant (??). The Disjunctive Kriging estimator of the function is then given by

\[
[f [Z(u)]]^{*}_{DK} = \sum_{j=0}^{\infty} f_j [H_j [Y(u)]]^{*}_{SK}
\]

(137)
where \([H_j [Y(u)]|_{SK}]^*\) is the estimated value of \(H_j [Y(u)]\) and is written as a weighted sum of Hermite polynomials evaluated at the sample values:

\[
[H_j [Y(u)]|_{SK}]^* = \sum_{\alpha=1}^{n(u)} \lambda_{\alpha j} H_j [Y(u_\alpha)].
\]

(138)

The weights \(\lambda_{\alpha j}\) are determined by solving a Simple Kriging system of the form (86) where the covariance between the random variables at different locations has been replaced by the covariance between the Hermite polynomials of the random variables at the different locations:

\[
\sum_{\beta=1}^{n(u)} \lambda_{\beta j}^K (u) Cov[H_j [Y(u_\alpha)], H_j [Y(u_\beta)]] = Cov[H_j [Y(u_\alpha)], H_j [Y(u)]],
\]

\(\alpha = 1, \ldots, n(u).\)

(139)

Using (53) and (70) the Simple Kriging system becomes

\[
\sum_{\beta=1}^{n(u)} \lambda_{\beta j}^K (u) [C(u_\alpha - u_\beta)]^j = [C(u_\alpha - u)]^j, \quad \alpha = 1, \ldots, n(u).
\]

(140)

As \(j\) increases, the kriging weights tend to zero and so the kriged estimator of \(H_j [Y(u)]\) at an unknown location rapidly tends to its mean (zero). Therefore in practice it is only necessary to krig a few polynomials to achieve the estimate.

Change of Support in Disjunctive Kriging

The target of estimation can be the block value of the attribute or a function of the attribute. As Disjunctive Kriging involves a non-linear transform of the original variable, the block value cannot be obtained by averaging a series of point estimates. As in the case for Indicator Kriging, estimates are calculated for the panel \(V(u)\) based on block support \(v\) using a change-of-support model to obtain the block distribution from the known point distribution.

The change-of-support model employed in Gaussian Disjunctive Kriging is known as the discrete Gaussian model. The support block size \(v\) is chosen as the minimum size upon which decisions may be based. The position of a sample inside a block is assumed to be random. In practice, the samples are relocated to the centre of the blocks so the block size is chosen such that any given block contains at most...
one sample. The location of a sample \(Z(u_n)\) is actually at \(u_n\), but is relocated to \(u_i\), where \(u_i\) is the centre of the block \(v(u_i)\) containing the sample. The Gaussian value \(Y_v(u_n)\) is associated with each block value \(Z_v(u_n)\) in the same way that we associated a Gaussian equivalent \(Y(u_n)\) with each sample value \(Z(u_n)\) using the anamorphosis function \(\Phi\). The block variable \(Z_v(u)\) is expressed as a function \(\Phi_v\) of another standard normal variable \(Y_v(u)\):

\[
Z_v(u) = \Phi_v[Y_v(u)]. \tag{141}
\]

In order to link the different blocks and samples we assume that any set of point Gaussian equivalents \(Y(u_n), Y(u_\beta), \ldots\) and of block Gaussian equivalents \(Y_v(u_\alpha), Y_v(u_\beta), \ldots\) is multivariate normal.

Cartier's relation (Rivoirard, 1994)

\[
E[Z(u)|Z_v(u)] = Z_v(u) \tag{142}
\]

where \(u\) denotes a point located at random inside the block \(v(u)\), means that the expected value of the grade of a point chosen at random given the block grade is equal to the block grade. Using the Hermite expansion of \(Z(u) = \Phi [Y(u)]\) given by (132) this relation can be written as

\[
Z_v(u) = \Phi_v[Y_v(u)]
\]

\[
= E[\Phi [Y(u)] | Y_v(u)]
\]

\[
= E \left[ \sum_{j=0}^{\infty} \phi_j H_j [Y(u)] | Y_v(u) \right] \text{ by (132)}
\]

\[
= \sum_{j=0}^{\infty} \phi_j E[H_j [Y(u)] | Y_v(u)]
\]

\[
= \sum_{j=0}^{\infty} \phi_j r^j H_j [Y_v(u)] \text{ by (52)} \tag{143}
\]

where \(r\) denotes the correlation coefficient of the standard bivariate normal pair \((Y(u), Y_v(u))\). Comparing this Hermite polynomial expansion of the block attribute variable to that of the point attribute variable (132), the anamorphosis coefficients for blocks is obtained by multiplying the corresponding point coefficients \(\phi_j\) by \(r^j\).

Using (65) and (66), we obtain for the point and block anamorphosis functions \(Z(u) = \Phi [Y(u)]\) and \(Z_v(u) = \Phi_v[Y_v(u)]\), whose anamorphosis coefficients are
given by $\phi_j$ and $\phi_j r^j$ respectively:

$$
\begin{align*}
\text{Cov} [Z (u_\alpha), Z (u_\beta)] &= \sum_{j=1}^{\infty} \phi_j^2 \left[ \text{Cov} [Y (u_\alpha), Y (u_\beta)] \right]^j, \\
\text{Cov} [Z (u_\alpha), Z_v (u_\beta)] &= \sum_{j=1}^{\infty} \phi_j^2 r^j \left[ \text{Cov} [Y (u_\alpha), Y_v (u_\beta)] \right]^j, \\
\text{Cov} [Z_v (u_\alpha), Z_v (u_\beta)] &= \sum_{j=1}^{\infty} \phi_j^2 r^j \left[ \text{Cov} [Y_v (u_\alpha), Y_v (u_\beta)] \right]^j.
\end{align*}
$$

As the covariance between any point chosen at random in a block with any other block or between any random point in one block with any random point in another block is just the covariance between the two blocks, we may also write

$$
\text{Cov} [Z (u_\alpha), Z_v (u_\beta)] = \text{Cov} [Z (u_\alpha), Z (u_\beta)] = \text{Cov} [Z_v (u_\alpha), Z_v (u_\beta)].
$$

Using $\text{Cov} [Y_v (u_\alpha), Y_v (u_\alpha)] = \text{Var} [Y_v (u_\alpha)] = 1$ and the results of (144) and (145), we define the discrete Gaussian change-of-support model by

$$
\begin{align*}
\text{Cov} [Y (u_\alpha), Y_v (u_\beta)] &= r \text{Cov} [Y_v (u_\alpha), Y_v (u_\beta)], \\
\text{Cov} [Y (u_\alpha), Y (u_\beta)] &= \begin{cases} 
 r^2 \text{Cov} [Y_v (u_\alpha), Y_v (u_\beta)], & \alpha \neq \beta, \\
 1, & \alpha = \beta.
\end{cases}
\end{align*}
$$

This change-of-support model allows us to express the kriging system in terms of block values $Y_v (u)$ rather than point values $Y (u)$. The kriging system for the panel is then obtained from the block kriging system by replacing the block variable $Y_v (u)$ by the sum of the variables for each block within the given panel. Estimates can then be made for each panel $V (u)$ on the basis of the $N (v)$ smaller blocks $v (u_i)$ of size $v$ within the panel.

The correlation coefficient $r$ of the pair $(Y (u), Y_v (u))$ is known as the change-of-support coefficient and is determined by the previously defined Kriging Relationship (124). Using the variance of a function of the standard normal variable expressed in terms of Hermite polynomials (59) where the coefficients of the block expansion are given by $\phi_j r^j$ the variability of blocks within the study region can be written as

$$
\sigma^2 (v (u), A) = \text{Var} [Z_v (u)] = \text{Var} [\Phi_r [Y_v (u)]] = \sum_{j=1}^{\infty} (\phi_j)^2 r^{2j}.
$$

As shown in the section on Change of Support in Indicator Kriging, $\sigma^2 (v (u), A)$ can be calculated from the estimated values of $\sigma^2 (v (u), A)$ and $\sigma^2 (u, A)$. The change-of-support coefficient $r$ can then be determined using (147). Note that $0 \leq r \leq 1$. 

45
Estimating Panel Tonnage and Mean Attribute Value above a Threshold

Estimates of the tonnage $T_V(u; z_k)$ and average attribute value $M_V(u; z_k)$ for the given cutoff, defined previously in (127) and (128) respectively, are obtained for each panel $V(u)$ based on block support $v$.

The tonnage for a panel $T_V(u; z_k)$ (127) is obtained from the sum of the Indicator Functions of the block attribute value $I_v(u; z_k)$, which, expressed in terms of Hermite polynomials, is given by

$$I_v(u; z_k) = I_v(u; y_k) = \sum_{j=0}^{\infty} c_j H_j \{Y_v(u)\}$$  \hspace{1cm} (148)

where $z_k = \Phi(y_k)$. The coefficients of the Hermite expansion are given by (9):

$$c_j = \frac{\langle I_v, H_j \rangle}{\|H_j\|^2_w}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{y^2}{2}} I_v(u; y_k) e^{\frac{dy^2}{2}} \frac{dy}{\sqrt{2\pi}} (e^{\frac{y^2}{2}}) dy$$

by (2), (20) and (22)

$$= \frac{1}{\sqrt{2\pi j!}} \int_{-\infty}^{y_k} dy \left( e^{-\frac{y^2}{2}} \right) dy$$

by (122)

$$= \begin{cases} \int_{-\infty}^{y_k} e^{-\frac{y^2}{2}} dy, & j = 0 \\ \frac{1}{\sqrt{2\pi j!}} \int_{-\infty}^{y_k} dy e^{-\frac{y^2}{2}} dy, & j = 1, 2, ... \end{cases}$$

$$= \begin{cases} g(y_k), & j = 0 \\ \frac{1}{\sqrt{2\pi}} g(y_k) H_{j-1}[y_k], & j = 1, 2, ... \end{cases}$$  \hspace{1cm} (149)

where $g(y_k)$ and $G(y_k)$ are defined previously by (43) and (44) respectively. The Indicator Function (148) can then be written as

$$I_v(u; z_k) = G(y_k) + \sum_{j=1}^{\infty} \frac{1}{\sqrt{j}} g(y_k) H_{j-1}[y_k] H_j \{Y_v(u)\}.$$  \hspace{1cm} (150)

