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Comparison and application of three decorrelation methods PCA, MAF and ACDC

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THE COMPARISON AND APPLICATION OF THREE DECORRELATION METHODS PCA, MAF AND ACDC.

BY

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Abstract

Geostatistics is a branch of applied mathematics that deals with spatially correlated data. Analysing and modelling spatially correlated data can be difficult and time consuming, especially for a multivariate data set. One of the techniques used to make analysis and modelling easier involves decorrelation, whereby a linear transformation on the sample variables is used to associate the spatially correlated variables with a set of decorrelated factors which are statistically and spatially independent. PCA was one of the first multivariate techniques and is mostly used as a data reduction technique. A popular alternative decorrelation technique often used in the mining industry is MAF. A study conducted by Bandarian (2008) found a relatively new decorrelation technique known as ACDC to be the method which produced the best spatial decorrelation for a multivariate moderately correlated data set consisting of four variables.

In this thesis the PCA, MAF and ACDC methods are described and then applied to a multivariate data set supplied by Rio Tinto's Iron Ore Operations. Secondly, we explore whether it is preferable for the data set to be standardised or transformed via Gaussian anamorphosis to normal scores before being decorrelated.

The data set consists of ten variables; however the three decorrelation methods were only applied to a subset of five variables (Fe, Al_2O_3, SiO_2, LOI and TiO_2) which have the greatest similarity from a statistical and spatial point of view. The three methods were applied to both standardised and normalised data. For ACDC, additional inputs such as weights, number of iterations, tolerance and an initial guess for the diagonalising matrix were explored and investigated in order to get the best spatial decorrelation results possible.

The overall best spatial decorrelation was achieved by performing ACDC on the standardised variables, using the matrix of eigenvectors of the correlation matrix as the initial guess for the diagonalising matrix as well as the first four experimental semivariogram matrices in the decorrelation. Transforming the variables to normal scores before decorrelation was found to be of no benefit, as the factors that were derived from the normalised variables with the exception of one, were not normally distributed following the decorrelation.

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1. Introduction

1.1 Background and Significance

Geostatistics is a branch of applied mathematics that deals with spatially correlated data. It originated in the early fifties in the mining industry, to help solve ore reserve estimation problems. The techniques used have evolved over time and are currently being used in areas such as petroleum geology, hydrogeology, hydrology, meteorology, oceanography, human geography, forestry, environmental control, landscape ecology and even epidemiology (Wackernagel, 2003). The main aim of geostatistics is to analyse, interpret, and derive a model from a sampled data set which may be spatially correlated in a study region, to provide accurate and reliable estimates of variables at unsampled locations. It is common that for each location under consideration there are several variables that may have to be analysed jointly.

There are a variety of multivariate geostatistical techniques used today, making analysis and modelling of several spatially correlated variables across a study region much easier. One of these techniques involves decorrelation, whereby a linear transformation of the sample variables is used to associate the spatially correlated variables with a set of decorrelated factors which are statistically and spatially independent. Univariate geostatistical techniques can then be used to model and possibly simulate the uncorrelated factors, decreasing the complexity and shortcomings of multivariate techniques, such as decreasing the size of cokriging systems used in multivariate estimations or simulations.

Principal component analysis (PCA) was one of the first multivariate techniques and is mostly used as a data reduction technique. Here the aim is to reduce a data set with a large number of variables to a smaller subset of uncorrelated factors, which accounts for a large proportion of the variability in the original variables. PCA is based on the eigenvector-eigenvalue decomposition of either the variance-covariance matrix or correlation matrix between variables (Desbarats & Dimitrakopoulos, 2000). However, the problem with PCA is that it only successfully decorrelates the factors at a lag spacing of zero. The factors will only be uncorrelated for all lags, other than zero, in the case of intrinsic correlation (Wackernagel, 2003). Most data sets do not exhibit intrinsic

correlation and therefore the PCA method is very limited and often does not provide the best decorrelation results.

The method of minimum/maximum autocorrelation factors (MAF) is another linear transformation technique based on PCA that decorrelates a set of variables into uncorrelated factors for all lag spacings, provided that the covariance function of the variables is characterised by a model of coregionalisation which consists of two structures to ensure orthogonality for all lag spacings. MAF was first developed by Switzer and Green (1984) as a data based approach used for multivariate spatial imaging. It was later shown by Desbarats and Dimitrakopoulos (2000) to be suitable for decorrelating variables in geostatical real data sets by applying the method to simulate a regionalised pore size distribution. The computational properties of MAF and limitations concerning a geostatistical context were later discussed by Vargas-Guzman and Dimitrakopoulos (2003) who also discuss extending the MAF approach to three covariance structures, but conclude that this is in general impossible. The method's current assumption of a two structure linear model of coregionalisation (2SLMC) can be restrictive as the model of a nugget plus one structure or two structures may be inadequate to model all spatial features (Bandarian, 2008). A recent study by Róndon and Tran (2008) in which the MAF method was used on a number of different data sets showing weak or non-linear correlations, also discusses a number of limitations and difficulties that may occur using the MAF method. A more general approach for spatial decorrelation is to approximately diagonalise a set of target matrices which originate from the experimental semivariogram matrices calculated at all relevant lag spacings. One of the methods which can be used to do so is the Alternating Columns and Diagonal Centres method, or more commonly known by its acronym ACDC. The ACDC method is a joint approximate diagonalisation (JAD) method. The ACDC method was first proposed by Yeredor in 2000 and is a relatively new linear transformation method. The ACDC method differs from the other JAD methods as it is not restricted to only finding an orthogonal diagonalising matrix (Yeredor, 2000).

A study performed by Bandarian (2008) illustrated and compared a variety of linear transformation methods using a subset of the Jura data set (Goovaerts, 1997), two of the methods which were considered where the MAF and ACDC. The subset consisted of four moderately correlated variables (Cd, Co, Cr and Ni). The results found the ACDC method to produce the better spatial decorrelation for the multivariate Jura subset,

thereby raising the question whether the ACDC method is the better linear transformation method to decorrelate any multivariate data set.

The linear transformation method, MAF (minimum/ maximum autocorrelation factors) is currently used in the mining industry to reduce complexity and time devoted to analysing and modelling multivariate data sets. Mining companies are often looking for the most cost effective methods which produce the best results. With this in mind even though most linear transformation methods only approximately diagonalise a multivariate data set, it would be cost effective to use the linear transformation method, whether it be ACDC or MAF, which produces the best spatial decorrelation, taking into account the time involved in using the linear transformation methods.

1.2 Aims and Objectives

The ultimate aim of this study is to compare the ACDC and MAF methods and determine if the ACDC method is able to approximately decorrelate a multivariate data set of more than four variables better than the currently used MAF method. Both methods will be applied to a multivariate data set from a channel iron ore deposit supplied by Rio Tinto's Iron Ore Operations. The factors obtained from both methods will be examined in order to determine which decorrelation method produces the best spatial decorrelation. Some of the variables in the data set are highly correlated. The effectiveness of both of the methods on the highly correlated data will also be considered.

The multivariate data set supplied by Rio Tinto consists of ten variables. A subset grouping all the variables which are statistically and spatially similar will be discussed in order to avoid variables which may be problematic. The most important variables are aluminium oxide, iron and silica which will need to be modelled jointly and hence have to be included in the subset, while there are other variables which may not be appropriate to add to the subset due to geological reasons. This will be discussed further in the thesis. Therefore, a suitable subset needs to be explored.

The ACDC algorithm, implemented in Matlab, allows for a variety of additional inputs besides the target matrices which could potentially affect the decorrelation results. The additional inputs such as weights, number of iterations, tolerance and an initial guess for the diagonalising matrix will be explored and investigated in order to get the best spatial decorrelation results possible using the ACDC method.

The decision to standardise the data set or to normalise the data before applying the methods is another interesting aspect which will be explored. This simple decision may have an effect on the decorrelation results for either method.

1.3 Thesis Outline

This thesis consists of five chapters and an Appendix. Chapter 2 discusses the theoretical framework significant to this study. This includes the multivariate random function model, linear model of co-regionalisation, a discussion of the linear transformation methods and finally how the spatial decorrelation will be assessed. Chapter 3 gives background information about the variables in the multivariate data set as well as a detailed exploratory data analysis of the data. The last few sections of Chapter 3 consist of the transformations of the variables and the investigation into suitable subsets. The results of the spatial decorrelation for all the methods are given in Chapter 4. The final chapter involves the discussion and conclusion.

1.4 Software

The main software packages used are Isatis and Matlab. Isatis is a geostastics software package which was mainly used to carry out exploratory data analysis, spatial data analysis and calculation of experimental semivariograms. The Gaussian anamorphosis function in Isatis was used to transform the original data to normally distributed data. The variables were also standardised using the corresponding population means and standard deviations calculated in Isatis. The MAF technique in Isatis was used to calculate the factors which were then analysed in Isatis. All the factors produced from ACDC, MAF and PCA were analysed in Isatis and SPSS.

Matlab is an engineering/mathematical software package in which the ACDC algorithm has been coded by Yeredor (2004). The target matrices produced in Isatis are run through the ACDC algorithm in Matlab to produce a transformation matrix that will approximately diagonalise the data. Matlab was furthermore used to calculate the spatial decorrelation assessment results for all the factors as well as the graphs showing the results. Microsoft Word and Excel were used for presentation and data preparation purposes. Finally SPSS was used to investigate the relationship between the variables.

1.5 Notation

The majority of the notation used in this thesis comes from Goovaerts (1997).

$\mathbf{A}$: study region

a : maximum range of the semivariogram

A^{-1}: ACDC transformation matrix

A_0: initial diagonalising matrix

b_{ij}^{l} : coefficients of the basic semivariogram model $g_l(\mathbf{h})$ in the linear model of co-regionalisation

B^{l} : co-regionalisation matrix containing the coefficients b_{ij}^{l} of the semivariogram model $g_l(\mathbf{h})$ in the corresponding linear model of co-regionalisation

B: matrix of correlation coefficient

$C(\mathbf{0})$: covariance value at separation distance $|\mathbf{h}|=0$

$C(\mathbf{h})$: covariance function of the random function for lag vector $\mathbf{h}$

$\hat{C}(\mathbf{h})$: experimental covariance function matrix of size $K \times K$

$\hat{C}_{ij}(\mathbf{h})$: experimental cross covariance between the two random function z_i and z_j for a lag vector $\mathbf{h}$

$\mathrm{C}_{\mathrm{LS}}(\cdot)$: objective function

D: diagonal matrix

$E\{\cdot\}$: expected values

$\mathbf{F}(\mathbf{u})$: factor values

$\Gamma(\mathbf{h})$: semivariogram matrix of size $K \times K$

$\hat{\Gamma}(\cdot)$: experimental semivariogram matrix of size $K \times K$

$g_l(\mathbf{h})$: lth basic semivariogram model in the linear model of co-regionalisation

$\hat{\gamma}_{ij}(\mathbf{h})$: experimental cross semivariogram between Z_i and Z_j at lag value **h**

$\gamma_{ij}(\mathbf{h})$: cross semivariogram between Z_i and Z_j at lag value **h**

h: separation vector

J: number of lag spacings

$\kappa(\mathbf{h})$: spatial diagonalisation efficiency at lag **h**.

$\bar{\kappa}$: average diagonalisation efficiency for all lags.

K: number of variables

Λ: eigenvalue matrix

λ: eigenvalue

L: number of models required to capture the spatial continuity of the attributes

m: lag means

subscript NS: normal scores data set

n: number of samples in the study region **A**

$N(\mathbf{h})$: is the number of pairs of data locations separated by the vector **h**

Q: PCA eigenvector matrix

$\hat{\rho}_{ij}$: experimental correlation coefficient between z_i and z_j

$\hat{\rho}_{ij}(\mathbf{h})$: cross correlogram between z_i and z_j for the lag vector **h**

$\hat{\sigma}_{ij}$: experimental covariance between z_i and z_j

σ^2: lag variance

subscript St: standardised data set

$\tau(\mathbf{h})$: quotient of the absolute deviation from diagonality and the sum of the factor main diagonal entries efficiency at lag **h**.

$\bar{\tau}$: the average quotient of the absolute deviation from diagonality and the sum of the factor main diagonal entries efficiency for all lags.

$\mathrm{Tr}\{\cdot\}$: trace of a matrix

$\mathbf{u}$: coordinate vector

$\mathbf{u}_\alpha$: datum location

$\varsigma(\mathbf{h})$: the measure of absolute deviation from diagonality for each lag $\mathbf{h}$

$\bar{\varsigma}$: the average measure of absolute deviation from diagonality for all lags

w_j: weight vector

X: MAF eigenvector matrix

X^T: MAF transformation matrix

$\boldsymbol{Z}$: multivariate random valued function

$z_i(\mathbf{u}_\alpha)$: z_i-datum values at location $\mathbf{u}_\alpha$

$z_i(\mathbf{u})$: z_i-datum values at location $\mathbf{u}$

$\boldsymbol{z}(\mathbf{u})$: vector of true values of K attributes at location $\mathbf{u}$

$z(\mathbf{u})$: true value at unsampled location $\mathbf{u}$

$\boldsymbol{Z}(\mathbf{u})$: vector of continuous random variable at location $\mathbf{u}$

$Z_i(\mathbf{u})$: ith continuous random variable at location $\mathbf{u}$

1.6 Acronyms and Abbreviations

The acronyms and abbreviations listed below are used in the content, Figure and Tables throughout the thesis.

ACDC:	Alternative Columns and Diagonal Centres method
Al_2O_3:	Aluminium oxide
CaO:	Calcium oxide
Fe:	Iron
JAD:	Joint Approximate Diagonalisation
LOI:	Loss on Ignition or The measurement of water content of the ore
MAF:	Maximum/minimum autocorrelation factors
MgO:	Magnesium oxide
Mn:	Manganese
P:	Phosphorus
PCA:	Principle component analysis
S:	Sulphur
SiO_2:	Silicon dioxide or silica
TiO_2:	Titanium dioxide or Titania
2SLMC:	Two structure linear model of coregionalisation

2 Theoretical Framework

In this chapter we discuss the theoretical framework appropriate for this study. The first part includes the geostatistical concepts relevant to the study, while the second part includes information about the linear model of co-regionalisation. The three linear transformation methods, PCA, MAF and ACDC, will also be discussed in this chapter along with the way in which the spatial decorrelation for each method will be assessed.

2.1 Multivariate Random Function

Geostatistics is based upon the concept of the random function, whereby a set of unknown values are regarded as realisations of spatially dependent random variables. A sample on a study region, **A**, consists of a set of measurements at specific locations for a number of attributes. The measurements in this region can be defined as

$$\{ z_i(\mathbf{u}_\alpha), \mathbf{u}_\alpha \in \mathbf{A}, \alpha=1,\ldots, n, i=1,\ldots, K\},$$

where $\mathbf{u}_\alpha$ is the α^{th} sampled location for n samples and z_i is defined as the i^{th} attribute of K attributes. The set of values the variable z_i attains on the study region **A** is defined as

$$\{z_i(\mathbf{u}): \mathbf{u} \in \mathbf{A}\}.$$

The value $z_i(\mathbf{u})$ can be thought of as being a realisation of the corresponding random variable $Z_i(\mathbf{u})$ at the location $\mathbf{u}$ in **A**. When we consider the study region as a whole, we have a set of usually dependent random variables, and can define a function from the study region **A** to the set $\{Z_i(\mathbf{u}): \mathbf{u} \in \mathbf{A}\}$, known as a random function.

In the multivariate case the vector, $\boldsymbol{z}(\mathbf{u}) = [z_1(\mathbf{u}), \ldots\ldots, z_K(\mathbf{u})]^T$ of K attributes at location $\mathbf{u}$ can be viewed as a realisation of the random variable valued vector $\boldsymbol{Z}(\mathbf{u}) = [Z_1(\mathbf{u}), \ldots\ldots, Z_K(\mathbf{u})]^T$. The multivariate random function can therefore be defined as

$$\boldsymbol{Z}: \mathbf{A} \rightarrow \{[Z_1(\mathbf{u}), \ldots\ldots, Z_K(\mathbf{u})]: \mathbf{u} \in \mathbf{A}\}.$$

Several assumptions need to be made about the multivariate random function. A random function is called stationary if for any separation vector **h,** the joint distributions of $[\boldsymbol{Z}(\mathbf{u}_1), \boldsymbol{Z}(\mathbf{u}_2) \ldots\ldots, \boldsymbol{Z}(\mathbf{u}_k)]$ and $[\boldsymbol{Z}(\mathbf{u}_1 + \mathbf{h}), \boldsymbol{Z}(\mathbf{u}_2 + \mathbf{h}) \ldots\ldots, \boldsymbol{Z}(\mathbf{u}_k + \mathbf{h})]$ are identical for any lag **h** and for any k. The assumption of stationarity is impossible to test and so

the weaker assumption of second order stationarity is used in practice. A random function is said to be second order stationary if the expected mean value

$$\mathbf{m} = E\{\boldsymbol{Z}(\mathbf{u})\},$$

exists and is invariant within **A**. Here $\mathbf{m} = [m_1(\mathbf{u}), \ldots\ldots, m_K(\mathbf{u})]^T$ and $E\{\cdot\}$ denotes the mathematical expectation. The covariance function

$$C(\mathbf{h}) = E\{[\boldsymbol{Z}(\mathbf{u}) - \mathbf{m}] \cdot [\boldsymbol{Z}(\mathbf{u}+\mathbf{h}) - \mathbf{m}]^T\}$$

only depends on the separation vector **h**. The covariance function must be a positive definite function. In many cases the assumption of second-order stationarity is not met and a weaker hypothesis, second order stationarity of the increments $\boldsymbol{Z}(\mathbf{u}) - \boldsymbol{Z}(\mathbf{u}+\mathbf{h})$ is assumed. When the increments are second-order stationary, the random function is said to be intrinsic stationary. In this case the mean

$$E\{\boldsymbol{Z}(\mathbf{u}+\mathbf{h}) - \boldsymbol{Z}(\mathbf{u})\}$$

exists and is equal to **0** and the semivariogram

$$\Gamma(\mathbf{h}) = \frac{1}{2} E\{[\boldsymbol{Z}(\mathbf{u}) - \boldsymbol{Z}(\mathbf{u}+\mathbf{h})] \cdot [\boldsymbol{Z}(\mathbf{u}) - \boldsymbol{Z}(\mathbf{u}+\mathbf{h})]^T\}$$

depends only on **h**. The semivariogram matrix, $\Gamma(\mathbf{h})$, is a $K \times K$ positive definite, symmetric matrix that contains the direct semivariograms results along the main diagonal and the experimental cross semivariogram off the diagonal. When the variance-covariance matrix $C(\mathbf{0})$ exists, the semivariogram matrix and covariance function matrix are related by

$$\Gamma(\mathbf{h}) = C(\mathbf{0}) - C(\mathbf{h}).$$

The semivariogram function is more commonly used in practise than the covariance function.

2.2 Experimental Measures of Bivariate Relations

The covariance and correlation coefficient are the most frequently used measures of bivariate relations. The experimental covariance $\hat{\sigma}_{ij}$ is a measure of the joint variation of z_i and z_j around their means and it is computed as

$$\hat{\sigma}_{ij} = \frac{1}{n} \sum_{\alpha=1}^{n} (z_i(\alpha) - m_i) \cdot (z_j(\alpha) - m_j),$$

where the arithmetic means of z_i and z_j are denoted by m_i and m_j, respectively. In the situation when $i = j$ the covariance becomes the variance.

The standardised form of the experimental covariance is the linear correlation coefficient $\hat{\rho}_{ij}$ which provides a measure of the linear relationship between two variables. The experimental correlation coefficient is calculated as

$$\hat{\rho}_{ij} = \frac{\sigma_{ij}}{\sigma_i \cdot \sigma_j} \quad \in [-1,1]$$

where σ_i and σ_j are the standard deviations of z_i and z_j, respectively. The correlation matrix B is a matrix of correlation coefficients $\hat{\rho}_{ij}$ for all pairs $i, j = 1 \ldots . K$. When the variables have been transformed to normal scores or standardised the correlation matrix is equivalent to the covariance matrix.

Spatial features of the data such as the location of extreme values, degree of continuity and spatial trends are often of considerable interest in geostatistics, and there are a variety of tools used to capture spatial continuity. In a multivariate data set consisting of several attributes, such as the data set that will be used for this project, there is a need to look at spatial cross continuity between measurements of different attributes. The cross covariance and cross correlation function are some of the measures of spatial continuity derived from the sample data that measure the similarities between colocated data. The experimental cross covariance function is the covariance between a pair of locations of different attributes, z_i and z_j, separated by a vector $\mathbf{h}$, which is also known as the lag. The experimental cross covariance function is defined as

$$\hat{C}_{ij}(\mathbf{h}) = \frac{1}{N(\mathbf{h})} \sum_{\alpha=1}^{N(\mathbf{h})} z_i(\mathbf{u}_\alpha) \cdot z_j(\mathbf{u}_\alpha + \mathbf{h}) - m_{i_{-\mathbf{h}}} m_{j_{+\mathbf{h}}},$$

with

$$m_{i_{-\mathbf{h}}} = \frac{1}{N(\mathbf{h})}\sum_{\alpha=1}^{N(\mathbf{h})} z_i(\mathbf{u}_\alpha), \text{ and } \quad m_{j_{+\mathbf{h}}} = \frac{1}{N(\mathbf{h})}\sum_{\alpha=1}^{N(\mathbf{h})} z_j(\mathbf{u}_\alpha + \mathbf{h}),$$

where $N(\mathbf{h})$ is the number of pairs of data locations separated by the vector $\mathbf{h}$, while $m_{i_{-\mathbf{h}}}$ and $m_{j_{+\mathbf{h}}}$ are the means of the z_i and z_j values. When *i=j* this is simply known as the experimental covariance function between data values of the same attribute separated by a vector $\mathbf{h}$. The cross correlogram is the standardised form of the covariance and is given by

$$\hat{\rho}_{ij}(\mathbf{h}) = \frac{C_{ij}(\mathbf{h})}{\sqrt{\sigma^2_{i_{-\mathbf{h}}}\sigma^2_{j_{+\mathbf{h}}}}} \in [-1,1]$$

with

$$\sigma^2_{i_{-\mathbf{h}}} = \frac{1}{N(\mathbf{h})}\sum_{\alpha=1}^{N(\mathbf{h})} [z_i(\mathbf{u}_\alpha) - m_{i_{-\mathbf{h}}}]^2 \quad \text{and} \quad \sigma^2_{j_{+\mathbf{h}}} = \frac{1}{N(\mathbf{h})}\sum_{\alpha=1}^{N(\mathbf{h})} [z_j(\mathbf{u}_\alpha + \mathbf{h}) - m_{j_{+\mathbf{h}}}]^2,$$

where $\sigma^2_{i_{-\mathbf{h}}}$ and $\sigma^2_{j_{+\mathbf{h}}}$ are the variances of z_i and z_j values. In the case where *i=j* the function is known as a correlogram and measures the similarities between data of the same attribute.

The experimental cross semivariogram is another measure of spatial continuity, however unlike the covariance and correlation function, the experimental cross semivariogram measures the average dissimilarity between data of different attributes which is separated by a vector $\mathbf{h}$. The experimental cross semivariogram between z_i and z_j at lag value $\mathbf{h}$ is defined as

$$\hat{\gamma}_{ij}(\mathbf{h}) = \frac{1}{2N(\mathbf{h})}\sum_{\alpha=1}^{N(\mathbf{h})} [z_i(\mathbf{u}_\alpha) - z_i(\mathbf{u}_\alpha + \mathbf{h})] \cdot [z_j(\mathbf{u}_\alpha) - z_j(\mathbf{u}_\alpha + \mathbf{h})].$$

A direct semivariogram is obtained when *i=j* for the function $\hat{\gamma}_{ij}(\mathbf{h})$. The semivariogram function and covariance function are known to be anisotropic if their values depend both on the distance $|\mathbf{h}|$ and direction of the lag vector $\mathbf{h}$. When the covariance and semivariogram values depend only on distance and not on direction they are said to be isotropic.

2.3 Linear Model of Co-regionalisation

Structural analysis and modelling is performed in order to be able to compute estimates at unsampled locations. From the experimental semivariograms and experimental cross semivariograms one only gets information for specific lag vectors, so a model for all lags is required. A model of co-regionalisation is a model constructed from the experimental semivariograms and cross semivariograms which provides estimates for the semivariogram or covariance for any lag **h**. A type of model of co-regionalisation is the linear model of co- regionalisation. This provides a method of modelling the cross semivariograms of a number of variables so that the variance of any possible linear combination of these variables is always positive (Isaaks and Srivastava, 1989). The linear model of co-regionalisation defines the semivariogram model function as a $K \times K$ matrix of linear combination of admissible models

$$\gamma_{ij}(\mathbf{h}) = \sum_{l=0}^{L} b_{ij}^{l} g_l(\mathbf{h}) \qquad i,j = 1, \ldots\ldots, K$$

where each model function $g_l(\mathbf{h})$ is an acceptable semivariogram model (a list of admissible models can be found in Goovaerts, pg 88, 1997), and the coefficients b_{ij}^{l} are the corresponding sills or slope coefficients of the model $g_l(\mathbf{h})$. The matrices $\mathrm{B}^{l} = [b_{ij}^{l}]$ are required to be positive semi-definite. The number L denotes the number of models or structures required to capture the spatial continuity of the attributes. Modelling the cross variograms via a linear model of co-regionalisation for a multivariate data set can be very difficult, time consuming, and sometimes inaccurate when basic models are used for all cross semivariograms. Therefore, there is a need to find a way to appropriately and efficiently decorrelate spatially dependent data.

2.4 Linear Transformation Methods

Transformation methods have long been used in geostatistics to spatially decorrelate data by transforming spatially correlated variables into a set of decorrelated factors which are statistically and spatially independent. The decorrelated factors derived from these methods are linear combinations of the original variables and are needed to produce a transformation matrix which approximately diagonalises the spatial covariance matrix for all lags.

2.4.1 PCA

Principal component analysis (PCA) is the most popular multivariate data analysis method and dates back to the early 1900's. PCA provides a linear transformation of a set of correlated variables into a set of statistically uncorrelated factors (Wackernagel, 2003). The variables are replaced by linear combinations called principal components which are uncorrelated at lag **0** (the vector **h** equals **0**). The PCA method is basically an eigenvalue problem, which consists of the extraction of the eigenvalues and corresponding eigenvectors of the positive definite symmetric correlation matrix B. The factors are obtained by pre-multiplying the vectors of the attributes by the transposed eigenvector matrix

$$\mathbf{F(u)} = \mathrm{Q}^{\mathrm{T}}\mathbf{Z(u)}$$

where the eigenvectors $\mathbf{q}_1, \ldots, \mathbf{q}_K$ of B make up the orthogonal matrix Q. The eigenvectors $\mathbf{q}_1, \ldots, \mathbf{q}_K$ in Q are arranged in decreasing order of magnitude of the corresponding eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_K$. The problem with PCA is that decorrelation is only guaranteed when the co-regionalisation matrices at different lag spacings are proportional, in other words it is only guaranteed when the spatial dependence of the variable under consideration can be modelled by a so-called intrinsic model of co-regionalisation. In practice this condition is rarely satisfied and therefore other methods may be better suited for decorrelation.

2.4.2 MAF

MAF decorrelates a set of variables into uncorrelated factors for all lag spacings provided that the covariance function of the variables is fully characterised by a two structure linear model of coregionalisation (2SLMC). This assumption can be restrictive as using a model consisting of either a nugget plus one structure or two structures may be inadequate to model all cross-semivariograms (Bandarian, 2008). For this thesis we will concentrate on the MAF method involving the experimental semivariogram matrices $\hat{\Gamma}(\cdot)$, in which the factors are derived via two successive PCA's.

The general formulation of MAF is first described and shown in terms of the assumed theoretical model. The assumption of MAF is that the semivariogram function $\Gamma(\mathbf{h})$ of a multivariate random function can be modelled by a 2SLMC such that

$$\Gamma(\mathbf{h}) = B_0 g_0(\mathbf{h}) + B_1 g_1(\mathbf{h}),$$

where B_0 and B_1 are the symmetric positive semi-definite co-regionalisation matrices which contain the sills of the semivariogram models $g_0(\mathbf{h})$ and $g_1(\mathbf{h})$. The coregionalisation matrices add up to the correlation matrix

$$B = B_0 + B_1,$$

only when the data are normalised or standardised. Therefore, as both co-regionalisation matrices are symmetric and therefore diagonalisable and B_1 is positive definite, then B_0 and $B_1 = B - B_0$ may be diagonalised simultaneously by congruence. Two matrices A and S are said to be congruent if there exists a non-singular matrix X, not necessarily orthogonal such that $S=X^TAX$. The 2SLMC can be expressed as

$$\Gamma(\mathbf{h}) = B_0 g_0(\mathbf{h}) + (B - B_0) g_1(\mathbf{h}) = B_0 g_0(\mathbf{h}) + B g_1(\mathbf{h}) - B_0 g_1(\mathbf{h}).$$

The first PCA of the MAF method involves orthogonally diagonalising the positive definite symmetric correlation matrix B such that

$$B = HDH^T,$$

where the columns of H are orthonormal eigenvectors of B and the corresponding eigenvalues $\lambda_1, \ldots, \lambda_K$, are arranged in order of decreasing magnitude to make up the diagonal matrix D.