The regularised variable

$$\frac{1}{N(v)} \sum_{i=1}^{N(v)} I_v(u_i; z_k)$$  \hspace{1cm} (151)

can be estimated without having to estimate $I_v(u_i; z_k)$ for each block $v(u_i)$ by replacing the kriging system for each block $v(u)$ by the system for the panel $V(u)$. The Simple Kriging system for the block $v(u)$ is of the type (86) obtained by replacing the point-to-point covariance values on the right hand side of (86) by
the point-to-block covariance values:

$$
\sum_{\beta=1}^{n(u)} \lambda_{\beta j}^{DK}(u) \text{Cov}[H_j | Y(u_\alpha), H_j | Y(u_\beta)]] = \text{Cov}[H_j | Y(u_\alpha), H_j | Y(u)],
$$

$$
\alpha = 1, \ldots, n(u).
$$

Using (53) we obtain

$$
\sum_{\beta=1}^{n(u)} \lambda_{\beta j}^{DK}(u) [\text{Cov}[Y(u_\alpha), Y(u_\beta)]]^{\beta} = [\text{Cov}[Y(u_\alpha), Y(u)]]^{\alpha},
$$

$$
\alpha = 1, \ldots, n(u).
$$

Then by the discrete Gaussian model (146), the block kriging system can be written as

$$
\lambda_{\alpha j} + \sum_{\beta=1}^{n(u)} \lambda_{\beta j} r^{2j} [\text{Cov}[Y_v(u_\alpha), Y_v(u_\beta)]^{\beta}] = r^j [\text{Cov}[Y_v(u_\alpha), Y_v(u)]]^{\alpha},
$$

$$
\alpha = 1, \ldots, n(u).
$$

The Simple Kriging system for the panel $V(u)$ is then obtained by replacing the block variable $Y_v(u)$ by the sum of the variables for each block within the given panel:

$$
\lambda_{\alpha j} + \sum_{\beta=1}^{n(u)} \lambda_{\beta j} r^{2j} [\text{Cov}[Y_v(u_\alpha), Y_v(u_\beta)]^{\beta}] = \frac{1}{N_v} \sum_{i=1}^{N(v)} \left( r^j [\text{Cov}[Y_v(u_\alpha), Y_v(u)]^{\alpha} \right),
$$

$$
\alpha = 1, \ldots, n(u).
$$

Using this kriging system the estimate of the regularised variable is given by

$$
\left[ \frac{1}{N(v)} \sum_{i=1}^{N(v)} \sum_{j=1}^{N(v)} I_v(u; z_k) \right]_{DK} = G(y_k) + \sum_{j=1}^{\infty} \frac{1}{\sqrt{j}} g(y_k) H_{j-1}[y_k] \left[ \frac{1}{N(v)} \sum_{i=1}^{N(v)} H_j | Y_v(u_i)] \right]_{SK}.
$$

Therefore we only need to krig $\sum_{i=1}^{N(v)} H_j | Y_v(u_i)]$ directly for each panel. The Disjunctive Kriging estimate of the tonnage above a threshold $z_k$ for a panel $V(u)$, using (127), is then given by

$$
[T_{V}(u; z_k)]_{DK} = 1 - G(y_k) - \sum_{j=1}^{\infty} \frac{1}{\sqrt{j}} g(y_k) H_{j-1}[y_k] \left[ \frac{1}{N(v)} \sum_{i=1}^{N(v)} H_j | Y_v(u_i)] \right]_{SK}.
$$
The average attribute value above a threshold for a panel (128) is obtained from the tonnage and attribute quantity of the panel. The attribute quantity $Q_v(u; z_k)$ (129) for a panel is given by

$$Q_v(u; z_k) = \frac{1}{N(u)} \sum_{i=1}^{N(u)} |Z_v(u_i) \{ 1 - I_v(u_i; z_k) \}|$$

which can be expressed in terms of Hermite Polynomials:

$$Q_v(u; z_k) = \sum_{j=0}^{\infty} q_j \left[ \frac{1}{N(u)} \sum_{i=1}^{N(u)} H_j[Y_v(u_i)] \{ 1 - I_v(u_i; y_k) \} \right]$$

The coefficients $q_j$ of the Hermite expansion can be written as

$$q_j = \left\langle \sum_{p=0}^{\infty} \phi_p H_p, H_j \right\rangle = \sum_{p=0}^{\infty} \phi_p \int_{y_k}^{\infty} e^{-y^2/2} H_p[y] H_j[y] \, dy.$$  

Therefore the Disjunctive Kriging estimator of the panel attribute quantity is given by

$$[Q_v(u; z_k)]_{DK} = \sum_{j=0}^{\infty} q_j \left[ \frac{1}{N} \sum_{i=1}^{N} H_j[Y_v(u_i)] \right]_{SK}$$

using the Simple Kriging system of (155). Note that we only need to krig the regularised variable $\frac{1}{N} \sum_{i=1}^{N} H_j[Y_v(u_i)]$ once to obtain the Disjunctive Kriging estimator of any function of the regularised variable that we wish to estimate. Using the Disjunctive Kriging estimates of the panel attribute quantity and the panel tonnage, the Disjunctive Kriging estimate of the average attribute value for the panel is given by

$$[M_v(u; z_k)]_{DK} = \frac{[Q_v(u; z_k)]_{DK}}{[T_v(u; z_k)]_{DK}}.$$
3 Data Analysis

Two suites of data were analysed in the course of this project for the purpose of comparing the results from three methods of kriging to be explored, namely Ordinary Kriging, Indicator Kriging and Disjunctive Kriging. One data suite (Moisture) is from the environmental science field and the other (True) is from the mining field.

3.1 Moisture Data Suite

The Moisture data set is an exhaustive data set obtained by sequential Gaussian simulation of soil samples taken originally in an uncropped field in an investigation of soil salinity and acidity in the Jimperding Brook area in Western Australia (Bloom & Kentwell, 1999). The data comprise 3600 moisture measurements located on a 2-dimensional square grid of size 60 metres by 60 metres with a grid spacing of 1.0 metre. A sample data set (Moisture100) consisting of 100 data points chosen randomly from the exhaustive Moisture data set, was used for estimation.

3.1.1 Statistical Description

Descriptive statistics for the moisture variable from Moisture and Moisture100 are shown in Table 1. These have similar means and standard deviations, but the sample data have a noticeably higher minimum and a noticeably lower maximum than the exhaustive data. Except for skewness and kurtosis, the sample data appear to reflect the summary statistics of the exhaustive data. Graphical summaries of the two data sets are shown in Figure 1 and Figure 2. The box plot of the Moisture summary indicates the presence of multiple outliers, including both extreme low and high values. These outliers are most likely a result that the data is simulated which may possibly be corrected by smoothing but this will not be undertaken in this study. A few high valued outliers are also evident in Moisture100. A normality test of the Moisture data indicates that the data are not normally distributed, with the skewness and kurtosis factors indicating positive skewness. Whilst the normality test of the Moisture100 data indicates that the data are most likely not normally distributed, the skewness and kurtosis factors are very small, indicating weak (positive) skewness.
Table 1: Descriptive statistics for \textit{Moisture} and \textit{Moisture100} data sets.

<table>
<thead>
<tr>
<th></th>
<th>Moisture</th>
<th>Moisture100</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>3600</td>
<td>100</td>
</tr>
<tr>
<td>Mean</td>
<td>11.796</td>
<td>11.581</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>1.901</td>
<td>1.678</td>
</tr>
<tr>
<td>Skewness</td>
<td>3.158</td>
<td>0.702</td>
</tr>
<tr>
<td>Kurtosis</td>
<td>27.898</td>
<td>0.852</td>
</tr>
<tr>
<td>Minimum</td>
<td>0.916</td>
<td>7.867</td>
</tr>
<tr>
<td>1st Quartile</td>
<td>10.626</td>
<td>10.414</td>
</tr>
<tr>
<td>Median</td>
<td>11.548</td>
<td>11.451</td>
</tr>
<tr>
<td>3rd Quartile</td>
<td>12.632</td>
<td>12.479</td>
</tr>
<tr>
<td>Maximum</td>
<td>38.511</td>
<td>17.139</td>
</tr>
</tbody>
</table>

Figure 1: Graphical summary of \textit{Moisture}.
Figure 2: Graphical summary of Moisture100.

The cumulative distribution functions of the exhaustive and sample moisture data are shown in Figure 3 and Figure 4 respectively. Inspection of the two graphs indicates that the Moisture100 data are representative of the Moisture data. The cumulative distribution function of the Moisture100 data will be used in the Indicator Kriging procedure to model the shape of the upper and lower tails beyond the estimated values of the cumulative distribution function.

Figure 3: Cumulative distribution function from Moisture.
3.1.2 Spatial Description

Plots of the moisture values of Moisture and Moisture100 are shown in Figure 5. The sample data reflect the regions of high values in the lower half and regions of low values in the upper half evident in the map of the exhaustive moisture values. However, they do not capture the region of high values along the upper edge of the Moisture map. Visual inspection does not suggest any evidence of anisotropy in either the sample or exhaustive data.

Figure 5: Plots of moisture values from Moisture (left) and Moisture100 (right).
In order to evaluate and compare the results of the various kriging procedures, estimates of panel proportions and mean values above given thresholds was obtained in each case. The block support size chosen was 1 metre by 1 metre and the panel size was chosen to be 5 metres by 5 metres. The thresholds used were the nine deciles, calculated using the convention of Isaaks & Srivastava (1989). The corresponding moisture values are shown in Table 2. Proportions of the panel values above each threshold and the mean panel value above the threshold were calculated for the Moisture data and are shown in Figure 6 and Figure 7 respectively. If the proportion of the panel values above the threshold is zero, then there is no corresponding mean panel value above the given threshold. This is indicated by a white panel on the map of the mean panel value above the threshold.

Table 2: Indicator thresholds for Moisture100.

<table>
<thead>
<tr>
<th>Decile</th>
<th>Threshold Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st</td>
<td>9.69</td>
</tr>
<tr>
<td>2nd</td>
<td>10.21</td>
</tr>
<tr>
<td>3rd</td>
<td>10.62</td>
</tr>
<tr>
<td>4th</td>
<td>10.93</td>
</tr>
<tr>
<td>5th</td>
<td>11.45</td>
</tr>
<tr>
<td>6th</td>
<td>11.94</td>
</tr>
<tr>
<td>7th</td>
<td>12.37</td>
</tr>
<tr>
<td>8th</td>
<td>12.85</td>
</tr>
<tr>
<td>9th</td>
<td>13.89</td>
</tr>
</tbody>
</table>
Figure 6: Panel proportions of moisture values from Moisture above specified thresholds.

Figure 6 indicates that the panels in the upper half of the study region generally have a lower proportion of values greater than the threshold for all thresholds. The panels showing the greatest proportion of values exceeding the given threshold are concentrated in the lower left hand corner of the study region. This means that generally the moisture values in the upper half of the study region have lower values than those in the lower half with the highest moisture values located in the lower left hand corner. Figure 7 indicates similar regions of high and low moisture values. These regions are reflected in the map of the exhaustive moisture data in Figure 5.
Figure 7: Panel mean moisture values of Moisture above specified thresholds.
3.1.3 Variography

Exploratory variography and variogram modelling were conducted on the sample moisture values of Moisture100 in order to apply the Ordinary Kriging, Indicator Kriging and Disjunctive Kriging procedures.

3.1.3.1 Variography of Moisture Values

Exploratory variography was performed on the sample moisture values to develop a model for use in the Ordinary Kriging and Disjunctive Kriging methods. The variogram surface of the sample data is shown in Figure 8 and indicates that there is no anisotropy evident in the sample moisture values. Therefore, an isotropic model was developed.

![Variogram Surface](image)

Figure 8: Variogram surface of Moisture100. (Lag spacing 6, Number of lags 7)

Calculation of the change-of-support factor requires a semivariogram model with total sill equal to the variance of the sample moisture values. Fitting a model of this form to the experimental semivariogram was not obvious by visual inspection of the experimental semivariogram (solid black circles) in Figure 10 where the sample variance is indicated by the dashed line. It was necessary to investigate and infer the model parameters from other measures of spatial continuity.

The covariance and correlogram models shown in Figure 9 indicate a model incorporating a nugget with a relative nugget effect of approximately 55% and two spherical structures at ranges 10 and 35 respectively. Using these models, an
isotropic semivariogram model was fitted with a nugget constant and two spherical structures. The relative nugget effect and the ranges used were those of the covariance and correlogram models. The semivariogram model and its parameters are shown in Figure 10 and Table 3 respectively.

Figure 9: Covariance (left) and correlogram (right) models of Moisture100.

Figure 10: Omnidirectional experimental semivariogram and semivariogram model of Moisture100. (Lag spacing 6, Number of lags 9)
Table 3: Semivariogram model parameters for Moisture100.

<table>
<thead>
<tr>
<th>Type</th>
<th>1st Structure</th>
<th>2nd Structure</th>
<th>3rd Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Range</td>
<td>-</td>
<td>10</td>
<td>35</td>
</tr>
<tr>
<td>Sill</td>
<td>1.6</td>
<td>0.16</td>
<td>1.04</td>
</tr>
</tbody>
</table>

3.1.3.2 Variography of Moisture Indicator Values

The Moisture100 data were coded into indicator variables according to the thresholds of Table 2 using the definition of \( i(u; z_k) \) (109). Exploratory variography was performed on the Moisture100 indicator data to develop a model for use in the Indicator Kriging method.

The variogram surfaces of the Moisture100 indicator data are shown in Figure 11. They suggest the possibility of anisotropy in the 3rd, 4th, 7th and 8th decile cutoffs. The variogram surfaces in the 3rd and 4th deciles suggest anisotropy with maximum spatial continuity parallel to the horizontal and those of the 7th and 8th deciles at an angle of 45\(^\circ\) taken clockwise from the horizontal. The direction of minimum spatial continuity is perpendicular to that of maximum spatial continuity. The presence of anisotropy was investigated via the directional semivariograms in the directions of maximum and minimum spatial continuity and in the intermediate directions (directions halfway between those of maximum and minimum spatial continuity), standardised via the variance of the indicator data shown in Table 4. Superimposition of the experimental directional semivariograms for the deciles indicated previously with the relevant isotropic model derived from the omnidirectional experimental semivariograms, as shown in Figure A1, Figure A2, Figure A3 and Figure A4 respectively in Appendix A, suggests that the spatial variability can be adequately modelled using an isotropic model. The experimental omnidirectional standardised semivariograms for the Moisture100 indicator data and the models fitted are shown in Figure 12 and their parameters are outlined in Table 5. The model in each case has a nugget constant and one exponential structure. The 9th decile was not used as the experimental semivariogram was too erratic.
Figure 11: Variogram surfaces of Moisture100 indicator data. (Lag spacing 6, Number of lags 7)

Table 4: Variance of Moisture100 indicator data.

<table>
<thead>
<tr>
<th>Threshold</th>
<th>Indicator Data Variance</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.69</td>
<td>0.090</td>
</tr>
<tr>
<td>10.21</td>
<td>0.160</td>
</tr>
<tr>
<td>10.62</td>
<td>0.210</td>
</tr>
<tr>
<td>10.93</td>
<td>0.242</td>
</tr>
<tr>
<td>11.45</td>
<td>0.250</td>
</tr>
<tr>
<td>11.94</td>
<td>0.240</td>
</tr>
<tr>
<td>12.37</td>
<td>0.210</td>
</tr>
<tr>
<td>12.85</td>
<td>0.154</td>
</tr>
<tr>
<td>13.89</td>
<td>0.090</td>
</tr>
</tbody>
</table>
Figure 12: Omnidirectional experimental semivariogram and semivariogram models of Moisture100 indicator data. (Lag spacing 6, Lag tolerance 3, Number of lags 9)
Table 5: Semivariogram model parameters for Moisture100 indicator data.

<table>
<thead>
<tr>
<th>Decile</th>
<th>Value</th>
<th>Nugget</th>
<th>Sill</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st</td>
<td>9.69</td>
<td>0.40</td>
<td>0.60</td>
<td>11</td>
</tr>
<tr>
<td>2nd</td>
<td>10.21</td>
<td>0.55</td>
<td>0.45</td>
<td>11</td>
</tr>
<tr>
<td>3rd</td>
<td>10.62</td>
<td>0.65</td>
<td>0.35</td>
<td>11</td>
</tr>
<tr>
<td>4th</td>
<td>10.93</td>
<td>0.65</td>
<td>0.35</td>
<td>17</td>
</tr>
<tr>
<td>5th</td>
<td>11.45</td>
<td>0.65</td>
<td>0.35</td>
<td>17</td>
</tr>
<tr>
<td>6th</td>
<td>11.94</td>
<td>0.70</td>
<td>0.30</td>
<td>21</td>
</tr>
<tr>
<td>7th</td>
<td>12.37</td>
<td>0.75</td>
<td>0.25</td>
<td>30</td>
</tr>
<tr>
<td>8th</td>
<td>12.85</td>
<td>0.50</td>
<td>0.50</td>
<td>30</td>
</tr>
</tbody>
</table>

3.1.3.3 Variography of Block Gaussian Moisture Variable

Disjunctive Kriging estimates for a panel requires a model of spatial dependence for the Gaussian variable $Y_v(u)$ (155). ISATIS develops the block anamorphosis for the chosen block support size $v$ and then uses this to calculate a discretised semivariogram for $Y_v(u)$ from the semivariogram model of the point variable $Z(u)$. The discretised semivariogram and the model fitted are shown in Figure 13 and the parameters for the model are given in Table 6. The model has a nugget constant and one spherical structure.

Table 6: Semivariogram model parameters block Gaussian moisture variable.

<table>
<thead>
<tr>
<th>Type</th>
<th>1st Structure</th>
<th>2nd Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Range</td>
<td>-</td>
<td>34</td>
</tr>
<tr>
<td>Sill</td>
<td>0.05</td>
<td>0.95</td>
</tr>
</tbody>
</table>
3.1.4 Cross Validation

Cross validation was performed on the Moisture100 data to test the semivariogram model and search parameters to be used for the kriging procedure. This procedure involves the removal of one datum at a time from the data set and re-estimation of this value from the remaining data. The interpolated values can then be compared with the actual values. Cross validation was performed with the GSLIB program KT3D using the semivariogram model obtained previously (Table 3) for the Moisture100 data and the parameter file (MoistXV.par) shown in Appendix C. Several search neighbourhoods were tested with no significant difference in their results, and the chosen search parameters are shown in Table 7. Plots of the sample moisture values, the cross validation estimates and the associated errors are shown in Figure 14. Inspection of the cross validation estimates indicates that the kriging procedure and model used were very successful in reproducing the sample moisture values. Errors of large magnitude were obtained for the extreme high and low values of the Moisture100 data and at locations where the moisture value to be estimated was surrounded by a number of moisture values quite different in magnitude.

Figure 13: Discretised semivariogram and semivariogram model for block Gaussian moisture variable.
Table 7: Search parameters used for Cross Validation of Moisture100.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of angular sectors</td>
<td>4</td>
</tr>
<tr>
<td>Minimum number of samples used for kriging a block</td>
<td>4</td>
</tr>
<tr>
<td>Maximum number of samples used for kriging a block</td>
<td>16</td>
</tr>
<tr>
<td>Maximum per sector</td>
<td>6</td>
</tr>
<tr>
<td>Search radius</td>
<td>15</td>
</tr>
</tbody>
</table>

Figure 14: Moisture100 data (left), cross validation estimates (centre) and estimation errors (right).

Graphical analysis of the estimation errors is shown in the plots of Figure 15. The normal plot and histogram of the estimation errors demonstrate that the errors are approximately normally distributed. The ordered plot of the errors and the plot of the errors versus the estimates shows no evidence of patterns or trends in the error values.
3.1.5 Ordinary Kriging Results

Ordinary Kriging was performed on Moisture100 to obtain estimates for blocks of the previously defined support size of 1 metre by 1 metre. Kriging was performed with the GSLIB program KT3D using the semivariogram model of the Moisture100 (Table 3) and the search parameters indicated previously for the cross validation procedure (Table 7). A block discretisation of 4 by 4 was used for each block. The parameter file used (MoistOK.par) is shown in Appendix C. The Ordinary Kriging block estimates along with the exhaustive moisture values and the associated errors are shown in Figure 16.

The Ordinary Kriging estimates highlight the smoothing nature of the kriging process. It is highly unlikely that any kriging process could reproduce the variability evident in the exhaustive moisture values. The estimation errors are much greater in magnitude than those observed for cross validation, most likely due to the more extreme values evident in the exhaustive moisture values than in the sample values. The largest errors correspond to the extreme high and low exhaustive moisture values and to those locations where the sample moisture values used for estimation
Figure 16: Moisture values (left), Ordinary Kriging block estimates (centre) and estimation errors (right) are quite different in magnitude to the actual moisture value being estimated.

For comparison with the results from other kriging processes, the Ordinary Kriging block estimates were converted into panel estimates for the previously defined panel size of 5 metres by 5 metres. Maps of the panel proportions and mean values above the thresholds of Table 2 for the Ordinary Kriging estimates are shown in Figure 17 and Figure 18 respectively.

The smoothing nature of Ordinary Kriging is evident in Figure 17 and Figure 18. As the values of the block estimates within each panel are very similar, there is a high chance that the proportion above a given threshold will be equal to either extreme of zero (all block estimates below threshold value) or one (all block estimates above threshold value). There is a clear boundary in the proportion maps separating the study region into two regions corresponding to panels with proportion zero and one. The boundary between the regions exhibits variability of proportions and corresponds to those panels that contain estimated block values very close to the threshold value of consideration. The proportion maps indicate that the panels in the lower half of the study region have higher values than those in the upper half, with the highest values being located in the lower left hand corner of the study region. These regions are consistent with the exhaustive moisture values (Figure 16).
Figure 17: Panel proportions of Moisture100 Ordinary Kriging block estimates above specified thresholds.

The regions of low and high values indicated in Figure 18 are the same as those indicated by the proportion maps with the higher values being located in the lower half of the study area, in particular the lower left hand corner. As stated previously, the white squares correspond to the locations where the proportion of moisture estimates above the threshold is zero and hence there is no respective mean value above that threshold. There are more missing values in the Ordinary Kriging mean value estimates than in the corresponding thresholds of the exhaustive moisture mean values (Figure 7). Only two panels have proportions greater than zero for the highest threshold of the Ordinary Kriging panel estimates.
Figure 18: Panel mean values of Moisture100 Ordinary Kriging block estimates above specified thresholds.
3.1.6 Indicator Kriging Results

Indicator Kriging was performed on *Moisture100* to obtain estimates of the proportion of the block values within each panel being above a given threshold and the mean value of the panel above that threshold. Point kriging was performed at the centres of the panels of size 5 metres by 5 metres with the GSLIB program IK3D using the semivariogram models developed for the *Moisture100* indicator data (Table 5). The point estimates were then adjusted to panel estimates using the GSLIB program POSTIK and implementing the affine correction method. The change-of-support factor required by POSTIK was calculated using (125) and the parameters obtained by the Gaussian Anamorphosis Modelling procedure of ISATIS. The parameters for the support correction are given in Table 8. The affine correction factor obtained was 0.413. It must be noted that when the variance adjustment factor is less than 0.7, the *indirect lognormal correction* may be more appropriate than the affine correction (Isaaks & Srivastava, 1989, pp. 486-7). However, for the purposes of this project only the affine correction was considered.

Table 8: Affine support correction parameters.

<table>
<thead>
<tr>
<th>Block size</th>
<th>1 x 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Block discretisation</td>
<td>4 x 4</td>
</tr>
<tr>
<td>Variogram sill</td>
<td>2.781</td>
</tr>
<tr>
<td>Gamma (v,v)</td>
<td>1.633</td>
</tr>
<tr>
<td>Affine correction factor</td>
<td>0.413</td>
</tr>
</tbody>
</table>

The search parameters used for the point Indicator Kriging process implemented in the IK3D program were the same as those indicated for Ordinary Kriging (Table 7). The post processing procedure implemented in the POSTIK program requires the specification of the minimum and maximum moisture values for the extrapolation of the cumulative distribution function. It also requires the models to be used for extrapolation below the first calculated cumulative distribution function value, above the last calculated cumulative distribution function value and between any two calculated cumulative distribution function values. These models and their
parameters were chosen by comparing the cumulative distribution function from *Moisture100* (Figure 4) with the cumulative distribution function of known linear, power and hyperbolic models (Goovaerts, 1997, pp. 279-82). The interpolation and extrapolation models and parameters used in the POSTIK program are given in Table 9. The parameter file used for the point kriging (MoistIK.par) and one example of the parameter files used for the post-processing procedure (PostMIKI.par) are shown in Appendix C. The Indicator Kriging estimates of the panel proportions and mean values above the thresholds of Table 2 are shown in Figures 19 and 20 respectively.