Premultiplying $\Gamma(\mathbf{h})$ by H^T and postmultiplying by H, one obtains

$$H^T\Gamma(\mathbf{h})H = Dg_1(\mathbf{h}) + H^TB_0H\big(g_0(\mathbf{h}) - g_1(\mathbf{h})\big).$$

Next, $H^T\Gamma(\mathbf{h})H$ is premultiplied by $D^{-\frac{1}{2}}$ and postmultiplied by $D^{-\frac{1}{2}}$. The 2SLMC is now able to be expressed as

$$\Gamma_w(\mathbf{h}) = W^T\Gamma(\mathbf{h})W = Ig_1(\mathbf{h}) + W^TB_0W\big(g_0(\mathbf{h}) - g_1(\mathbf{h})\big),$$

where $W = HD^{-\frac{1}{2}}$.

The initial transformation matrix W only decorrelates the $\mathbf{W(u)} = W^T\boldsymbol{Z}(\mathbf{u})$ factors at lag zero, like a PCA transformation matrix would. Therefore, unless intrinsic correlation occurs the factors would still be correlated for all lags other than zero.

The matrix W^TB_0W and $\Gamma_w(\mathbf{h})$ are symmetric as

$$(W^TB_0W)^T = W^TB_0W$$

and

$$(\Gamma_w(\mathbf{h}))^T = \Big(Ig_1(\mathbf{h}) + W^TB_0W\big(g_0(\mathbf{h}) - g_1(\mathbf{h})\big)\Big)^T$$

$$= \big(Ig_1(\mathbf{h})\big)^T + \Big(W^TB_0W\big(g_0(\mathbf{h}) - g_1(\mathbf{h})\big)\Big)^T$$

$$= Ig_1(\mathbf{h}) + W^TB_0W\big(g_0(\mathbf{h}) - g_1(\mathbf{h})\big) = \boldsymbol{\Gamma}_w(\mathbf{h}).$$

The second PCA is carried out on the symmetric matrix $\Gamma_w(\mathbf{h})$, resulting in the calculation of the orthonormal eigenvectors C and a diagonal matrix of corresponding eigenvalues D_1. The transpose of the eigenvector C^T is able to orthogonally diagonalise the factors $\mathbf{M(u)} = C^T\mathbf{W(u)}$ for all lags (Desbarats & Dimmitrakopos, 2000). The orthonormal eigenvectors that would be calculated from the decomposition of W^TB_0W would be similar to C. Both eigenvectors are independent of the lag $\mathbf{h}$. Therefore, the orthogonal diagonalisation of $\Gamma_w(\mathbf{h})$ is

$$\Gamma_w(\mathbf{h}) = C[D_1g_0(\mathbf{h}) + (I - D_1)g_1(\mathbf{h})]C^T,$$

where the orthogonal matrix of eigenvectors is denoted as C and the diagonal matrix of corresponding eigenvalues is denoted as $[D_1g_0(\mathbf{h}) + (I - D_1)g_1(\mathbf{h})]$.

The transformation matrix A^T is a combination of the two decompositions and is calculated as

$$A^T = C^T D^{-1/2} H^T$$

where $A^T B A = I$ as $H^T H = C^T C = I$. Since the theorecical LMC is not available in practice the correlation matrix, which is equivalent to the covariance matrix in the case of standardised or normalised data, and the semivariogram matrix at a lag close to the sample spacing are used to derive A (Bandarian & Mueller, 2008, p. 1173). The transformation matrix A^T simultaneously diagonalises B and semivariogram matrix chosen producing orthogonal factors at a lag of zero and lag of the semivariogram matrix, regardless of the suitability of the 2SLMC.

The MAF factors are produced by putting

$$\mathbf{F(u)} = A^T \boldsymbol{Z}(\mathbf{u}).$$

As observed earlier, MAF can be very restrictive as the assumption of a 2SLMC being able to model all the cross variogram factors is not always realistic. The MAF method does not cope well with poorly correlated variables and non linearity between variables (Rondon & Tran, 2008). For this reason the correlation coefficients and linearity between the variables has been included in the analysis of the data set in order to check for such limitation.

2.4.3 ACDC

A more general and recent approach for spatial decorrelation is to approximately diagonalise a set of target matrices which originate from the experimental semivariogram matrices calculated at all lag spacings. One of the methods which can be used to do so is the Alternating Columns and Diagonal Centres method, or more commonly known by its acronym ACDC. The ACDC method is a joint approximate diagonalisation (JAD) method. Given a family of symmetric, positive definite matrices $(M_1, M_2, \ldots., M_J)$ the method iteratively determines a non orthogonal diagonalising matrix A and a family of diagonal matrices $\Lambda_1, \Lambda_2, \ldots., \Lambda_J$ such that

$$M_j \approx A \Lambda_j A^T \quad j = 1,2, \ldots., J$$

where J denotes the number of $K \times K$ matrices and $\mathrm{M}_j = \Gamma(\mathbf{h})_j$. When the experimental semivariogram matrices $\hat{\Gamma}(\mathbf{h})_j$ are used then the matrix A and diagonal matrices $\Lambda_1, \Lambda_2, \ldots, \Lambda_J$ are estimates and denoted as $\widehat{\mathrm{A}}$ and $\widehat{\Lambda}_1, \widehat{\Lambda}_2, \ldots, \widehat{\Lambda}_J$. The ACDC algorithm aims to minimise the objective function

$$\mathrm{C_{LS}}\left(\widehat{\mathrm{A}}, \widehat{\Lambda}_1, \widehat{\Lambda}_2, \ldots, \widehat{\Lambda}_J\right) = \sum_{j=1}^{J} \mathrm{w}_j \ \mathrm{Tr}\left\{\left(\widehat{\mathrm{M}}_j - \widehat{\mathrm{A}}\widehat{\Lambda}_j\widehat{\mathrm{A}}^{\mathrm{T}}\right)^{\mathrm{T}}\left(\widehat{\mathrm{M}}_j - \widehat{\mathrm{A}}\widehat{\Lambda}_j\widehat{\mathrm{A}}^{\mathrm{T}}\right)\right\}$$

where $\mathrm{w}_1, \ldots, \mathrm{w}_J$ are non-negative weights and $\mathrm{Tr}\left\{\left(\widehat{\mathrm{M}}_j - \widehat{\mathrm{A}}\widehat{\Lambda}_j\widehat{\mathrm{A}}^{\mathrm{T}}\right)^{\mathrm{T}}\left(\widehat{\mathrm{M}}_j - \widehat{\mathrm{A}}\widehat{\Lambda}_j\widehat{\mathrm{A}}^{\mathrm{T}}\right)\right\}$ denotes the trace of $\left(\widehat{\mathrm{M}}_j - \widehat{\mathrm{A}}\widehat{\Lambda}_j\widehat{\mathrm{A}}^{\mathrm{T}}\right)^{\mathrm{T}}\left(\widehat{\mathrm{M}}_j - \widehat{\mathrm{A}}\widehat{\Lambda}_j\widehat{\mathrm{A}}^{\mathrm{T}}\right)$ defined as the sum of the entries on its main diagonal. The weights enable some of the matrices to have more of an impact on the approximate diagonalisation than others. The algorithm alternates between two phases, the alternating column phase (AC) and the diagonal centres phase (DC). The AC phase consists of minimising the $\mathrm{C_{LS}}\left(\widehat{\mathrm{A}}, \widehat{\Lambda}_1, \widehat{\Lambda}_2, \ldots, \widehat{\Lambda}_J\right)$ with respect to a particular column of the diagonalising matrix $\widehat{\mathrm{A}}$, while keeping its other columns and diagonal matrices $\widehat{\Lambda}_1, \widehat{\Lambda}_2, \ldots, \widehat{\Lambda}_J$ fixed (Yeredor, 2000). The DC phase consists of minimising the $\mathrm{C_{LS}}\left(\widehat{\mathrm{A}}, \widehat{\Lambda}_1, \widehat{\Lambda}_2, \ldots, \widehat{\Lambda}_J\right)$ with respect to the diagonal matrices $\widehat{\Lambda}_1, \widehat{\Lambda}_2, \ldots, \widehat{\Lambda}_J$, while the diagonalising matrix $\widehat{\mathrm{A}}$ remains fixed (Yeredor, 2000).

The AC phase minimises $\mathrm{C_{LS}}$ with respect to a particular column l of $\widehat{\mathrm{A}}$ $(1 \leq l \leq K)$ calculated by the following quadratic equation

$$\mathrm{P} = \sum_{j=1}^{J} \mathrm{w}_j \hat{\lambda}_l^{(j)} \left[\widehat{\mathrm{M}}_j - \sum_{\substack{k=1 \\ k \neq l}}^{K} \hat{\lambda}_k^{(j)} \hat{\mathbf{a}}_k \hat{\mathbf{a}}_k^{\mathrm{T}}\right],$$

where $\hat{\mathbf{a}}_k$ denotes the k^{th} column of the diagonalising matrix $\widehat{\mathrm{A}} = [\hat{\mathbf{a}}_1, \hat{\mathbf{a}}_2, \ldots, \hat{\mathbf{a}}_k]$ and $\hat{\lambda}_k^{(j)}$ denotes the corresponding k^{th} diagonal value of $\widehat{\Lambda}_j$ while $\hat{\lambda}_l^{(j)}$is the corresponding diagonal value for the l^{th} column. The unit-norm eigenvectors $\boldsymbol{\alpha}$ and largest eigenvalue of P are calculated and if $\mu<0$ then set $\hat{\mathbf{a}}_l = 0$, otherwise set

$$\hat{\mathbf{a}}_l = \frac{\alpha\sqrt{\mu}}{\sqrt{\Sigma_{j=1}^{J} \mathrm{w}_j (\lambda_l^{(j)})^2}}.$$

This is done to determine if P is negative definite as if it is then the $\hat{\mathbf{a}}_l$ is set to zero to attain minimisation of $\mathrm{C_{LS}}$ with respects to $\hat{\mathbf{a}}_l$.

The DC phase minimise the C_{LS} with respect to the diagonal matrices $\widehat{\Lambda}_1, \widehat{\Lambda}_2, \ldots, \widehat{\Lambda}_J$. For $j = 1,2, \ldots, J$ the diagonal matrices are calculated by

$$\widehat{\Lambda}_j = \text{diag}\left\{\left[(\widehat{A}^T \widehat{A})^* \odot (\widehat{A}^T \widehat{A})\right]^{-1} \text{diag}\{\widehat{A}^T \widehat{M}_j \widehat{A}\}\right\}$$

where $\odot$ denotes Hadamard's (element wise) product and the superscript * represents conjugation, however this is not needed in the case of the semi-positive matrices.

The ACDC algorithm alternates between the AC and DC phase until a pre-specified tolerance or number of iterations has been reached. The initial phase of the algorithm depends on the inputs added to the algorithm. If an initial guess for the diagonal matrices is made then the AC phase is run first. In most cases where an initial guess of the diagonal matrices or diagonalising matrix is not made, the DC phase is run first. The diagonalising matrix is automatically set to the identity matrix so that the first DC phase will be able to calculate the corresponding diagonal matrices (Yeredor, 2000). The AC phase is then run over all J columns of the diagonalising matrix, minimising the objective function with respect to the corresponding diagonal matrices. The improved diagonalising matrix is then used in the DC phase to minimise the objective with respect to the new calculated diagonalising matrix.

Intelligent initial guesses for the diagonal matrices or diagonalisation matrix may possibly improve the quality of the ACDC algorithm. An intelligent guess for the diagonalisation matrix would be the matrix that diagonalises the correlation matrix. The reason being that the the ACDC method would just be improving the diagonalising matrix in which the transpose is already used as the PCA transformation matrix to approximately decorrelate variables. The other reason is because it is very easy and simple to calculate and is the basis for a few methods.

Once the matrix $\widehat{A}$ has been determined, the factors are computed by putting

$$\mathbf{F(u)} = \widehat{A}^{-1} \boldsymbol{Z(u)}.$$

A Matlab program that implements the algorithm was published by Yeredor (2004). This program was used extensively throughout this thesis. The additional inputs such as weights, number of iterations, initial guesses for the diagonalising matrix and tolerance were explored to investigate the impact they made on the ACDC decorrelation results. It was hoped that the additional specified inputs would improve the quality of the

decorrelation resulting from the ACDC algorithm. The impact of the additional inputs and results on the data set will be discussed further on in the thesis using the multivariate data set supplied by Rio Tinto.

2.5 Methods Used to Assess Spatial Decorrelation.

There are a variety of ways to assess how successfully the factors have been spatially decorrelated. For a visual assessment the cross semivariogram for each factor pair will be graphed in order to detect any remaining spatial correlation. Perfect decorrelation is shown when the experimental cross semivariogram factors are at zero for all lags. A quantitative method used to measure spatial decorrelation is to calculate the absolute deviation from diagonality $\varsigma(\mathbf{h})$, the quotient of the absolute deviation from diagonality and the sum of the factor main diagonal entries $\tau(\mathbf{h})$, and the spatial diagonalisation efficiency $\kappa(\mathbf{h})$.

The deviation from diagonality at lag $\mathbf{h}$, $\varsigma(\mathbf{h})$, is the sum of squares of the off-diagonal elements of the factor experimental semivariogam matrix for all lag spacings,

$$\varsigma(\mathbf{h}) = \sum_{k=1}^{K}\sum_{j\neq k}^{K}(\hat{\gamma}_F(\mathbf{h};k,j))^2,\ |\mathbf{h}| > 0\,.$$

where $\hat{\gamma}_F$ denotes the experimental semivariogram for the factors. Perfect spatial decorrelation occurs when $\varsigma(\mathbf{h}) = 0$ for all separation distances. A global measure is given by the average $\bar{\zeta}$ of $\varsigma(\mathbf{h})$ calculated at J lag spacings,

$$\bar{\zeta} = \frac{1}{J}\sum_{j=1}^{J}\zeta(\mathbf{h}_j).$$

The measure of spatial decorrelation, $\tau(\mathbf{h})$, compares the absolute sum of off-diagonal elements of the factor experimental semivariogram matrix $\hat{\Gamma}_F(\mathbf{h})$ with the absolute sum of the diagonal elements calculated at each lag spacing $\mathbf{h}$ (Tercan, 1999). The formula for $\tau(\mathbf{h})$ along with the average $\bar{\tau}$, of $\tau(\mathbf{h})$ calculated at J lag spacings, are given by

$$\tau(\mathbf{h}) = \frac{\sum_{k=1}^{K}\sum_{j\neq k}^{K}|\hat{\gamma}_F\,(\mathbf{h};k;j)|}{\sum_{k=1}^{K}|\hat{\gamma}_F\,(\mathbf{h};k;k)|},\ |\mathbf{h}| > 0$$

and

$$\bar{\tau} = \frac{1}{J}\sum_{j=1}^{J}\tau(\mathbf{h}_j),$$

respectively. For perfect decorrelation to occur $\tau(\mathbf{h})$=0 for all lags $\mathbf{h}$.