Table 9: Indicator Kriging post processing parameters for *Moisture100*.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum value</td>
<td>0</td>
</tr>
<tr>
<td>Maximum value</td>
<td>40</td>
</tr>
<tr>
<td>Lower tail model</td>
<td>Power</td>
</tr>
<tr>
<td>Middle model</td>
<td>Linear</td>
</tr>
<tr>
<td>Upper tail model</td>
<td>Hyperbolic</td>
</tr>
</tbody>
</table>

The proportion maps of the lower thresholds display a boundary below which the panel proportions are all zero. Similarly, the proportion maps of the higher thresholds display a boundary above which the panel proportions are all one. In the areas where the proportions are not exactly zero or one, the maps show much more variability than was evident in the Ordinary Kriging proportion maps. Like the proportion maps for the exhaustive moisture values (Figure 6) and those for the Ordinary Kriging estimates (Figure 17), the proportion maps for the Indicator Kriging estimates indicate that the panels in the lower half of the study region have higher values than those in the upper half with the highest values being located in the lower left-hand corner of the study region.
Figure 19: Indicator Kriging estimates from Moisture100 of panel proportions above specified thresholds.

Figure 20 indicates the same regions of high and low moisture values as Figure 19, which is consistent with the exhaustive values (Figure 5). The lower mean values of the Indicator Kriging estimates, located in the upper half of the study region, are generally lower than those of the exhaustive values. Similarly, the higher mean values of the Indicator Kriging estimates in the lower half of the study region are generally higher than those of the exhaustive values. This could be attributed to the extrapolation parameters used in the Indicator Kriging post processing procedure. There are more missing values in the Indicator Kriging mean value estimates than in the corresponding thresholds of the exhaustive moisture mean values (Figure 7) but fewer than those obtained from the Ordinary Kriging procedure (Figure 18).
Figure 20: Indicator Kriging estimates from Moisture100 of panel mean values above specified thresholds.

As mentioned previously, since the affine correction factor used in this analysis was 0.413, there is reason to believe that the indirect lognormal correction method may have been more appropriate. This may account for the inability of the Indicator Kriging estimates to adequately capture the features of the actual moisture values.
3.1.7 Disjunctive Kriging Results

Disjunctive Kriging was performed on *Moisture100* using the program ISATIS. Estimates of the proportion of 1 metre by 1 metre blocks within a panel of size 5 metres by 5 metres above a given threshold and the mean value above that threshold for the panel were obtained. The Gaussian Anamorphosis Modelling procedure of the ISATIS program was used to obtain the block correction factor for the change of support. The parameters used for this procedure are given in Table 10. The block correction factor obtained was 0.648.

Table 10: Gaussian anamorphosis modelling of *Moisture100*.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Hermite polynomials</td>
<td>30</td>
</tr>
<tr>
<td>Block size</td>
<td>1 x 1</td>
</tr>
<tr>
<td>Block discretisation</td>
<td>4 x 4</td>
</tr>
<tr>
<td>Variogram sill</td>
<td>2.781</td>
</tr>
<tr>
<td>Gamma (v,v)</td>
<td>1.633</td>
</tr>
<tr>
<td>Block variance</td>
<td>1.147</td>
</tr>
<tr>
<td>Block correction factor</td>
<td>0.648</td>
</tr>
</tbody>
</table>

The block anamorphosis obtained was used to build a discretised semivariogram for the block Gaussian variable, which was then modelled (Figure 13, Table 6). Disjunctive Kriging was then performed using this semivariogram model and the search parameters indicated in Table 11, similar to those used in the Ordinary Kriging and Indicator Kriging procedures (Table 7). The Disjunctive Kriging estimates of the panel proportions and mean values above the specified thresholds (Table 2) are shown in Figures 21 and 22 respectively.

Like the proportion maps for the Indicator Kriging estimates, those for the Disjunctive Kriging estimates display a region where the panel proportions are zero for the lower thresholds, and for the higher thresholds a region where the panel proportions are one. In the regions where the proportions lie between zero and one, the maps show much more variability than was evident in the Ordinary Kriging
Table 11: Search parameters used for Disjunctive Kriging of Moisture %.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of kriged polynomials</td>
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</tr>
<tr>
<td>Panel size</td>
<td>5 x 5</td>
</tr>
<tr>
<td>Panel discretisation</td>
<td>5 x 5</td>
</tr>
<tr>
<td>Number of angular sectors</td>
<td>4</td>
</tr>
<tr>
<td>Minimum number per sector</td>
<td>4</td>
</tr>
<tr>
<td>Optimum number per sector</td>
<td>8</td>
</tr>
<tr>
<td>Search radius</td>
<td>15</td>
</tr>
</tbody>
</table>

proportion maps but less variability than in those obtained from Indicator Kriging. Figure 21 indicates that the panels in the lower half of the study region have higher values than those in the upper half with the highest values being located in the lower left hand corner of the study area. This is consistent with the exhaustive moisture values (Figure 5).

The regions of low and high values indicated by Figure 22 are the same as those indicated by the Figure 21 and the actual moisture values. The Disjunctive Kriging mean panel values do not display the extreme low and high mean values as shown by the Indicator Kriging estimates.
Figure 21: Disjunctive Kriging estimates from Moisture100 of panel proportions above specified thresholds.
Figure 22: Disjunctive Kriging estimates from Moisture100 of panel mean values above specified thresholds.
3.1.8 Comparison of Kriging Results

Comparing the maps of the proportions and mean values of panels above the specified thresholds shown previously for the three different kriging methods and those of the exhaustive moisture values enables us to evaluate and compare the different kriging procedures. The proportion and mean value maps of the three kriging methods all correctly indicated the locations of low and high moisture values evident in the Moisture data.

The proportion maps of the Indicator Kriging and Disjunctive Kriging estimates reflect the proportions evident for the Moisture values although the variability of the Indicator Kriging proportion estimates is much greater than those obtained using Disjunctive Kriging. The Ordinary Kriging estimates fail to reflect the extent of variability evident in the Moisture proportions. It must be noted that the proportions for the Ordinary Kriging method were derived from calculated small block estimates whereas the other kriging methods involved a direct estimate of the proportion itself. The Disjunctive Kriging proportion estimates appear to have captured the features of the Moisture values most accurately of the kriging methods employed.

The maps of mean values of all three kriging methods appear to reflect those of the Moisture mean values. All kriging methods display many more missing values than the actual moisture values where the associated proportion above the threshold is zero, with the Ordinary Kriging map showing the greatest number of missing values. The Ordinary Kriging estimates show lower mean values than Moisture in the upper half of the study region corresponding to the area of low moisture values. The Indicator Kriging mean values display greater extremes of high and low values than is evident in Moisture. Of the three kriging methods employed, the Disjunctive Kriging mean value estimates appear to reflect the features of the actual moisture values most accurately.
The mean square errors for the proportions and mean values above the specified thresholds were calculated for the three kriging methods. In the case of the mean values, only the panels where the proportion above the threshold was greater than zero were taken into account. Plots of the mean square errors for the panel proportions and panel mean values are shown in Figure 23.

![Panel Proportions (moisture)](image)

![Panel Mean Values (moisture)](image)

Figure 23: Mean square errors of panel proportions (left) and panel mean values (right) of moisture data.

The mean square errors of the panel proportions are greater for the middle thresholds and lower for the extreme thresholds. The Disjunctive Kriging proportion estimates have the lowest mean square error for every threshold. This supports the previous observation that the Disjunctive Kriging proportion estimates appear to have captured the features of the Moisture proportions most accurately. The Indicator Kriging mean square errors are slightly greater than those of the Disjunctive Kriging estimates at all thresholds. The Ordinary Kriging estimates have significantly higher mean square errors for the middle thresholds. The Indicator Kriging proportion estimates have the highest mean square error for the highest threshold and the two lowest thresholds whilst the Ordinary Kriging proportion estimates show the highest mean square error for the remaining thresholds. This is consistent with the observation that the Indicator Kriging estimates exhibit greater extreme values and the Ordinary Kriging block estimates within panels display significant smoothing. The larger mean square errors of the Indicator Kriging estimates at the extreme thresholds may also be attributed to the affine correction procedure.
implemented as it is often only considered adequate for cutoffs of interest close to the mean (Isaaks & Srivastava, 1989, p. 472).

The Disjunctive Kriging mean value estimates have the lowest mean square error for the four lowest thresholds and the second highest threshold. Whilst the Ordinary Kriging panel estimates have the lowest mean square error for the fifth, sixth and seventh deciles, inspection of the mean value maps indicate that for these thresholds the Disjunctive Kriging estimates have significantly fewer missing values and visually appear to reflect the mean values of Moisture more accurately. The Indicator Kriging mean value estimates have the highest mean square error for all thresholds except the median and the highest threshold, which supports the observation that the Indicator Kriging mean value estimates exhibit greater variability. The Ordinary Kriging estimates have an extremely high mean square error for the highest threshold, which can be attributed to the inclusion of only two panel values for that threshold. The mean value estimates of all three kriging methods display a greater number of missing values than the Moisture means, with the number of missing values significantly greater for the higher thresholds. This contributes to the greater mean square errors evident for all kriging methods at the higher thresholds.

The various kriging results may also be compared by plotting the average mean value above a threshold against the average proportion above that threshold, shown in Figure 24. Inspection of this plot indicates that all three kriging methods reflect the shape of the Moisture curve. All three kriging estimators are reasonably accurate at the lower thresholds corresponding to higher proportions and lower mean values. The differences between the kriging results are more pronounced at the higher thresholds. The Indicator Kriging method overestimates the Moisture values at the higher thresholds whilst both the Ordinary Kriging and Disjunctive Kriging methods underestimate at the higher thresholds. It must be noted that the average mean value for each threshold is calculated using only those panels where a valid estimate is obtained. Therefore, the mean values of the Ordinary Kriging estimates are calculated using significantly fewer panel values than those of the other kriging estimates and the actual moisture values. In particular, the
curve of the Ordinary Kriging estimates deviates from the shape of the Moisture curve quite dramatically at the highest threshold where only one panel is used to obtain the average mean value for the study region (Figure 18).

Figure 24: Mean value above threshold versus proportion above threshold for Moisture data and kriging estimates.

3.2 True Data Suite

The True data set is a two-dimensional exhaustive reference data set included with the GSLIB software library (Deutsch & Journel, 1998). The data comprise 2500 measurements located on a regular 50 mile by 50 mile grid with a grid spacing of 1 mile. The True data set contains two variables, primary and secondary, but this project will be concerned only with the primary variable, whose values have been simulated to match a low nugget isotropic variogram and are highly positively skewed. They exhibit properties commonly associated with a gold mineralisation. Two sample data sets are also provided with the GSLIB software. The one used in this project for the purpose of estimation is True97, a sample of 97 values on a pseudo-regular grid taken from the True data.
3.2.1 Statistical Description

Descriptive statistics for the primary values of *True* and *True97* are shown in Table 12. The two data sets have similar minimum values, but the maximum of the sample data is considerably lower than that of the exhaustive data. Both data sets are positively skewed and display similar means, however the standard deviation of the sample data is slightly lower than that of the exhaustive data.

Table 12: Descriptive statistics for *True* and *True97* primary values.

<table>
<thead>
<tr>
<th></th>
<th>True</th>
<th>True97</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>2500</td>
<td>97</td>
</tr>
<tr>
<td>Mean</td>
<td>2.580</td>
<td>2.211</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>5.152</td>
<td>3.191</td>
</tr>
<tr>
<td>Skewness</td>
<td>6.836</td>
<td>3.063</td>
</tr>
<tr>
<td>Kurtosis</td>
<td>81.598</td>
<td>11.550</td>
</tr>
<tr>
<td>Minimum</td>
<td>0.010</td>
<td>0.000</td>
</tr>
<tr>
<td>1st Quartile</td>
<td>0.340</td>
<td>0.335</td>
</tr>
<tr>
<td>Median</td>
<td>0.960</td>
<td>1.020</td>
</tr>
<tr>
<td>3rd Quartile</td>
<td>2.560</td>
<td>2.610</td>
</tr>
<tr>
<td>Maximum</td>
<td>102.700</td>
<td>18.760</td>
</tr>
</tbody>
</table>

Graphical summaries of the two data sets are shown in Figure 25 and Figure 26. The histograms and boxplots of both data sets indicate that the data are positively skewed, which is supported by their significant positive skewness and kurtosis factors.

The cumulative distribution functions from the primary values of *True* and *True97* are shown in Figure 27 and Figure 28 respectively. Inspection of the two graphs indicates that the sample data are representative of the exhaustive data. The cumulative distribution function from the *True97* data will be used in the Indicator Kriging procedure to model the shape of the upper and lower tails beyond the estimated values of the cumulative distribution function.
Figure 25: Graphical summary of primary values of True data set.

Figure 26: Graphical summary of primary values of True97 data set.
Figure 27: Cumulative distribution function of primary values of *True* data set.

Figure 28: Cumulative distribution function of primary values of *True97* data set.
3.2.2 Spatial Description

Plots of the True and True97 primary data are shown in Figure 29. The sample values reflect the regions of low values evident in the exhaustive data but do not appear to reflect all the regions of high values evident in the exhaustive data. In particular, they do not reflect the two regions of high primary values evident in the lower right hand corner of the exhaustive data and they do not adequately reflect the size of the high valued regions in the centre of the study region. Visual inspection does not suggest any evidence of anisotropy in either of the data sets.

Figure 29: Plots of primary values from True (left) and True97 (right).

As previously shown for the Moisture data suite, estimates of panel proportions and mean values above given thresholds was obtained from each kriging procedure using the sample data as well as the corresponding values for the True primary values. The block support size chosen for the primary values was 1 mile by 1 mile and the panel size chosen was 5 miles by 5 miles. The nine deciles were chosen as the thresholds, calculated using the convention of Isaaks & Srivastava (1989) and are shown in Table 13 along with the corresponding primary values. The panel proportions and mean values above given thresholds for the primary values of the exhaustive data are shown in Figure 30 and Figure 31 respectively. As indicated for the moisture values, where the proportion of the panel value being above the threshold is zero there is no corresponding mean value above the given threshold, indicated by a white panel on the map of the mean value above the threshold.
### Table 13: Indicator thresholds for True97.

<table>
<thead>
<tr>
<th>Decile</th>
<th>Threshold Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st</td>
<td>0.15</td>
</tr>
<tr>
<td>2nd</td>
<td>0.27</td>
</tr>
<tr>
<td>3rd</td>
<td>0.45</td>
</tr>
<tr>
<td>4th</td>
<td>0.83</td>
</tr>
<tr>
<td>5th</td>
<td>1.02</td>
</tr>
<tr>
<td>6th</td>
<td>1.38</td>
</tr>
<tr>
<td>7th</td>
<td>2.07</td>
</tr>
<tr>
<td>8th</td>
<td>3.16</td>
</tr>
<tr>
<td>9th</td>
<td>6.29</td>
</tr>
</tbody>
</table>

Figure 30 indicates a region of high primary values covering the centre and right hand corner of the upper half of the study region evident by the higher proportions in this region. There is a region of low primary values in the upper left hand corner and two or three regions of low primary values in the lower half of the study region evident by the lower proportions in these regions. Figure 31 indicates similar regions of low primary values evident by the blue panels in the lower thresholds and white panels in the upper thresholds. The large region of orange and/or red squares located in the upper centre and right hand corner of the study region for all thresholds indicates the presence of high primary values. The regions of high and low primary values indicated by Figure 30 and Figure 31 are reflected in the map of the exhaustive primary data (Figure 29).
Figure 30: Panel proportions of primary values from True above specified thresholds.
Figure 31: Panel mean primary values of True above specified thresholds.
3.2.3 Variography

Exploratory variography and variogram modelling was conducted on the primary values of True97 in order to apply the same kriging procedures as those indicated previously for the moisture data.

3.2.3.1 Variography of Primary Values

Exploratory variography was performed on the True97 primary data to develop a model for use in the Ordinary Kriging and Disjunctive Kriging methods. The variogram surface of the sample primary values is shown in Figure 32 and indicates no anisotropy in the sample values. Therefore, an isotropic model was developed.

![Figure 32: Variogram surface of Primary values of True97 data set. (Lag spacing 3, Number of lags 8)](image)

The covariance and correlogram models shown in Figure 33 were used to help infer the semivariogram model parameters. Both models had a small nugget with relative nugget effect of approximately 10% and two spherical structures at ranges 7.5 and 20 respectively. The second spherical structure was not required for the semivariogram model as the total sill of the semivariogram model was fitted to the sample variance, as required by the change-of-support factor calculation. The nugget fitted for the semivariogram model had a slightly greater relative nugget effect of 25%. The model fitted to the experimental semivariogram is shown in Figure 34 and the parameters for the model are given in Table 14.
Figure 33: Covariance (left) and correlogram (right) models for *True97* primary values.

Figure 34: Omnidirectional semivariogram model for *True97* primary values. (Lag spacing 3, Lag tolerance 1.5, Number of lags 11)

Table 14: Semivariogram model parameters for *True97*.

<table>
<thead>
<tr>
<th>1st Structure</th>
<th>2nd Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Nugget</td>
</tr>
<tr>
<td>Range</td>
<td>-</td>
</tr>
<tr>
<td>Sill</td>
<td>2.70</td>
</tr>
</tbody>
</table>
3.2.3.2 Variography of Primary Indicator Values

The True97 data were coded into indicator variables using the definition of $i(u; z_k)$ (109) and the threshold values of Table 13. Exploratory variography was performed on the True97 primary indicator values to develop a model for use in the Indicator Kriging method.

The variogram surfaces of the Primary indicator data of the True97 data set are shown in Figure 35. Inspection of the variogram surfaces suggests the possibility of anisotropy in the 4th, 5th and 6th deciles. The variogram surfaces of the 4th and 6th deciles suggest anisotropy with maximum spatial continuity at an angle of 45° taken clockwise from the horizontal and that of the 5th decile at an angle of 30° taken clockwise from the horizontal. The direction of minimum spatial continuity is perpendicular to that of maximum spatial continuity. The standardised directional semivariograms were calculated in the directions of maximum and minimum spatial continuity and in the intermediate directions for these deciles, standardised by dividing by the indicator data variance given in Table 15.

Table 15: Variance of True97 indicator data.

<table>
<thead>
<tr>
<th>Threshold</th>
<th>Indicator Data Variance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.15</td>
<td>0.084</td>
</tr>
<tr>
<td>0.27</td>
<td>0.158</td>
</tr>
<tr>
<td>0.45</td>
<td>0.210</td>
</tr>
<tr>
<td>0.83</td>
<td>0.240</td>
</tr>
<tr>
<td>1.02</td>
<td>0.250</td>
</tr>
<tr>
<td>1.38</td>
<td>0.238</td>
</tr>
<tr>
<td>2.07</td>
<td>0.216</td>
</tr>
<tr>
<td>3.16</td>
<td>0.158</td>
</tr>
<tr>
<td>6.29</td>
<td>0.084</td>
</tr>
</tbody>
</table>
Figure 35: Variogram surfaces of Primary indicator data of True97 data set. (Lag spacing 3, Number of lags 6)

The directional semivariograms of the 4th, 5th and 6th deciles are shown in Appendix B by Figure D1, Figure D2 and Figure D3 respectively, superimposed with the relevant isotropic model derived from the omnidirectional experimental semivariograms. The isotropic model fits reasonably well to the directional semivariograms which suggests that the spatial variability can be adequately modelled using an isotropic model. The isotropic models fitted to the experimental semivariograms have a nugget constant and one spherical structure. As the indicator semivariograms for the 8th and 9th deciles were quite erratic, the parameters for their models were inferred from the corresponding correlogram models shown in Figure 36. The experimental omnidirectional semivariograms for the primary indicator data of True97 and the isotropic models fitted to the experimental semivariograms are shown in Figure 37 and the parameters for the model are given in Table 16.
Figure 36: Correlogram models for the 8th (left) and 9th (right) deciles of the True97 primary values.

Table 16: Semivariogram model parameters for True97 indicator data.

<table>
<thead>
<tr>
<th>Threshold</th>
<th>Semivariogram model</th>
<th>Spherical Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Decile</td>
<td>Value</td>
<td>Nugget</td>
</tr>
<tr>
<td>1st</td>
<td>0.15</td>
<td>0.10</td>
</tr>
<tr>
<td>2nd</td>
<td>0.27</td>
<td>0.30</td>
</tr>
<tr>
<td>3rd</td>
<td>0.45</td>
<td>0.30</td>
</tr>
<tr>
<td>4th</td>
<td>0.83</td>
<td>0.35</td>
</tr>
<tr>
<td>5th</td>
<td>1.02</td>
<td>0.35</td>
</tr>
<tr>
<td>6th</td>
<td>1.38</td>
<td>0.35</td>
</tr>
<tr>
<td>7th</td>
<td>2.07</td>
<td>0.40</td>
</tr>
<tr>
<td>8th</td>
<td>3.16</td>
<td>0.15</td>
</tr>
<tr>
<td>9th</td>
<td>6.29</td>
<td>0.35</td>
</tr>
</tbody>
</table>
Figure 37: Omnidirectional semivariograms and semivariogram models of primary indicator values of *True97*. (Lag spacing 3, Lag tolerance 1.5, Number of lags 11)
3.2.3.3 Variography of Block Gaussian Primary Variable

The ISATIS program was used to develop the block anamorphosis for the chosen block support size \( v \) which was then used to calculate a discretised semivariogram for the block Gaussian \( Y_v(u) \) from the semivariogram model of the point variable \( Z(u) \) as required to obtain Disjunctive Kriging estimates for a panel (155). The discretised semivariogram and the model fitted are shown in Figure 38 and the parameters for the model are given in Table 17. The model has a nugget constant and one spherical structure.

![Figure 38: Discretised semivariogram and semivariogram model for block Gaussian primary variable.](image)

Table 17: Semivariogram model parameters for block Gaussian primary variable.

<table>
<thead>
<tr>
<th>Type</th>
<th>1st Structure</th>
<th>2nd Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nugget</td>
<td>-</td>
<td>0.05</td>
</tr>
<tr>
<td>Sill</td>
<td>0.95</td>
<td>0.95</td>
</tr>
<tr>
<td>Range</td>
<td>7</td>
<td></td>
</tr>
</tbody>
</table>
3.2.4 Cross Validation

Cross validation was performed on the True97 primary data to test the semivariogram model and search parameters used for the kriging procedure and was performed using the GSLIB program KT3D. The semivariogram model obtained previously for the True97 primary values (Table 14) was used and the parameter file (TrueXV.par) is shown in Appendix C. Several search neighbourhoods were tested with no significant difference in their results, and the search parameters chosen are shown in Table 18.