Finally, the spatial decorrelation efficiency function at lag $\mathbf{h}$, $\kappa(\mathbf{h})$, compares the sum of squares of the off diagonal elements of the factor experimental semivariogram matrix $\hat{\Gamma}_F(\mathbf{h})$ to the sum of squares of the off diagonal elements of the sample experimental semivariogram matrix $\hat{\Gamma}_z(\mathbf{h})$ (Tercan, 1999). It is given by

$$\kappa(\mathbf{h}) = 1 - \frac{\sum_{k=1}^{K}\sum_{j\neq k}^{K}(\hat{\gamma}_F(\mathbf{h};k,j))^2}{\sum_{k=1}^{K}\sum_{j\neq k}^{K}(\hat{\gamma}_z(\mathbf{h};k,j))^2}, |\mathbf{h}| > 0.$$

Perfect spatial decorrelation for all separation distances or lags $\mathbf{h}$ occurs when $\kappa(\mathbf{h})=1$. A set of matrices may be considered to be nearly in diagonal form if $\kappa(\mathbf{h}) \geq 0.9$ for all lags $\mathbf{h}$ (Xie, Myers & Long, 1995). The average of $\kappa(\mathbf{h})$ for all J lag spacing is given as

$$\bar{\kappa} = \frac{1}{J}\sum_{j=1}^{J}\kappa(\mathbf{h}_j).$$

The average calculated for J lag spacings quantifies the overall spatial decorrelation.

3 Analysis

This chapter discusses the exploratory and spatial analysis of the data set supplied by Rio Tinto. The two ways in which the ten variables have been transformed will also be discussed in this chapter. The last section of this chapter discusses the similarity and differences between the ten variables in order to determine a suitable subset which will be approximately decorrelated.

3.1 Data Set Background

The data set which will be used for the study has been supplied by Rio Tinto's Iron Ore operation in Western Australia. The compositional data set contains ten variables; aluminium oxide (Al_2O_3), calcium oxide (CaO), iron (Fe), the measurement of water content of the ore (LOI), magnesium oxide (MgO), manganese (Mn), phosphorus (P), sulphur (S), silicon dioxide or silica (SiO_2) and titanium dioxide or titania (TiO_2). The 1885 sample measurements for each of these ten attributes come from one mining bench in a channel iron deposit in the Pilbara region, located in the northwest of Western Australia, approximately 1,100 km north of Perth. The assays are from sampling of blast hole cuttings, where the patterns of the blast hole locations represent different phases of mining. The original co-ordinates have been transformed, but otherwise all other measurements are in meters. The ten variables influence the mining of iron ore as well as the extraction of iron, and therefore need to be analysed and modelled in order to successfully produce iron and subsequently steel.

The most important variables, in terms of saleable products, are iron, alumina and silica. The iron content is important because it is the iron element in the ore which is predominantly used to make steel. The main concern for mining companies would be to identify, concentrate and mine in areas of the region which are rich in iron. Aluminium (Al), present in Al_2O_3, has a number of adverse effects on the furnace operation involved in producing iron and steel, reducing the quality of iron. Aluminium is also very difficult to reduce once present. Therefore, it is important to identify the locations of major Al_2O_3 concentrations in relation to iron, as potential clients are interested in a high iron quality. Silica promotes the formation of gray iron which is a type of iron less brittle and easier to finish than the more common white iron. Gray iron is preferred for casting and is often used for housing structures while white iron is the starting material for malleable cast iron. Thus, by mining companies knowing where areas of high silica

concentrations are in relation to iron deposits, they are more capable of producing a higher quality of white and gray iron (Liddelow & Dinsdale, 1996).

The iron mineralisation occurs within the Hamersley Iron Province. The geology of this Province is characterised by a 2,500 million year old group of late Archaean and early Proterozoic rock formations known as the 'Hamersley Group'. The Hamersley group was formed as a result of volcanic activity, which introduced basalt rock into the area. Throughout its formation, ongoing transportation and weathering of the Hamersley group led to the existence of sedimentary rocks, such as sandstone. Also during this period, rocks with different chemical compositions were deposited in layers (Rio Tinto Iron Ore, 2009)

3.2 Exploratory Data Analysis

The summary statistics of the ten raw variables are given in Table 1. Each variable comprises of 1885 observations, with no missing data. Except for Mn and Fe, the variables are positively skewed. The severity of skewness differs for each variable, with CaO being the most skewed and Mn being the least skewed. The kurtoses for all ten variables are positive, indicating that the distributions are more peaked than a normal distribution. The severity of peaks differ for each variable, with the CaO distribution being the most peaked and S being the least peaked, compared to a normal distribution. This is further illustrated in the histograms shown in Figure 1. The histogram for Mn shows that the Mn distribution may be discrete.

Table 1- Summary statistic for the ten variables.

	Al_2O_3	CaO	Fe	LOI	MgO	Mn	P	S	SiO_2	TiO_2
Mean	1.561	0.059	56.887	9.75	0.077	0.02	0.034	0.007	7.131	0.106
Median	1.21	0.06	57.18	9.73	0.07	0.02	0.033	0.007	6.97	0.07
Standard Deviation	1.202	0.026	1.96	0.411	0.027	0.006	0.007	0.003	1.752	0.102
Variance	1.446	0.001	3.84	0.169	0.001	0	0	0	3.069	0.01
Kurtosis	17.595	161.846	12.967	5.479	18.622	6.716	7.566	3.681	6.676	14.681
Skewness	3.077	8.957	-2.194	0.302	2.612	-0.229	1.521	0.981	1.11	2.932
Range	13.02	0.61	22.27	4.4	0.32	0.06	0.057	0.017	17.46	0.85
Minimum	0.33	0.03	38.21	7.34	0.03	0	0.022	0.002	3.49	0.01
Lower Quartile	0.84	0.04	56.12	9.49	0.06	0.02	0.03	0.005	5.9	0.05
Upper Quartile	1.87	0.07	58.1	9.98	0.09	0.02	0.037	0.009	8.07	0.13
Maximum	13.35	0.64	60.48	11.74	0.35	0.06	0.079	0.019	20.95	0.86
Count	1885	1885	1885	1885	1885	1885	1885	1885	1885	1885

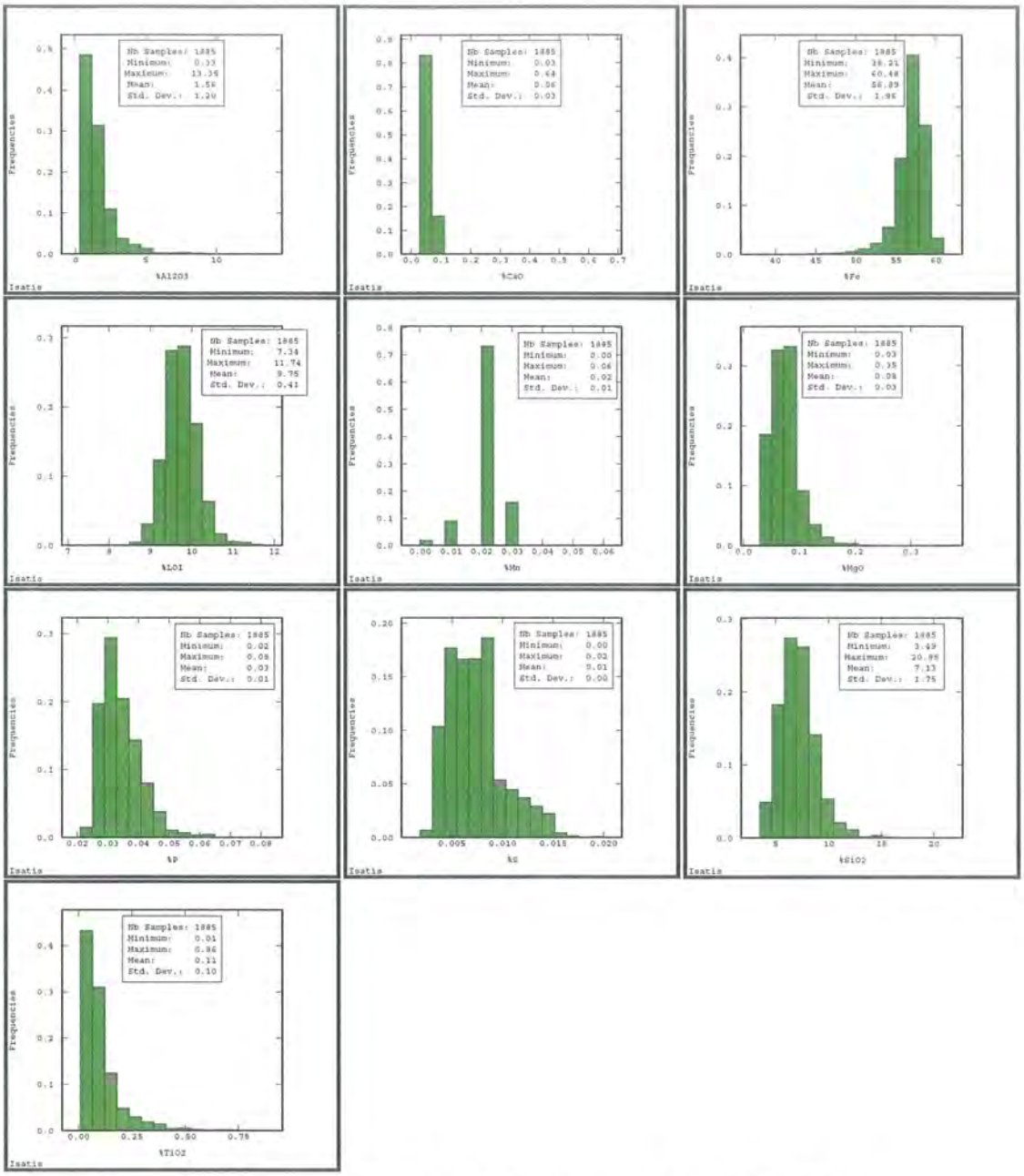

Figure 1-The histograms for each of the ten variables, in alphabetical order.

Shown in Figure 2 are the qq plots which are plotted against a lognormal distribution for all variables, except Mn which is plotted against a normal distribution. The qq plots of Al_2O_3, loss on ignition LOI and SiO_2 give the impression of following a lognormal distribution. The qq plot for Mn shows that it may be discrete while the qq plots for S, CaO, MgO and TiO_2 indicate that these variables do not follow a lognormal distribution. A χ^2 goodness of fit test with twenty two degrees of freedom, using twenty five classes was performed. The results showed that at a five percent significance level SiO_2 was the only variable which showed significant evidence that it is lognormal (experimental χ^2 (30.55) < theoretical value (33.92)).

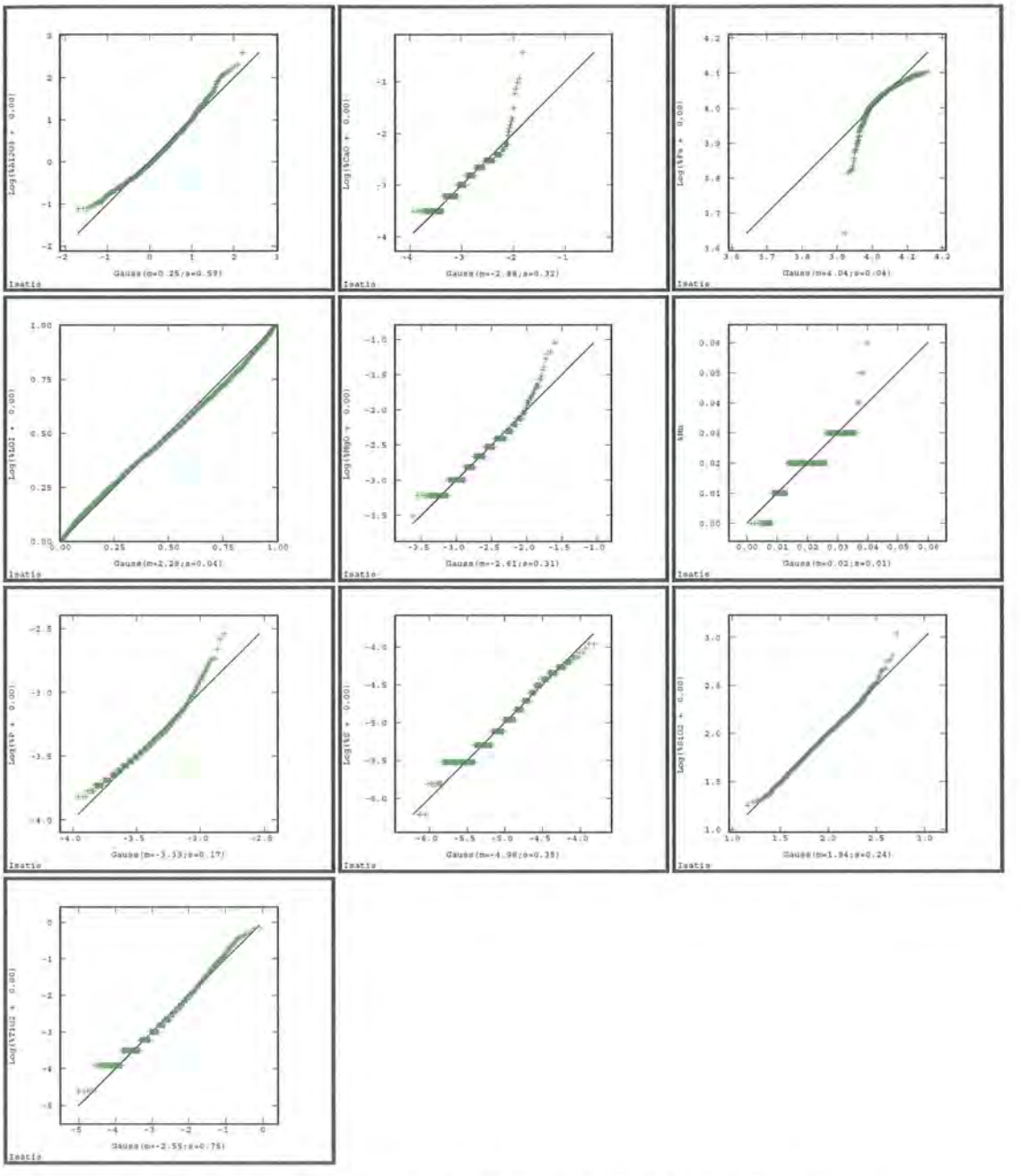

Figure 2- The qq plots for each of the ten variables, in alphabetical order.

The matrix of the correlation coefficients is shown in Table 2. The highlighted red fields indicate the variables which are highly correlated ($r > 0.7$). The highest correlation co-efficient is between Al_2O_3 and TiO_2, with a correlation of 0.916. The lowest correlation co-efficient (in terms of absolute value) is between Fe and S, with a correlation of only -0.002. S and P are poorly correlated with all the variables, while CaO is poorly correlated with all the variables, except MgO. Al_2O_3 and Fe have the highest correlation, with being moderately or highly correlated with all the variables except for CaO, S and P. Mn has a mixture of moderate and poor correlations with other variables. MgO, SiO_2 and TiO_2 have a mixture of linear correlation strengths.

Table 2- Correlation co-efficient matrix between the ten variables. The highlighted cells represent a correlation coefficient higher than 0.7.

	Al_2O_3	CaO	Fe	LOI	MgO	Mn	P	S	SiO_2	TiO_2
Al_2O_3	1	0.256	-0.85	0.51	0.583	-0.502	0.241	-0.106	0.541	0.916
CaO	0.256	1	-0.169	0.003	0.704	-0.121	-0.018	-0.402	0.089	0.176
Fe	-0.85	-0.169	1	-0.465	-0.483	0.556	0.019	-0.002	-0.882	-0.753
LOI	0.51	0.003	-0.465	1	0.248	-0.545	0.239	-0.017	0.165	0.364
MgO	0.583	0.704	-0.483	0.248	1	-0.364	0.069	-0.424	0.316	0.424
Mn	-0.502	-0.121	0.556	-0.545	-0.364	1	0.007	0.138	-0.423	-0.313
P	0.241	-0.018	0.019	0.239	0.069	0.007	1	-0.034	-0.258	0.278
S	-0.106	-0.402	-0.002	-0.017	-0.424	0.138	-0.034	1	0.067	-0.024
SiO_2	0.541	0.089	-0.882	0.165	0.316	-0.423	-0.258	0.067	1	0.471
TiO_2	0.916	0.176	-0.753	0.364	0.424	-0.313	0.278	-0.024	0.471	1

The base map showing the sample locations is displayed in Figure 3. The base map of the study region shows that some areas of the region have been sampled extensively while other areas, in particular the centre, have not been sampled as densely.

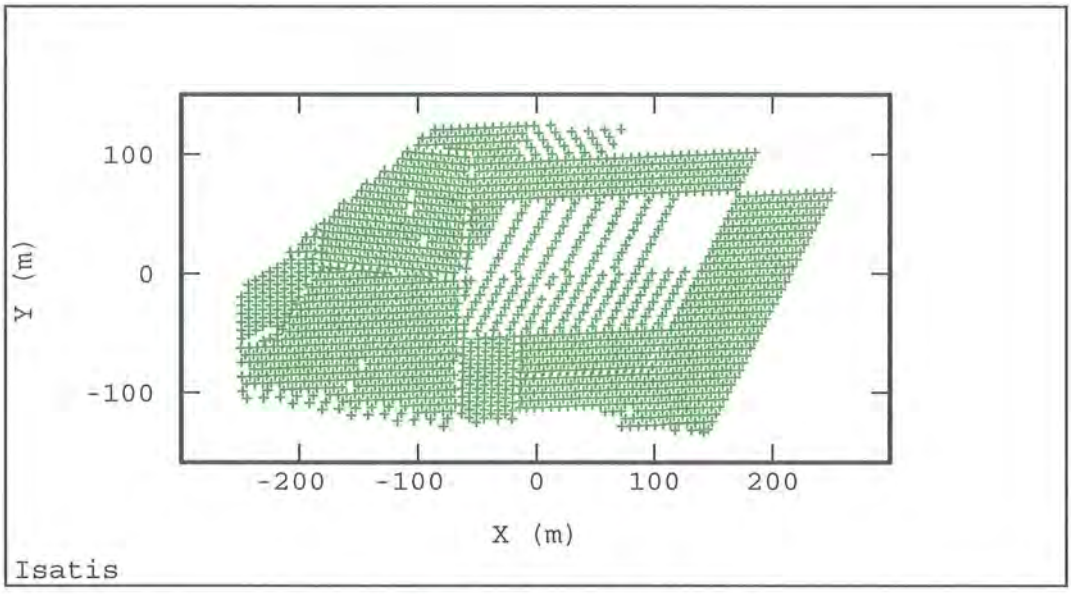

Figure 3-Base map for study region.

The spatial maps for each of the ten variables are shown in Figure 4. The colour scales were defined via the corresponding deciles for each variable, except for Mn which was based on the seven discrete values observed. The spatial map for Fe shows a region of very high values on the western border. The spatial maps for Al_2O_3, TiO_2, P and LOI do not show any distinct areas of very high or very low values. For SiO_2 lower concentrations are located on the western border. The spatial map for CaO shows that the higher values are more concentrated on the western border, while the very low values are more concentrated in an area in the south east. This is opposite for S. The

spatial map for Mn appears to have predominantly lower values. The very low values of MgO are mainly concentrated in an area in the south east of the spatial map.

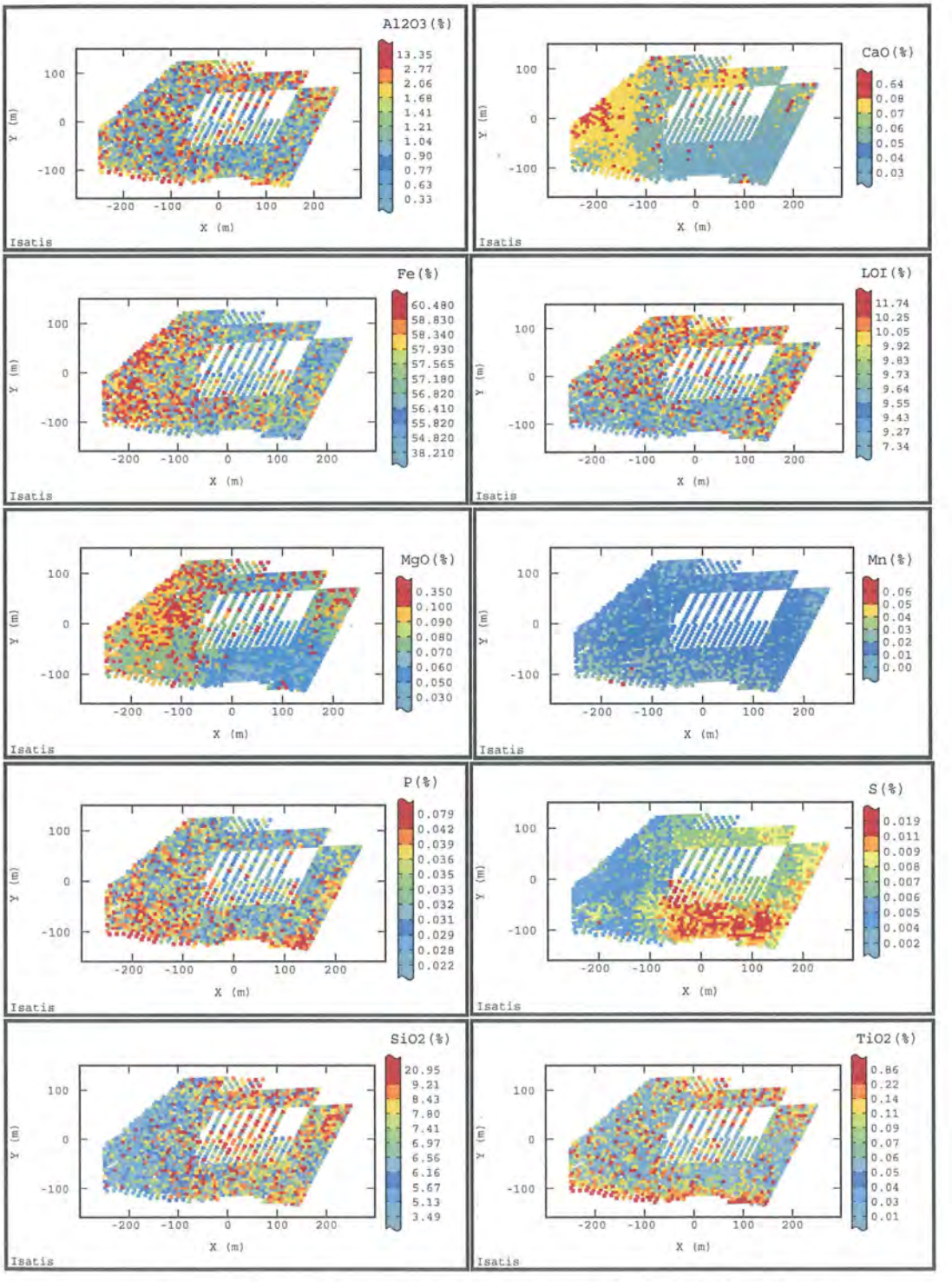

Figure 4- The spatial maps for each of the ten variables in alphabetical order.

3.3 Spatial Analysis

The experimental semivariogram maps for each of the ten original variables were calculated in order to identify the spatial features of each of the ten variables. An average lag spacing of 15m using fifteen lags was used to obtain the experimental semivariogram maps shown in Figure 5. It is clear from the experimental semivariogram maps that the ten variables do not exhibit the same spatial behaviour. Some of the variables such as LOI, SiO_2, Al_2O_3 and Fe, appear to be isotropic or weakly anisotropic, MgO and CaO appear to exhibit stronger anisotropy than LOI, SiO_2, Al_2O_3 and Fe. The variables which exhibit the strongest anisotropy are Mn, P and S. There is not a single direction of greatest continuity instead the direction of greatest continuity varies from N20° to N100° depending on the variable.

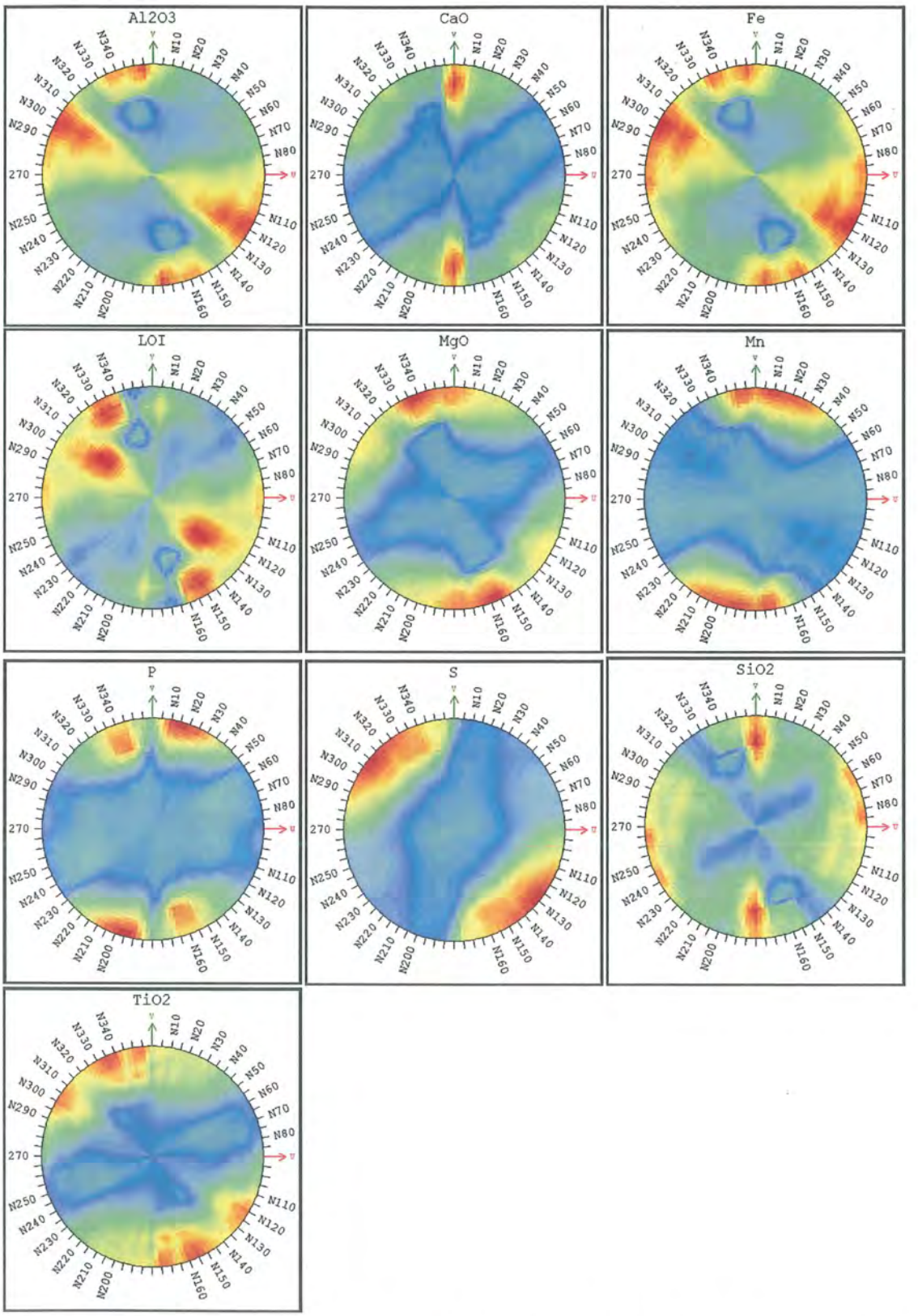

Figure 5- The spatial maps for each of the ten variables in alphabetical order. The red shows areas of high semivariances and the blue shows areas of low semivariances.