Table 18: Search parameters used for Cross Validation of True97 primary data.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of angular sectors</td>
<td>4</td>
</tr>
<tr>
<td>Minimum number of samples used for kriging a block</td>
<td>4</td>
</tr>
<tr>
<td>Maximum number of samples used for kriging a block</td>
<td>16</td>
</tr>
<tr>
<td>Maximum per sector</td>
<td>6</td>
</tr>
<tr>
<td>Search radius</td>
<td>15</td>
</tr>
</tbody>
</table>

Plots of the True97 primary values, the cross validation estimates and the associated errors are shown in Figure 39. Inspection of the cross validation estimates indicates that the kriging procedure has successfully reproduced the key features of the sample primary values. Inspection of the map of errors indicates that the majority of the errors are between -1 and 1 in value as is demonstrated by the large number of light orange and yellow squares present on the error map. Errors of large magnitude correspond to locations of extreme high and low True97 primary values or to locations where the primary value to be estimated was surrounded by a number of values extremely different in magnitude. The greatest negative error obtained was significantly greater in magnitude than the greatest positive error.
Figure 39: Primary values of True97, cross validation estimates and estimation errors.

A graphical analysis of the estimation errors is shown in the plots of Figure 40. The normal plot and histogram of the estimation errors show that the errors are not normally distributed. This can be attributed to the presence of errors of large magnitude, both positive and negative. The ordered plot of the errors and the plot of the errors versus the estimates demonstrates clear evidence of a pattern or trend in the errors which can also be partially attributed to the errors of large magnitude, both positive and negative. Although there is clear evidence that the cross validation process has produced errors that are neither normally distributed nor devoid of patterns or trends, there is still reason to believe that the kriging process and model used is valid. This is evident from the ability of the process to adequately capture the key features of the True97 primary values as shown in Figure 39. The kriging process only fails to adequately reproduce the primary values of the True97 data set for locations where the sample primary value is surrounded by significantly different primary values, or where the sample primary value is exceptionally large. In the first case, reproduction of a value in a neighbourhood of significantly different values is impossible via the kriging process and in the second case, exceptionally large values are a direct result of the significant positive skewness of the data set.
3.2.5 Ordinary Kriging Results

Ordinary Kriging was performed on the True97 primary data to obtain estimates of 1 mile by 1 mile blocks. Using the GSLIB program KT3D with the semivariogram model developed for the sample primary values (Table 14) and the search parameters developed in the cross validation procedure (Table 18) kriging estimates were obtained. A block discretisation of 4 by 4 was used for each block. The parameter file used (TrueOK.par) is shown in Appendix C. The exhaustive primary values, Ordinary Kriging block estimates and estimation errors are shown in Figure 41.

Figure 41: True primary values (left), Ordinary Kriging block estimates (centre) and estimation errors (right).
The Ordinary Kriging estimates of the primary values reflect the regions of high and low primary values evident in the True primary data. The smoothing nature of the kriging process is evident in the Ordinary Kriging block estimates. A range of errors much greater in magnitude than those evident in the cross validation estimates is observed for the Ordinary Kriging estimates. The majority of the errors were between the values of -2 and 2. Like the cross validation process, the greatest negative error value obtained was significantly greater in magnitude than the greatest positive error value. The errors of greatest magnitude were obtained in the locations of high sample primary values.

As outlined previously for the moisture data, in order to make comparisons with estimates from the other kriging methods and with the exhaustive primary values, the Ordinary Kriging block estimates were converted into panel estimates. Proportions of blocks within panels above a given threshold and the mean value above that threshold for the previously defined panel size of 5 miles by 5 miles were calculated using the thresholds outlined previously (Table 13). Maps of these values are shown in Figure 42 and Figure 43 respectively.

Figure 42 displays many panels where the proportion of block values above the threshold is one for the lower thresholds and zero for the higher thresholds. This highlights the smoothing nature of the kriging process as blocks within a given panel display similar values. Two or three distinct regions of higher valued primary values are evident in the lower half of the study region, and one region in the upper left hand corner, evident from the lower proportions in those regions. Similarly there is evidence of lower valued primary regions in the upper right hand corner and along the lower left hand edge with higher proportions in those regions than in the rest of the study region. These regions of high and low primary values agree with the exhaustive primary values (Figure 41). Similar regions of high and low primary values are evident in Figure 43.
Figure 42: Panel proportions of True97 Ordinary Kriging block primary estimates above specified thresholds.
Figure 43: Panel mean values of True97 Ordinary Kriging block primary estimates above specified thresholds.

3.2.6 Indicator Kriging Results

Indicator Kriging was performed on the True97 primary values to obtain estimates of the proportion of a given panel of size 5 miles by 5 miles being above a given threshold and the mean value above that threshold. The GSLIB program IK3D was used to perform point kriging at the centres of the panels of size 5 miles by 5 miles using the semivariogram models developed for the True indicator data (Table 16). The point estimates were then corrected to panel estimates accounting for change of support using POSTIK and implementing affine correction. The change-of-support factor was calculated using (125) and the parameters obtained in the Gaussian Anamorphosis Modelling procedure implemented using ISATIS. The support correction parameters are given in Table 19. The affine correction
factor obtained was 0.745.

Table 19: Affine support correction parameters for *True97*.

<table>
<thead>
<tr>
<th>Block size</th>
<th>1m x 1m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Block discretisation</td>
<td>4 x 4</td>
</tr>
<tr>
<td>Variogram sill</td>
<td>10.070</td>
</tr>
<tr>
<td>Gamma (v,v)</td>
<td>2.563</td>
</tr>
<tr>
<td>Affine correction factor</td>
<td>0.745</td>
</tr>
</tbody>
</table>

The point Indicator Kriging process used the same search parameters as those implemented in the Ordinary Kriging procedure (Table 18). The models to be used for extrapolation and interpolation of cumulative distribution function values in the POSTIK program are given in Table 20 and were chosen by comparing the cumulative distribution function of the sample primary data (Figure 28) with the cumulative distribution function of known models (Goovaerts, 1997, pp.279-82). The parameter file used for the point kriging (TrueIK.par) and one example of the parameter files used for the post processing procedure (PostTIK1.par) are shown in Appendix C.

The Indicator Kriging estimates of the proportion and mean values above the thresholds are shown in Figure 44 and Figure 45 respectively. The proportion maps of the lower thresholds display a region where the panel proportions are zero and for the higher thresholds a couple of regions where the panel proportions are one. Figure 44 indicates a region of high primary values in the upper right hand corner and along the lower left hand edge evident by the higher proportions in these regions. Two or three regions of lower valued primary values are evident in the lower half as well as one region in the upper left hand corner by the comparatively low proportions in these regions. Similar regions of high and low primary values are evident in Figure 45. These regions reflect those evident in the exhaustive primary values (Figure 29). There are significantly fewer missing values in the Indicator Kriging mean value estimates than the corresponding thresholds of the Ordinary Kriging estimates.
Table 20: Indicator Kriging post processing parameters for True97.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum value</td>
<td>0</td>
</tr>
<tr>
<td>Maximum value</td>
<td>100</td>
</tr>
<tr>
<td>Lower tail model</td>
<td>Linear</td>
</tr>
<tr>
<td>Middle model</td>
<td>Linear</td>
</tr>
<tr>
<td>Upper tail model</td>
<td>Hyperbolic  3.0</td>
</tr>
</tbody>
</table>

Figure 44: Indicator Kriging estimates from True97 of panel proportions above specified thresholds.
Figure 45: Indicator Kriging estimates from True97 of panel mean values above specified thresholds.
3.2.7 Disjunctive Kriging Results

Disjunctive Kriging was performed on the True97 primary data using the program ISATIS. Estimates were obtained of the proportion of 1 mile by 1 mile blocks, within a panel of 5 miles by 5 miles, above a given threshold and the mean value above that threshold for the panel. The thresholds used were the previously defined deciles (Table 13). The first step was to perform the Gaussian Anamorphosis Modelling in order to obtain the block correction factor for the change of support. The parameters used for this procedure are outlined in Table 21. The block correction factor obtained was 0.902.

Table 21: Gaussian anamorphosis modelling of True97 primary data.

<table>
<thead>
<tr>
<th>Number of Hermite polynomials</th>
<th>30</th>
</tr>
</thead>
<tbody>
<tr>
<td>Block size</td>
<td>1m x 1m</td>
</tr>
<tr>
<td>Block discretisation</td>
<td>4 x 4</td>
</tr>
<tr>
<td>Punctual variance (Anamorphosis)</td>
<td>9.943</td>
</tr>
<tr>
<td>Variogram sill</td>
<td>10.070</td>
</tr>
<tr>
<td>Gamma (v,v)</td>
<td>2.563</td>
</tr>
<tr>
<td>Block variance</td>
<td>7.412</td>
</tr>
<tr>
<td>Block correction factor</td>
<td>0.902</td>
</tr>
</tbody>
</table>

The anamorphosis was used to build a semivariogram model for the block Gaussian variable shown in Figure 38. The Disjunctive Kriging was then performed using the semivariogram model for the block Gaussian variable (Figure 38, Table 17) along with the search parameters indicated in Table 22, similar to those used in the Ordinary Kriging and Indicator Kriging procedures.
Table 22: Search parameters for Disjunctive Kriging of True97 Primary values.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of kriged polynomials</td>
<td>10</td>
</tr>
<tr>
<td>Panel size</td>
<td>5m x 5m</td>
</tr>
<tr>
<td>Panel discretisation</td>
<td>5 x 5</td>
</tr>
<tr>
<td>Number of angular sectors</td>
<td>4</td>
</tr>
<tr>
<td>Minimum number per sector</td>
<td>4</td>
</tr>
<tr>
<td>Optimum number per sector</td>
<td>8</td>
</tr>
<tr>
<td>Search radius</td>
<td>15</td>
</tr>
</tbody>
</table>

Disjunctive Kriging estimates of the panel proportions and mean values above the specified thresholds are shown in Figure 46 and Figure 47 respectively. These maps indicate regions of high primary values in the upper right hand corner and along the lower left hand edge and regions of lower valued primary values in the lower half and the upper left hand corner. These are consistent with the exhaustive primary data (Figure 29).
Figure 46: Disjunctive Kriging estimates from True97 of panel proportions above specified thresholds.
Figure 47: Disjunctive Kriging estimates from True97 of panel mean values above specified thresholds.

3.2.8 Comparison of Kriging Results

The proportion and mean value maps of the three kriging methods all correctly indicated the locations of low and high primary values evident in the exhaustive primary data. The proportion maps of the Indicator Kriging and Disjunctive Kriging estimates reflect the proportions evident for the exhaustive primary values whilst the proportion maps of the Ordinary Kriging estimates fail to reflect the extent of variability evident in the proportion map of the True primary data. Again it must be noted that the proportions for the Ordinary Kriging method were derived from calculated small block estimates unlike the other kriging methods which involved a direct estimate of the proportion itself. The Indicator Kriging and Disjunctive
Kriging proportion estimates appear to have captured the features of the actual primary values quite similarly.

The maps of mean values of all three kriging methods appear to reflect that of the actual primary values. The Indicator Kriging estimates show a similar number of missing values as the exhaustive primary values where the associated proportion above the threshold is zero, whereas the Ordinary Kriging estimates display many more missing values and the Disjunctive Kriging estimates show slightly less missing values.