3.4 Transforming the Data Set

Two types of transformations were applied to the data set. The first was a Gaussian anamorphosis and the resultant transformation set will be denoted by subscript NS. The other transformation involved the raw data set to be standardised by subtracting the mean from each value in the variable and dividing the difference by the standard deviation. For the mean and standard deviation values used for each variable, refer to Table 1. The resultant standardised data will be denoted by subscript St. Both transformation methods are similar as they both transform the original variables into variables which have a mean close to zero and standard deviation close to one. The two transformation methods differ as standardising the raw data does not change the shape of the original distribution, while the transformation of the raw data to normal scores changes the original distribution of the variables into a normal distribution. In addition, standardisation is a linear transformation, while the Gaussian anamorphosis is non-linear. The histograms of the standardised variables are shown in Figure A1 in Appendix 1. By comparing the histograms in Figure A1 with the histograms of the raw data in Figure 1 it is clear that the shape of the distributions of the variables have not changed.

The transformation of the raw variables to normal scores was done in Isatis using Gaussian anamorphosis. The Gaussian anamorphosis fit is shown in Figure 6, while Table 3 contains the minimum, maximum and number of polynomials used for each variable, as well as the theoretical mean and variance, and the difference between the actual mean and theoretical mean. The parameters for each variable are shown in Appendix 2.1.

Table 3- Minimum, maximum and number of polynomials used for each Gaussian anamorphosis fit.

	Min	Max	Number of polynomials	Theoretical Mean	% error between Means	Theoretical Variance	% error between Variances
Al_2O_3	0	14	60	1.56	0.06406	1.445	0.06307
CaO	0	0.7	40	0.06	1.69492	0.001	32.70000
Fe	37	62	60	56.89	0.00527	3.836	0.09977
LOI	7	12	50	9.75	0.00000	0.169	0.12249
MgO	0	0.4	40	0.08	3.89610	0.001	27.80000
Mn	0	0.07	50	0.02	0.00000	0.000	0.00000
P	0	0.081	50	0.03	11.76471	0.000	0.00000
S	0	0.022	40	0.01	42.85714	0.000	0.00000
SiO_2	3	22	40	7.13	0.01402	3.067	0.06918
TiO_2	0	0.88	50	0.11	3.77358	0.010	4.00000

The criteria used to determine the number of polynomials were to compare the theoretical means and variances to the actual mean and variance, shown in Table 1 and a visual inspection of the Gaussian anamorphosis fit for each variable. The smaller the percentage error the better, however even though there appear to be a few high percentage errors the slight decrease in percentage error when using a larger number of polynomials does not warrant using the larger number of polynomials. The small percentage difference shows how similar the actual means and variances are to the theoretical mean and variance values, justifying the number of polynomials chosen. The allowable range for the transformed variable was set to [-4,4]. The histograms showing that the variables have a normal distribution with a mean of zero and standard variation of approximately one can be viewed in Figure A2 in Appendix 2.

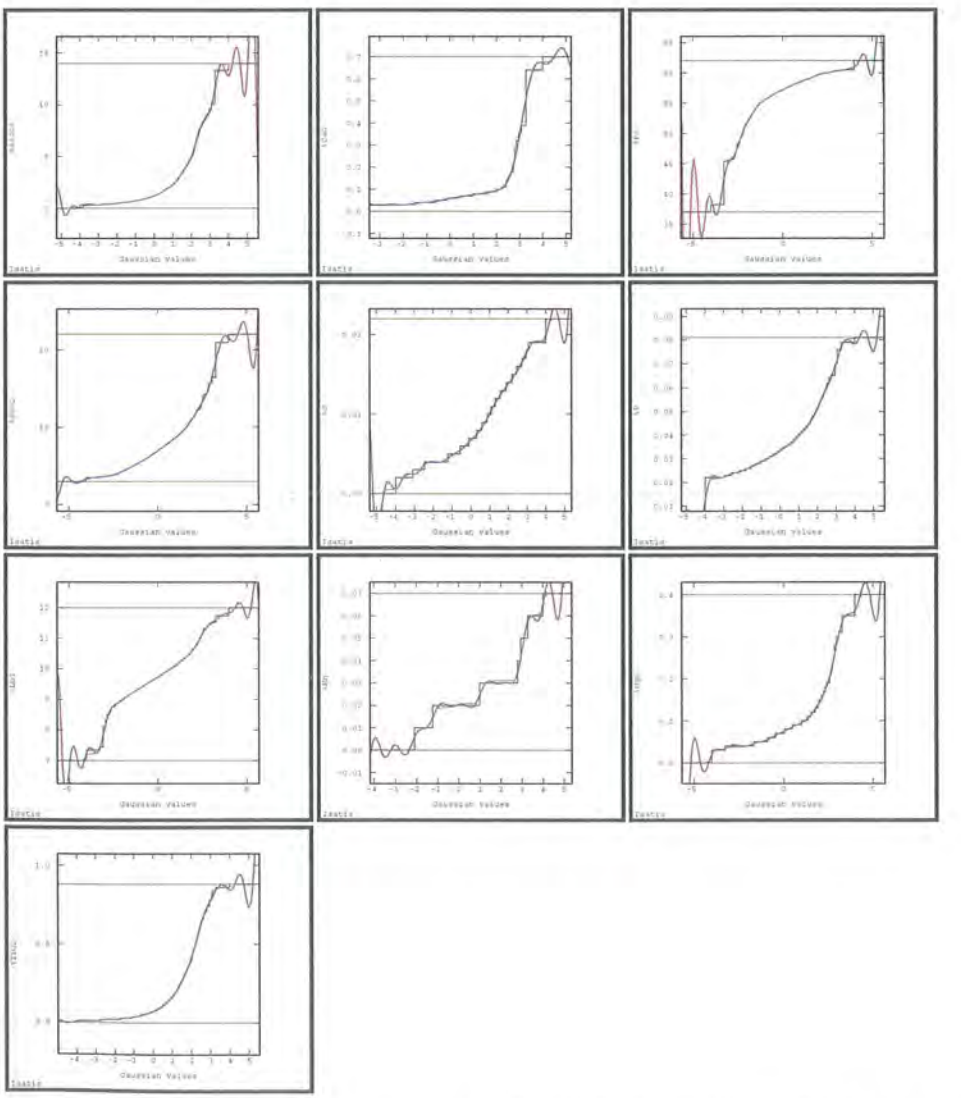

Figure 6-Gaussian anamorphosis for each of the ten variables in alphabetical order.

3.5 Subsets

The exploratory and spatial data analysis has shown how diverse the ten variables are; therefore using the MAF and ACDC algorithm on all ten variables may not be practical for simulation or kriging. Instead a subset of variables needed to be selected. As the most important variables, in terms of saleable products, are Fe, Al_2O_3 and SiO_2, the subset has to contain these three variables.

A Principal Component Analysis (PCA) and factor analysis using the correlation matrix in SPSS was performed on the ten normal score variables. The normal scores were used since the PCA and factor analysis are more robust when the distributions of the variables are normal. The scree plot and correlation circle in Figure 7 show that most of the information concerning the variability of the ten normal score variables is contained in the first two principal components. The correlation circle of the two factors shows that LOI, Al_2O_3, TiO_2 and SiO_2 are closely related. This relationship is further highlighted by the factor pattern matrix shown in Table 4. The factor pattern matrix contains the correlation coefficient between the variables and factors, therefore measuring the importance of the variables to the factors, independent of the other variables.

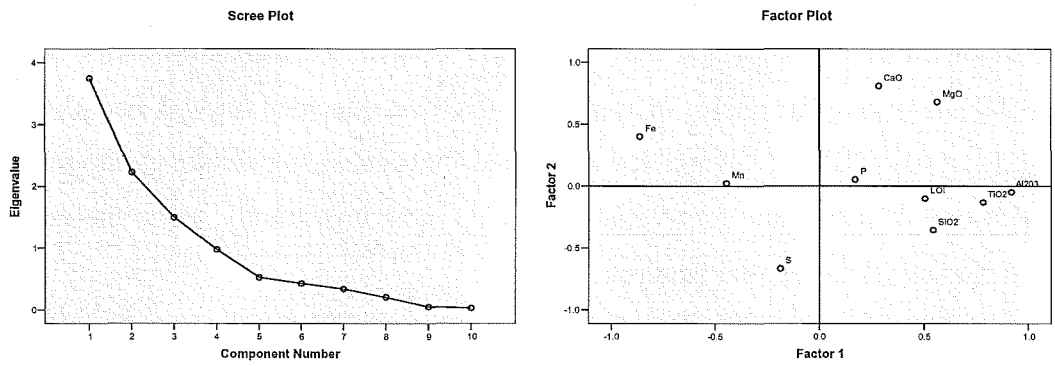

Figure 7- The scree plot (left) and correlation circle (right).

The factor pattern matrix in Table 4 has fewer loadings than the original factor matrix and therefore is easier to interpret as it only shows the highest loading for each variable. The table shows that most of the variability for Fe, Al_2O_3, TiO_2, SiO_2, LOI and Mn is present in factor one, while the variability for CaO, MgO and S can be explained in factor two. The variability of P must be explained in one of the other factors, showing that the statistical aspects of the variable are different to all the other variables. It would be logical to produce two subsets, the first subset would consist of the group of

variables similar to that shown in factor one while the other subset would consist of the variables shown in factor two, leaving P out.

Table 4- Factor pattern matrix for the two factors.

	Factor	
	1	2
Fe	-0.964	
Al_2O_3	0.879	
TiO_2	0.784	
SiO_2	0.649	
LOI	0.511	
Mn	-0.427	
P		
CaO		0.867
MgO		0.802
S		-0.702

The PCA and factor analysis is a good way to determine which variables can be grouped with each other, yet the spatial and statistical analysis has to be considered also before a subset can be decided on. The group of variables shown in factor one appears to make up a reasonable subset, with the exception of Mn. The reason for excluding Mn from the subset is that it is statistically and spatial very different from the other variables. The main concern with Mn is that it has a discrete distribution and will have many detection limit values which may affect the normal score transformation and hence the decorrelation. The subset of variables which was decided on was Fe, Al_2O_3, SiO_2, LOI and TiO_2. These five variables were choosen because they make up the most reasonable subset of more than four variables, which most importantly, show the most similarity in statistical and spatial features.

3.6 Linearity

The MAF method does not cope well with non linear correlations or poorly correlated variables (Rondón & Tran, 2008). Therefore, the correlation of the normal scores and standardised variables were checked by examining the scatter plots between the five variables in the subset, as shown in Figures 8 and 9. The corresponding correlation coefficients are displayed in Table 5 and Table 6. The scatter plots and correlation coefficients indicate varying degrees of linearity in the bivariate relationships between the five variables. Linearity between the variables is better shown on the scatter plots between the normal score variables than the scatter plots of the standardised variables. The reason for this is that the normal score variables no longer have the extreme values that the standardised variables have, as the presence of extreme values affects the correlation coefficients and the shape of the scatter diagrams.

Table 5- The correlation coefficients for the five transformed normal scores.

NS	Al_2O_3	Fe	SiO_2	TiO_2	LOI
Al_2O_3	1	-0.70229	0.3954	0.92189	0.52522
Fe	-0.70229	1	-0.88765	-0.66213	-0.43529
SiO_2	0.3954	-0.88765	1	0.39257	0.13802
TiO_2	0.92189	-0.66213	0.39257	1	0.3887
LOI	0.52522	-0.43529	0.13802	0.3887	1

Table 6- The correlation coefficients for the five standardised variables.

St	Al_2O_3	Fe	SiO_2	TiO_2	LOI
Al_2O_3	1	-0.84969	0.54139	0.91626	0.51003
Fe	-0.84969	1	-0.88243	-0.75286	-0.46455
SiO_2	0.54139	-0.88243	1	0.47099	0.16513
TiO_2	0.91626	-0.75286	0.47099	1	0.36436
LOI	0.51003	-0.46455	0.16513	0.36436	1

There is little difference in the correlation coefficients between the normal score variables and standardised variables. Both of the tables show LOI to have the poorest correlation with the other variables. This is further illustrated by the weak linear relationship in the scatter plots which involve LOI. The scatter plots of SiO_2 with TiO_2 and Al_2O_3 also show only weak correlation. The correlation coefficient between Al_2O_3 and Fe show the two variables to have a strong negative relationship; however the scatter plot between the two variables does not appear linear, with the upper values showing a linear relationship but not the lower values.

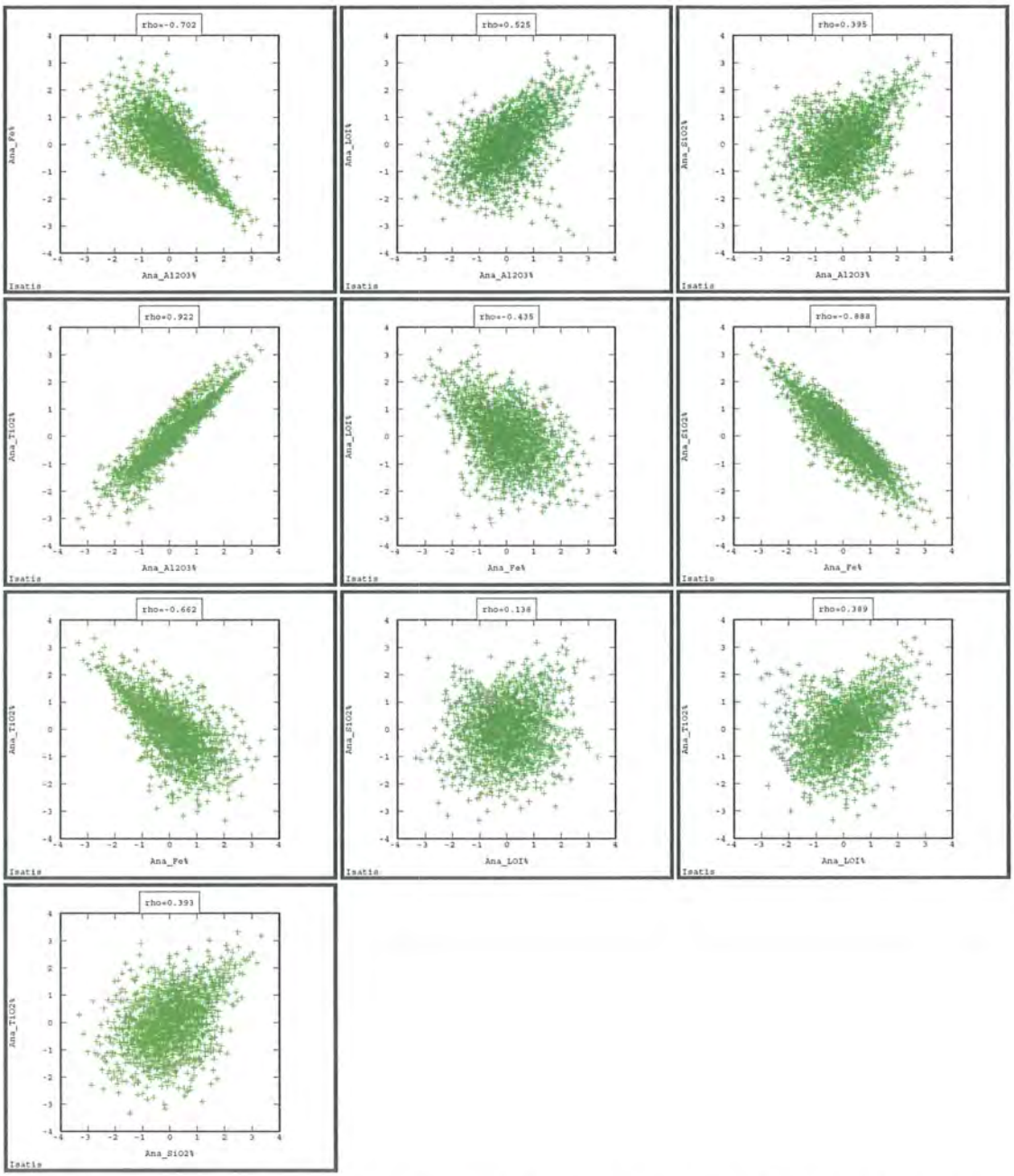

Figure 8- The scatter plots and correlation coefficients between each of the five transformed normal score variables in the subset.