The mean square errors for the proportions and mean values above the specified threshold were calculated for each threshold. Panel mean values were only used where the panel proportion was greater than zero. Plots of the mean square errors for the panel proportions and panel mean values are shown in Figure 48.

![Figure 48: Mean square errors of panel proportions (left) and panel mean values (right) of primary data.](image)

The mean square errors of the proportions are higher for the middle thresholds. The Indicator Kriging and Disjunctive Kriging proportion estimates have very similar mean square errors for all thresholds. The Ordinary Kriging proportion estimates have the highest mean square error for every threshold. In particular, the Ordinary Kriging proportion estimates are considerably higher than those of the Indicator Kriging and Disjunctive Kriging estimates for the middle thresholds.
The three kriging methods have very similar mean square errors for the mean value estimates of the lower thresholds. The mean square errors increase with increasing thresholds. For the higher thresholds the Ordinary Kriging mean value estimates have the highest mean square error and the Disjunctive Kriging mean value estimates have the lowest mean square error.

Plots of the average mean value above a threshold against the average proportion above that threshold for the three kriging methods are shown in Figure 49. Observation of the plot indicates that all three kriging methods are reasonably accurate at the lower thresholds corresponding to the higher proportions and lower mean values. The differences between the kriging results is more pronounced at the higher thresholds. All three kriging methods underestimate the primary values at the higher thresholds, with the Ordinary Kriging results underestimating by a larger margin than the other kriging methods. It must be noted that the average mean value for each threshold is calculated using only those panels where a valid estimate was obtained. Therefore, the mean values of the Ordinary Kriging estimates were calculated using significantly less panel values than those of the other kriging estimates and of the actual primary values.

Figure 49: Mean value above threshold versus proportion above threshold for kriging estimates and actual values of True data set.
4 Discussion and Conclusions

Panel estimates based on the blocks within a panel can be obtained even when the available sample data refers to point data. This is achieved by using a change-of-support model which adjusts the known point distribution of values to the theoretical block distribution. The use of change-of-support models stems from the inability of linear kriging methods to produce accurate estimates for blocks of larger size than the support of the available sample data. The estimates obtained for panels based on the linear estimation of the blocks within the panel have very low precision. Nonlinear methods provide a solution to this problem by producing estimates for collection of blocks (panels), where the point support sample data has been used to provide a model of the theoretical block spatial dependence. Indicator Kriging and Disjunctive Kriging are examples of such methods, which apply linear estimation methods to nonlinear transforms of the variable of interest.

Three kriging methods were investigated in the course of this project, namely Ordinary Kriging, Indicator Kriging and Disjunctive Kriging. The Disjunctive Kriging method was chosen as an application of an orthogonal family of functions known as the Hermite Polynomials. The more commonly used methods of Ordinary Kriging and Indicator Kriging were chosen as methods of comparison.

Two suites of data were used for the purposes of analysis in this project. The moisture data originated from soil measurements and showed weak positive skewness. The primary data were simulated gold mineralisation values that were highly positively skewed. The data suites comprise sample data used in the estimation process for each kriging procedure, together with exhaustive data used for the purpose of comparison of these kriging procedures. Both sets of sample data were representative of their corresponding exhaustive data.

The results obtained from the three kriging procedures were estimates of the proportion of values above a threshold, and the mean value above that threshold for the panels in the study region. In each case the set of thresholds used comprised the nine deciles of the sample values. The values of panel proportions and panel mean values were directly estimated from the Indicator Kriging and Disjunctive Kriging.
methods using change-of-support models based on the distribution of smaller blocks within the panels. As Ordinary Kriging cannot derive these estimates directly, Ordinary Kriging block estimates for blocks of the support size were calculated and then converted into values of panel proportions and panel mean values in order to provide comparative estimates. The estimates obtained from the three kriging methods for the moisture and primary data were consistent with the exhaustive values. However, the estimates obtained using Ordinary Kriging were significantly smoothed and this supports the use of nonlinear methods such as Indicator Kriging and Disjunctive Kriging.

The results were analysed in a number of ways. The maps of the panel proportions and panel mean values from each kriging method were compared visually with one another and against the corresponding maps from the exhaustive data. The mean square errors of the estimated panel proportions and panel mean values from those of the exhaustive data were calculated for each of the kriging methods and compared. Plots of the average panel proportions versus the average panel mean values for each of the thresholds were constructed for the three kriging methods and compared with the corresponding plots from the exhaustive values.

The Indicator Kriging change-of-support model implemented involved affine correction of the variance. However, it must be noted that affine correction is a simplistic method of variance reduction. The rule of thumb is that affine correction is appropriate for factors greater than 0.7. The variance adjustment factor calculated for the moisture data was 0.413. For this reason the Indicator Kriging results for moisture need to be treated with caution. However, since the Indicator Kriging estimates for the moisture data adequately captured the features of the exhaustive data and were comparable to the estimates from the other kriging methods, the use of the affine correction appears to have been reasonable in this case.

Comparison of plots of the panel proportions and panel mean values above a series of thresholds indicated that those obtained from Indicator Kriging and Disjunctive Kriging captured the features of the exhaustive sets quite accurately, whilst those of the Ordinary Kriging panel estimates failed to reflect the extent of variability evident in the exhaustive data proportions and mean values. As the
Ordinary Kriging block estimates within a given panel displayed little variability, the panel proportions obtained for each threshold were mostly ones or zeroes, highlighting the smoothing nature of the kriging process. The Indicator Kriging panel proportions and mean values of the moisture data displayed greater extremes than was evident for the exhaustive values. This may be a consequence of the extrapolation models used within the Indicator Kriging procedure that were inferred from the cumulative distribution function of the sample values. Of the three kriging methods, the plots of the Disjunctive Kriging estimates of panel proportions and panel mean values appear to reflect the features of the exhaustive values most accurately.

Panel mean values display missing values for panels where the proportion of the values in the panel above the particular threshold is zero. The locations of missing values evident in the panel mean values of the exhaustive data are reflected in the kriging estimates. The Ordinary Kriging process produced many more missing values than was evident in the exhaustive data whilst the Indicator Kriging process only produced more missing values in the case of the moisture data. The Disjunctive Kriging mean value estimates showed more missing values for the moisture data than the exhaustive data but fewer missing values for the primary data.

Comparison of the mean square errors for the panel proportions of the three kriging methods indicate that generally the mean square errors were greater for the middle thresholds and lower for the extreme thresholds. Panel estimates derived from Ordinary Kriging generally showed greater mean square errors at all thresholds than those from the Indicator Kriging and Disjunctive Kriging estimates. In particular, the Ordinary Kriging mean square errors were significantly greater for the middle thresholds. The mean square estimation errors of the Indicator Kriging and Disjunctive Kriging methods were quite similar for the primary data whilst those for the Indicator Kriging panel estimates were slightly higher for the moisture data. The magnitude of the mean square errors obtained for the two data sets were similar.

Mean square errors of the estimated panel mean values were greater for higher thresholds. For the primary data there was little difference between the mean
square errors obtained from the three kriging methods at the lower thresholds. As threshold values increased, Ordinary Kriging panel estimates produced the highest mean square errors and Disjunctive Kriging estimates produced the lowest mean square errors. For the moisture data the Indicator Kriging method generally produced slightly higher mean square errors. The magnitude of the mean square errors obtained for the panel mean values were significantly greater than those obtained for the panel proportions.

Plots of the average panel mean value versus the average panel proportion for the study region provided useful comparisons of the kriging results. All three kriging methods reproduced the shape of the corresponding curve of the exhaustive data for both sets of data. The curves of the three kriging methods were similar at the lower thresholds, corresponding to higher proportions and lower mean values. Differences between the curves were more pronounced for the higher thresholds. All three kriging methods underestimated the mean value for a given proportion above a threshold in the case of the primary data. For the moisture data the Ordinary Kriging and Disjunctive Kriging estimates underestimated the mean value for a given proportion whilst the Indicator Kriging estimates overestimated the mean value.

All three kriging methods capture the shape of the curve of panel proportions versus panel mean values. Mean square errors of the kriging estimates indicate that generally the Ordinary Kriging estimates deviate considerably more from the exhaustive data than those of the Indicator Kriging and Disjunctive Kriging methods. The mean square errors of the Disjunctive Kriging method are generally slightly lower than the corresponding Indicator Kriging estimates. Visually, plots of the panel proportions and panel mean values for the exhaustive data are reproduced most accurately by the Disjunctive Kriging method and least accurately by the Ordinary Kriging method.

Comparing panel estimates of the moisture and primary data from the three kriging methods indicated that generally the estimates obtained using Ordinary Kriging were the least accurate. Mean square estimation errors along with plots of
the estimates themselves and curves relating the estimates to the exhaustive values indicated that those obtained using Disjunctive Kriging were the most accurate.

The Ordinary Kriging method required the modelling of only one semivariogram for each data set whilst the Indicator Kriging method involved the modelling of nine semivariograms for each data set and the inference of extrapolation models for the cumulative distribution function values. The Disjunctive Kriging method required the modelling of two semivariograms as well as the calculation of change-of-support parameters. The modelling of an extra semivariogram in Disjunctive Kriging by comparison with Ordinary Kriging was justified by a significant increase in estimation accuracy. However the additional modelling required by Indicator Kriging did not produce any additional benefits. The Disjunctive Kriging primary estimates and the Indicator Kriging primary estimates were quite similar, and the Disjunctive Kriging moisture estimates reflected the features of the actual moisture values more accurately than the Indicator Kriging moisture estimates. In summary, the Disjunctive Kriging method was found to produce more accurate estimates than the more commonly used methods of Ordinary Kriging and Indicator Kriging and this supports the use of Disjunctive Kriging in fields where geostatistics is used. However, the use of Disjunctive Kriging in these fields may be limited by the use of more familiar methods, such as Indicator Kriging, which produce useful results and whose implementation is understood by their users. The software requirements of implementing the Disjunctive Kriging method is also a major consideration for users.
References


114


Appendices
Appendix A: Moisture Indicator Directional Semivariograms

Figure A1: Directional standardised semivariograms for 3rd decile of Moisture100 indicator data.

Figure A2: Directional standardised semivariograms for 4th decile of Moisture100 indicator data.
Figure A3: Directional standardised semivariograms for 7th decile of Moisture100 indicator data.

Figure A4: Directional standardised semivariograms for 8th decile of Moisture100 indicator data.
Appendix B: True Indicator Directional Semivariograms

Figure B1: Directional standardised semivariograms for 4th decile of True97 indicator data.