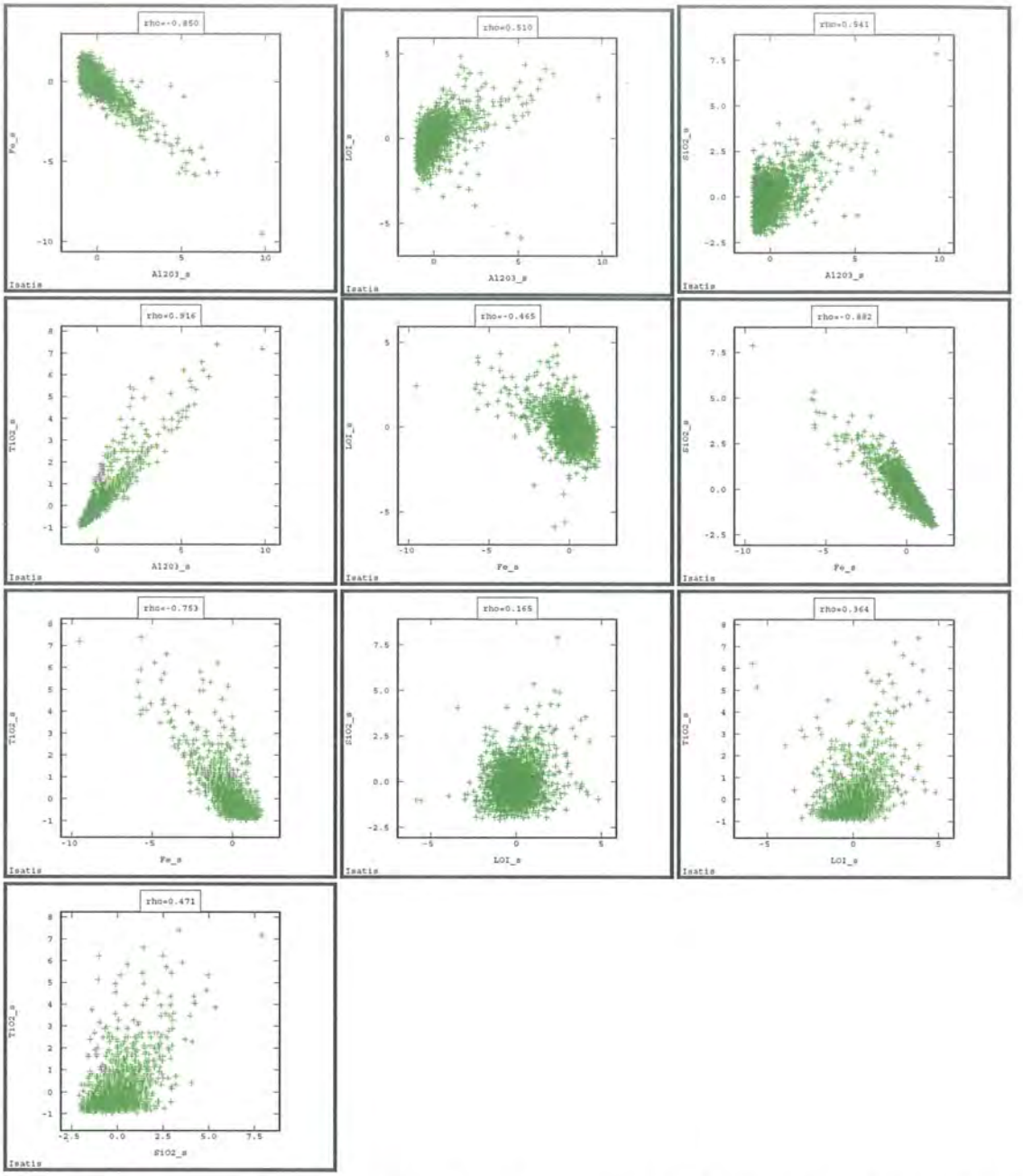

Figure 9- The scatter plots and correlation coefficients between each of the five standardised variables in the subset.

3.7 Analysis of Experimental Semivariograms.

The experimental cross semivariogram of the normal scores and standardised subset are shown in Figure 10. The figures show that the experimental cross semivariograms are correlated as expected. The experimental direct semivariogram of the normal scores and standardised subset is shown in Figure 11. A 3SLMC consisting of a nugget and two acceptable semivariogram models would be appropriate to capture the spatial variability of the variables.

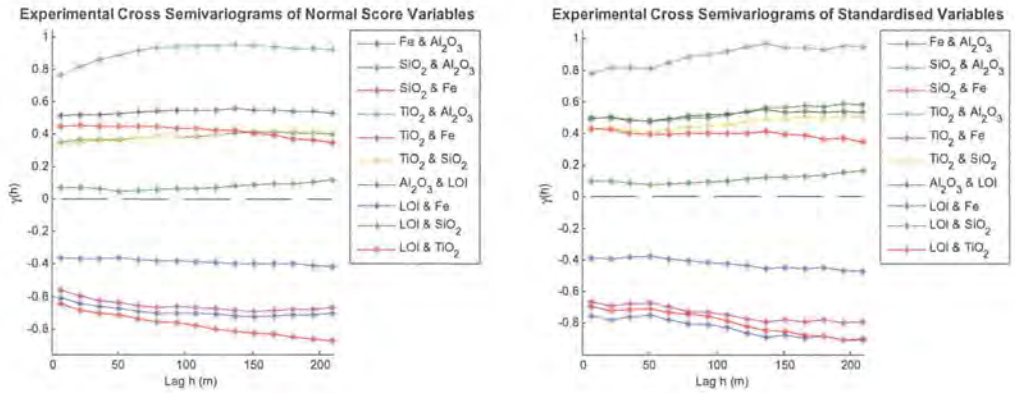

Figure 10- The experimental cross semivariograms of the five normal scores (left) and standardised (right) variables.

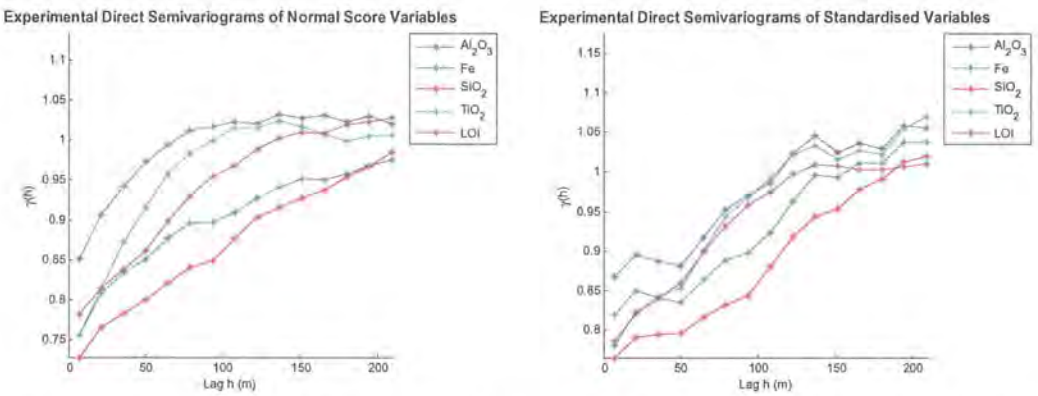

Figure 11- The experimental direct semivariograms of the five normal scores (left) and standardised (right) variables.

The average distance for each lag and experimental semivariogram matrices using the normal scores and standardised variables can be viewed in Table A1 and A2 in Appendix 3. The corresponding eigenvalues for each of the experimental semivariogram matrices are also shown in Tables A1 and A2. The eigenvalues for each experimental semivariogram matrix are positive demonstrating that the experimental semivariogram matrices, using the five normal scores and standardised variables respectively, are positive definite.

4 Results

In this chapter the results obtained throughout the study are presented. The average spatial decorrelation results, transformation matrix and analysis of the factors for each method will first be discussed separately. The final section will compare the spatial decorrelation results and experimental cross semivariograms for all the methods.

4.1 Decorrelation Results

The PCA, MAF and ACDC methods were applied to the normal scores and standardised variables for the subset, Al_2O_3, Fe, SiO_2, TiO_2 and LOI to determine which of the methods decorrelates the subset better. The factors produced from each method were assessed for spatial decorrelation using a number of criteria. These criteria include a visual assessment of the experimental cross semivariograms of the factors and plots of the absolute deviation from diagonality $\varsigma(\mathbf{h})$, the quotient of the absolute deviation from diagonality and the sum of the factor main diagonal entries $\tau(\mathbf{h})$ and the spatial diagonalisation efficiency $\kappa(\mathbf{h})$ for every lag. The final criterion is a comparison of $\bar{\zeta}$, the average absolute deviation from diagonality for all lags, $\bar{\tau}$, an average of the quotient of the absolute deviation from diagonality and the sum of the factor main diagonal entries for all lags, and $\bar{\kappa}$, the average spatial diagonalisation efficiency for all lags.

4.1.1 PCA Decorrelation Results

The PCA transformation using the normal scores and standardised scores was computed using Isatis. The correlation matrix of the normal scores is

$$B_{NS}=\begin{bmatrix} 1 & -0.702 & 0.395 & 0.922 & 0.525 \\ -0.702 & 1 & -0.888 & -0.662 & -0.435 \\ 0.395 & -0.888 & 1 & 0.393 & 0.138 \\ 0.922 & -0.662 & 0.393 & 1 & 0.389 \\ 0.525 & -0.435 & 0.138 & 0.389 & 1 \end{bmatrix}.$$

The diagonal matrix of eigenvalues $D_{PCA_{NS}}$ and matrix of eigenvectors Q_{NS} of B_{NS} are

$$D_{PCA_{NS}} = \begin{bmatrix} 3.2545 & 0 & 0 & 0 & 0 \\ 0 & 1.0122 & 0 & 0 & 0 \\ 0 & 0 & 0.6400 & 0 & 0 \\ 0 & 0 & 0 & 0.0657 & 0 \\ 0 & 0 & 0 & 0 & 0.0277 \end{bmatrix},$$

and

$$Q_{NS} = \begin{bmatrix} 0.4995 & -0.2914 & -0.3244 & 0.7085 & 0.2416 \\ -0.5131 & -0.3250 & -0.1737 & -0.1130 & 0.7670 \\ 0.3927 & 0.6743 & 0.2085 & -0.1020 & 0.5807 \\ 0.4789 & -0.2269 & -0.5185 & -0.6711 & 0.0079 \\ 0.3220 & -0.5507 & 0.7432 & -0.1566 & 0.1273 \end{bmatrix},$$

respectively. The PCA transformation matrix when using the normal score variables is the transpose of the eigenvector matrix Q and was calculated to be

$$Q_{NS}^{T} = \begin{bmatrix} 0.4995 & -0.5131 & 0.3927 & 0.4789 & 0.3220 \\ -0.2914 & -0.3250 & 0.6743 & -0.2269 & -0.5507 \\ -0.3244 & -0.1737 & 0.2085 & -0.5185 & 0.7432 \\ 0.7085 & -0.1130 & -0.1020 & -0.6711 & -0.1566 \\ 0.2416 & 0.7670 & 0.5807 & 0.0079 & 0.1273 \end{bmatrix}.$$

The histograms of the PCA factors using the normal scores subset are shown in Figure 12. The distributions of the factors do not appear to follow a normal distribution. This is supported by Kolmogorov-Smirnov statistics with a Lilliefors significance level test of normality, in Table 7, showing that there is significant evidence that the factors are not normally distributed (sig.<0.05). The scatter plots and corresponding correlation coefficients between the factors, shown in Appendix 4.1, confirm that the factors are uncorrelated.

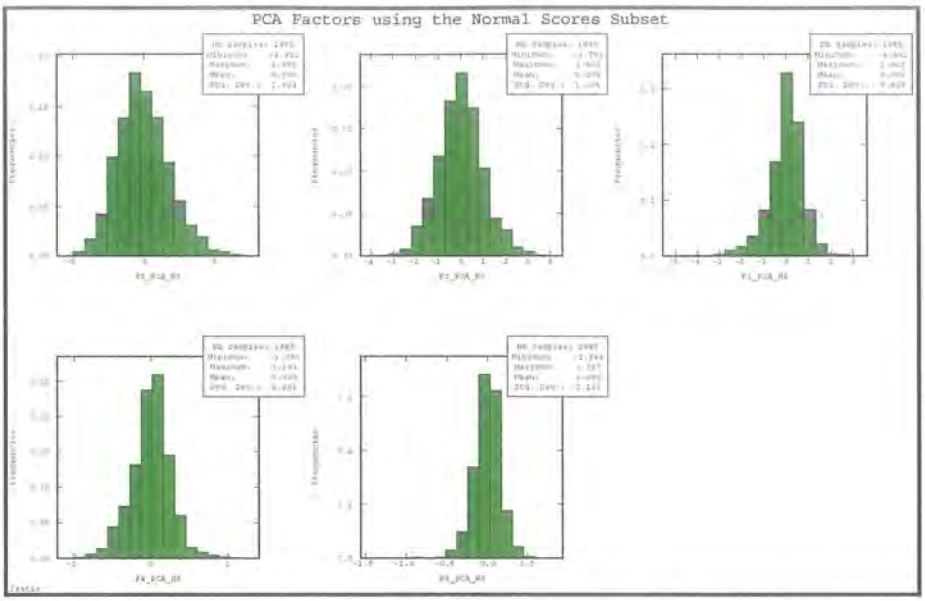

Figure 12- The histograms of the PCA factors using the normal scores subset.