Figure B2: Directional standardised semivariograms for 5th decile of True97 indicator data.
Figure B3: Directional standardised semivariograms for 6th decile of True97 indicator data.
Appendix C: GSLIB Parameter Files
MoistXV.par
Parameters for KT3D
*************************
START OF PARAMETERS:
Moisture100.dat \ file with data
 1 2 0 3 0 \ columns for X, Y, Z, var, sec var
-1.0e21 1.0e21 \ trimming limits
1 \ option: 0=grid, 1=cross, 2=jackknife
nodata.dat \ file with jackknife data
 1 2 0 3 0 \ columns for X,Y,Z, var and sec var
3 \ debugging level: 0,1,2,3
MoistureXV.dbg \ file for debugging output
MoistureXV.dat \ file for kriged output
60 0.5 1.0 \ nx,xmin,xsiz
60 0.5 1.0 \ ny,ynmin,ysiz
1 0.5 1.0 \ nz,zmin,zsiz
1 1 1 \ x,y and z block discretization
4 16 \ min, max data for kriging
6 \ max per octant (0-> not used)
15.0 15.0 15.0 \ maximum search radii
0.0 0.0 0.0 \ angles for search ellipsoid
1 11.581 \ 0=SK, 1=OK, 2=non-st SK, 3=exdrift
0 0 0 0 0 0 0 0 \ drift: x,y,z,xx,yy,zz,xy,xz,zy
0 \ 0, variable; 1, estimate trend
nodata.dat \ gridded file with drift/mean
data \ column number in gridded file
2 1.6 \ ust, nugget effect
1 0.16 0.0 0.0 0.0 \ it,cc,ang1,ang2,ang3
10.0 10.0 10.0 \ a_lmax, a_lmin, a_vert
1 1.04 0.0 0.0 0.0 \ it,cc,ang1,ang2,ang3
35.0 35.0 35.0 \ a_lmax, a_lmin, a_vert
MoistOK.par
Parameters for KT3D
***************

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Moisture100.dat  \file with data
1 2 0 3 0 \ columns for X, Y, Z, var, sec var
-1.0e21 1.0e21 \ trimming limits
0 \option: 0=grid, 1=cross, 2=jackknife
nodata.dat \file with jackknife data
1 2 0 3 0 \ columns for X,Y,Z, var and sec var
3 \debugging level: 0,1,2,3
MoistureOK.dbg \file for debugging output
MoistureOK.dat \file for kriged output
60 0.5 1.0 \nx,xmn,xsiz
60 0.5 1.0 \ny,ymn,ysiz
1 0.5 1.0 \nz,zmn,zsiz
4 4 4 \x,y and z block discretization
2 16 \min, max data for kriging
8 \max per octant (0-> not used)
15.0 15.0 15.0 \maximum search radii
0.0 0.0 0.0 \angles for search ellipsoid
1 11.581 \0=SK, 1=OK, 2=non-st SK, 3=exdrift
0 0 0 0 0 0 0 0 \drift: x,y,z,xx,yy,zz,xy,xz,zy
0 \0, variable: 1, estimate trend
nodata.dat \gridded file with drift/menu
1 \ column number in gridded file
2 1.6 \nst, nugget effect
1 0.16 0.0 0.0 0.0 \it,cc,ang1,ang2,ang3
10.0 10.0 10.0 \a_lmax, a_lmin, a_vert
1 1.04 0.0 0.0 0.0 \it,cc,ang1,ang2,ang3
35.0 35.0 35.0 \a_lmax, a_lmin, a_vert

124
MoistIK.par
Parameters for IK3D

START OF PARAMETERS:

1 \(1=\text{continuous(cdf), } 0=\text{categorical(pdf)}\)
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nodata.dat \(\text{file with jackknife data}\)
1 2 0 3 \(\text{columns for } X,Y,Z, vr\)
8 \(\text{number thresholds/categories}\)
9.69 10.21 10.62 10.93 11.45
11.94 12.37 12.85 \(\text{thresholds/categories}\)
0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 \(\text{global cdf/pdf}\)
m100i.dat \(\text{file with data}\)
1 2 0 3 \(\text{columns for } X,Y,Z \text{and variable}\)
nodata.ik \(\text{file with soft indicator input}\)
1 2 0 3 4 5 6 \(\text{columns for } X,Y,Z \text{and indicators}\)
-1.0e21 1.0e21 \(\text{trimming limits}\)
2 \(\text{debugging level: } 0,1,2,3\)
MoistIK.dbg \(\text{file for debugging output}\)
MoistIK.dat \(\text{file for kriging output}\)
12 2.5 5.0 \(\text{nx, xmn, xsiz}\)
12 2.5 5.0 \(\text{ny, ymn, ysiz}\)
1 0.0 1.0 \(\text{nz, zmn, zsiz}\)
2 16 \(\text{min, max data for kriging}\)
15.0 15.0 15.0 \(\text{maximum search radii}\)
0.0 0.0 0.0 \(\text{angles for search ellipsoid}\)
8 \(\text{max per octant (0-> not used)}\)
0 11.45 \(\text{0=full IK, 1=Median IK (threshold num)}\)
1 \(\text{0(SK), 1=OK}\)
1 0.40 \(\text{One nest, nugget effect}\)
2 0.60 0.0 0.0 0.0 \(\text{it, ce, ang1, ang2, ang3}\)
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**PostMIK1.par**

Parameters for POSTIK

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2 9.69 \(\text{output option, output parameter}\)

8 \(\text{number of thresholds}\)

9.69 10.21 10.62 10.93 11.45

11.94 12.37 12.85 \(\text{the thresholds}\)

1 1 0.413 \(\text{volume support?}, \text{type}, \text{varred}\)

nodata.dat \(\text{file with global distribution}\)

1 0 -1.0 1.0e21 \(\text{ivr}, \text{iwt}, \text{tmin, tmax}\)

0.0 40.0 \(\text{minimum and maximum Z value}\)

2 2.5 \(\text{lower tail: option, parameter}\)

1 1.0 \(\text{middle: option, parameter}\)

4 5.0 \(\text{upper tail: option, parameter}\)

50 \(\text{maximum discretization}\)
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Columns for X, Y, Z, var, sec var  
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Trimming limits  
0  
Option: 0 = grid, 1 = cross, 2 = jackknife  

**nodata.dat**  
File with jackknife data  
1 2 0 3 0  
Columns for X, Y, Z, var and sec var  
3  
Debugging level: 0, 1, 2, 3  

**TrueXV.dbg**  
File for debugging output  

**TrueXV.dat**  
File for kriged output  
50 0.5 1.0  
xmin, xsiz  
50 0.5 1.0  
ymin, ysiz  
1 0.5 1.0  
zmin, zsiz  
1 1 1  
x, y and z block discretization  
4 16  
Min, max data for kriging  
6  
Max per octant (0 -> not used)  
15.0 15.0 15.0  
Maximum search radii  
0.0 0.0 0.0  
Angles for search ellipsoid  
1 2.211  
0 = SK, 1 = OK, 2 = non-st SK, 3 = exdrift  
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Drift: x, y, z, xx, yy, zz, xy, xz, yz  
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0, variable; 1, estimate trend  

**nodata.dat**  
Gridded file with drift/mean  
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Column number in gridded file  
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Nugget, nugget effect  
1 7.37 0.0 0.0 0.0  
It, cc, ang1, ang2, ang3  
7.5 7.5 7.5  
a_hmax, a_hmin, a_vert
**TrueOK.par**

Parameters for K`T3D

***************

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-nodata.dat

file with trimming limits
-1.0e21 1.0e21

file with jackknife data
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file with debugging output
TrueOK.dbg
TrueOK.dat

file for debugging output
1 2 0 3 0

file for kriged output
50 0.5 1.0
50 0.5 1.0
1 0.5 1.0
3

x, y and z block discretization
4 4 4

min, max data for kriging
2 16

max per octant (0-> not used)
12.0 12.0 12.0

maximum search radii
0.0 0.0 0.0

angles for search ellipsoid
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0=SK,1=OK,2=non-st SK,3=exdrift
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drift: x,y,z,xx,yy,zz,xy,xz,zy
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variable; 1, estimate trend

file with drift/mean
nodata.dat

grid file with grid
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grid number in grid file
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nst, nugget effect
1 2.7

0.0 0.0 0.0

it, cc, ang1, ang2, ang3
7.5 7.5 7.5

a_hmax, a_hmin, a_vert
```
### TrueIK.par

**Parameters for IK3D**

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</table>
```

- **1**: Continuous (cdf), 0 = categorical (pdf)
- **0**: Option: 0 = grid, 1 = cross, 2 = jackknife
- **nodata.dat**: File with jackknife data
- **1 2 0 3**: Columns for X, Y, Z, vr
- **9**: Number thresholds/categories
- **0.15 0.27 0.45 0.83 1.02 1.38 2.07 3.16 6.29**: Thresholds / categories
- **0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9**: Global cdf / pdf
- **True97i.dat**: File with data
- **1 2 0 3**: Columns for X, Y, Z and variable
- **nodata.ik**: File with soft indicator input
- **1 2 0 3 4 5 6**: Columns for X, Y, Z and indicators
- **-1.0e21 1.0e21**: Trimming limits
- **2**: Debugging level: 0, 1, 2, 3
- **TrueIK.dbg**: File for debugging output
- **TrueIK.dat**: File for kriging output
- **10 2.5 5.0**: Nx, xmn, xsiz
- **10 2.5 5.0**: Ny, ymn, ysiz
- **1 0.0 1.0**: Nz, zmn, zsiz
- **4 16**: Min, max data for kriging
- **15.0 15.0 15.0**: Maximum search radii
- **0.0 0.0 0.0**: Angles for search ellipsoid
- **6**: Max per octant (0 -> not used)
- **0 1.02**: 0 = full IK, 1 = Median IK (threshold num)
- **1**: 0 = SK, 1 = OK
- **1 0.10**: One nst, nugget effect
- **1 0.90 0.0 0.0 0.0**: It, cc, ang1, ang2, ang3
\begin{verbatim}
7.5 7.5 0.0  \ a_hmax, a_hmin, a_vert
1 0.30  \ Two nst, nugget effect
1 0.70 0.0 0.0 0.0  \ it,cc,ang1,ang2,ang3
7.5 7.5 0.0  \ a_hmax, a_hmin, a_vert
1 0.30  \ Three nst, nugget effect
1 0.70 0.0 0.0 0.0  \ it,cc,ang1,ang2,ang3
7.5 7.5 0.0  \ a_hmax, a_hmin, a_vert
1 0.35  \ Four nst, nugget effect
1 0.65 0.0 0.0 0.0  \ it,cc,ang1,ang2,ang3
7.5 7.5 0.0  \ a_hmax, a_hmin, a_vert
1 0.35  \ Five nst, nugget effect
1 0.65 0.0 0.0 0.0  \ it,cc,ang1,ang2,ang3
9.5 9.5 0.0  \ a_hmax, a_hmin, a_vert
1 0.35  \ Six nst, nugget effect
1 0.65 0.0 0.0 0.0  \ it,cc,ang1,ang2,ang3
10.0 10.0 0.0  \ a_hmax, a_hmin, a_vert
1 0.40  \ Seven nst, nugget effect
1 0.60 0.0 0.0 0.0  \ it,cc,ang1,ang2,ang3
10.0 10.0 0.0  \ a_hmax, a_hmin, a_vert
1 0.15  \ Eight nst, nugget effect
1 0.85 0.0 0.0 0.0  \ it,cc,ang1,ang2,ang3
9.5 9.5 0.0  \ a_hmax, a_hmin, a_vert
1 0.35  \ Nine nst, nugget effect
1 0.65 0.0 0.0 0.0  \ it,cc,ang1,ang2,ang3
8.0 8.0 0.0  \ a_hmax, a_hmin, a_vert
\end{verbatim}
PostTIK1.par
Parameters for POSTIK

START OF PARAMETERS:

TrueK.dat \file with 1K3D output (continuous)
PostIK1.dat \file for output
2 0.15 \output option, output parameter
9 \number of thresholds
0.15 0.27 0.45 0.83 1.02 1.38
2.07 3.16 6.29 \the thresholds
1 1 0.745 \volume support?, type, varred
nodata.dat \file with global distribution
1 0 -1.0 1.0e21 \ivr, iwt, tmin, tmax
0.0 100.0 \minimum and maximum Z value
1 1.0 \lower tail: option, parameter
1 1.0 \middle: option, parameter
4 3 \upper tail: option, parameter
50 \maximum discretization