Table 7- The Kolmogorov-Smirnov statistics test of normality results for all the PCA factors using the normal scores subset.

	Kolmogorov-Smirnov		
	Statistic	df	Sig.
F1_PCA_NS	0.032457	1885	0
F2_PCA_NS	0.022559	1885	0.026
F3_PCA_NS	0.084104	1885	0
F4_PCA_NS	0.047189	1885	0
F5_PCA_NS	0.037647	1885	0

The correlation matrix for the standardised scores is

$$B_{St}=\begin{bmatrix} 1 & -0.85 & 0.541 & 0.916 & 0.510 \\ -0.85 & 1 & -0.882 & -0.753 & -0.465 \\ 0.541 & -0.882 & 1 & 0.471 & 0.165 \\ 0.916 & -0.753 & 0.471 & 1 & 0.364 \\ 0.510 & -0.465 & 0.165 & 0.364 & 1 \end{bmatrix}.$$

The diagonal matrix of eigenvalues $D_{PCA_{St}}$ and matrix of eigenvectors Q_{St} of B_{St} are

$$D_{PCA_{St}}=\begin{bmatrix} 3.4632 & 0 & 0 & 0 & 0 \\ 0 & 0.8857 & 0 & 0 & 0 \\ 0 & 0 & 0.5774 & 0 & 0 \\ 0 & 0 & 0 & 0.0659 & 0 \\ 0 & 0 & 0 & 0 & 0.0078 \end{bmatrix},$$

and

$$Q_{St}=\begin{bmatrix} 0.505 & 0.1385 & -0.3394 & -0.6989 & -0.3494 \\ -0.5197 & 0.1936 & -0.2077 & 0.1586 & -0.79 \\ 0.4069 & -0.5783 & 0.467 & 0.1988 & -0.4923 \\ 0.4688 & 0.0715 & -0.5987 & 0.6455 & -0.0038 \\ 0.2992 & 0.777 & 0.5149 & 0.1736 & -0.1069 \end{bmatrix},$$

respectively. The PCA transpose matrix when using the subset which had been standardised is

$$Q_{St}^{T}=\begin{bmatrix} 0.505 & -0.5197 & 0.4069 & 0.4688 & 0.2992 \\ 0.1385 & 0.1936 & -0.5783 & 0.0715 & 0.777 \\ -0.3394 & -0.2077 & 0.467 & -0.5987 & 0.5149 \\ -0.6989 & 0.1586 & 0.1988 & 0.6455 & 0.1736 \\ -0.3494 & -0.79 & -0.4923 & -0.0038 & -0.1069 \end{bmatrix}.$$

The histograms of the PCA factors using the standardised subset are shown in Figure 13. The distributions of the factors do not appear to follow a normal distribution, with factors 1 and 3 appearing severely skewed and factors 2, 4 and 5 appearing as though they may be slightly skewed. The scatter plots and corresponding correlation coefficients between the factors, shown in Appendix 4.2, confirm that the factors are uncorrelated.

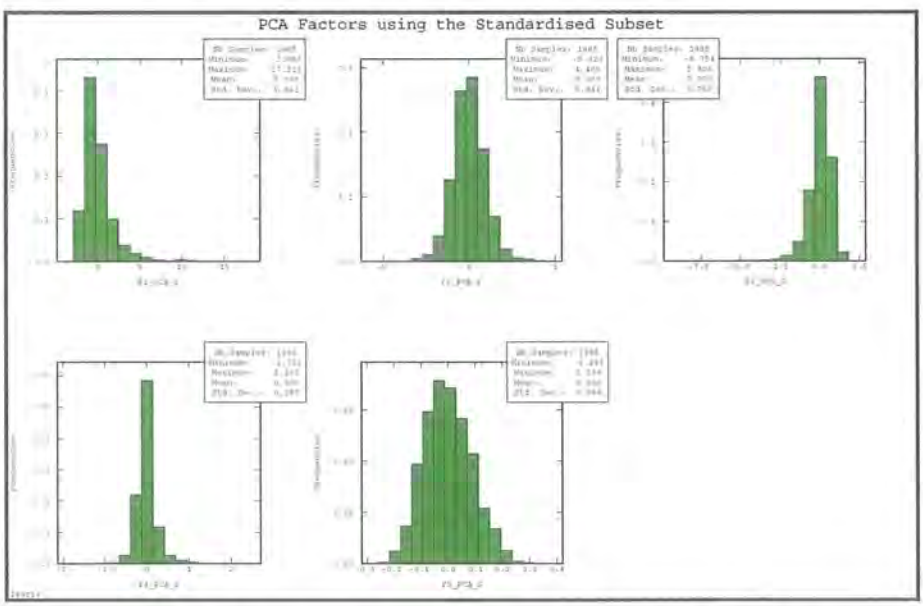

Figure 13- The histograms of the PCA factors using the standardised subset.

The measures of spatial decorrelation from the PCA transformation can be viewed in Table 8.

Table 8-The PCA average spatial decorrelation measures using both the normal scores and standardised subset.

		$\bar{\zeta}$	$\bar{\tau}$	$\bar{\kappa}$
Normal Scores Subset	PCA	0.0393	0.1168	0.9938
Standardised Subset	PCA	0.0182	0.076	0.9975

4.1.2 MAF Decorrelation Results

The MAF transformation was computed using Isatis. The MAF was performed using the corresponding correlation matrix and the experimental semivariogram matrix for a lag spacing of 15m. The correlation matrix of the normal scores used in the MAF method is denoted as B_{NS} and the correlation matrix for the standardised score is denoted as B_{St}. The choice of 15m was made because this lag spacing best reflected the data spacing. The experimental variance/covariance matrix of the normal scores for a lag spacing of 15m (**h**=15m) used in the MAF is

$$\hat{C}(\mathbf{h})_{NS}=\begin{bmatrix} 1.81595 & -1.29358 & 0.72332 & 1.63417 & 1.03795 \\ -1.29358 & 1.61754 & -1.36892 & -1.19928 & -0.73897 \\ 0.72332 & -1.36892 & 1.53154 & 0.69563 & 0.144 \\ 1.63417 & -1.19928 & 0.69563 & 1.63087 & 0.90966 \\ 1.03795 & -0.73897 & 0.144 & 0.90966 & 1.63043 \end{bmatrix},$$

and the experimental variance/covariance matrix for the standardised scores is

$$\hat{C}(\mathbf{h})_{St}=\begin{bmatrix} 1.78711 & -1.55377 & 1.00519 & 1.62297 & 0.99212 \\ -1.55377 & 1.69742 & -1.43589 & -1.37398 & -0.78994 \\ 1.00519 & -1.43589 & 1.58067 & 0.8607 & 0.19738 \\ 1.62297 & -1.37398 & 0.8607 & 1.64359 & 0.8461 \\ 0.99212 & -0.78994 & 0.19738 & 0.8461 & 1.64241 \end{bmatrix}.$$

The MAF transformation matrix for the normal scores subset is

$$X_{NS}^{T}=\begin{bmatrix} -1.3636 & 1.8751 & 0.0589 & 1.9508 & -0.9432 \\ -0.4533 & 0.8892 & -4.0597 & 0.9263 & -1.8273 \\ -0.6262 & -0.2707 & -2.9026 & 0.9741 & -1.7503 \\ 1.8943 & -1.0675 & -1.2877 & -0.7616 & 0.6582 \\ -0.6058 & -0.3019 & -1.1859 & -0.2511 & 0.475 \end{bmatrix},$$

while the MAF transformation matrix using the standardised subset is

$$X_S^T = \begin{bmatrix} -1.564 & 3.369 & -2.0569 & -2.0027 & -1.1812 \\ -0.1431 & 3.2215 & -7.8644 & -2.1563 & -2.0236 \\ -0.2403 & 1.002 & -5.0363 & -1.8031 & -1.7193 \\ 2.0505 & -1.06 & -1.0208 & 0.3565 & 0.7166 \\ -0.429 & -0.1816 & -1.6203 & -0.0204 & 0.5043 \end{bmatrix}.$$

The histograms of the MAF factors using the normal scores subset and standardised subset are displayed in Figure 14 and Figure 15, respectively. MAF factor 2 using the normal scores subset appears to be the only MAF factor which may follow a normal distribution. This is confirmed by the Kolmogorov-Smirnov statistics with a Lilliefors significance level test of normality (see Table 9) showing that at a 5% significance level there is enough evidence to suggest that factor 2 may be normally distributed (sig.>0.05). The distributions of the MAF factors using the standardised subset appear to be skewed, with factor 4 showing to be severely skewed.

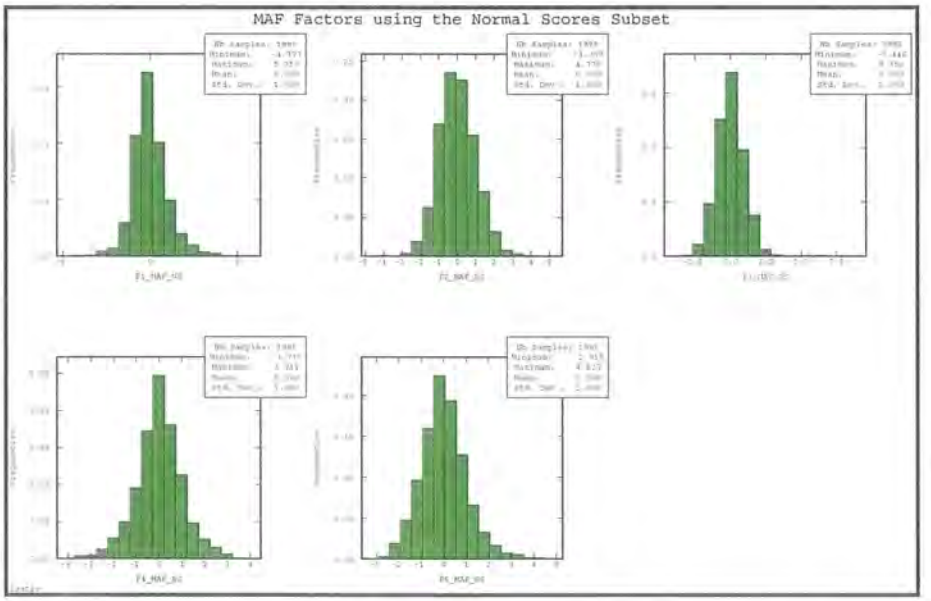

Figure 14- The histograms of the MAF factors using the normal scores subset.

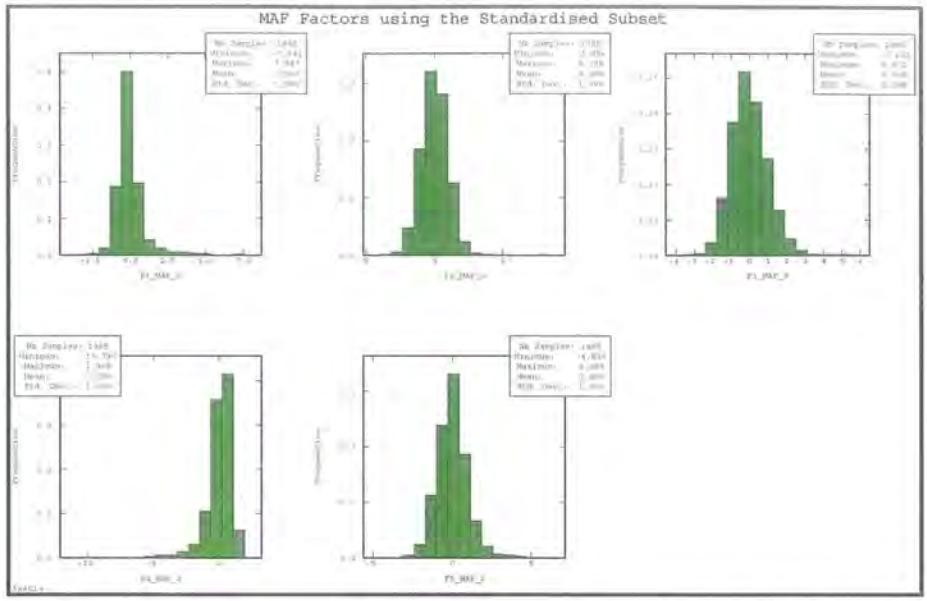

Figure 15- The histograms of the MAF factors using the standardised subset.

Table 9- The Kolmogorov-Smirnov statistics test of normality results for all the MAF factors using the normal scores subset

	Kolmogorov-Smirnov		
	Statistic	Df	Sig.
F1_MAF_NS	0.06471	1885	0
F2_MAF_NS	0.020641	1885	0.059
F3_MAF_NS	0.0309	1885	0
F4_MAF_NS	0.039033	1885	0
F5_MAF_NS	0.039735	1885	0

The scatter plots and corresponding correlation coefficients between the MAF factors using the normal scores and standardised variables are shown in Appendix 4.3 and 4.4, respectively. The scatter plots and corresponding correlation coefficients confirm that the factors are uncorrelated.

The results of the average spatial decorrelation measures for the MAF factors using the normal score subset and standardised subset are shown in Table 10. The spatial decorrelation from the MAF transformation performed better than that from PCA (Table 8) for all the measures, except for $\bar{\tau}$ using the standardised subset.

Table 10- The MAF average spatial decorrelation measures using both the normal score subset and standardised subset.

		$\bar{\zeta}$	$\bar{\tau}$	$\bar{\kappa}$
Normal Scores Subset	MAF	0.0164	0.0907	0.9976
Standardised Subset	MAF	0.0177	0.0797	0.9978

4.1.3 ACDC Decorrelation Results

The ACDC method was performed in Matlab. The target matrices to be diagonalised consisted of fifteen symmetric positive definite matrices, calculated from the experimental semivariograms of the five normal scores or standardised variables respectively using a lag spacing of 15m. The ACDC function in Matlab was executed initially using the call [A,D,Nit,Cls]=acdc(M,w,TOL), where A is the diagonalising matrix, D is the $K \times J$ matrix of diagonal values, Nit is the number of full iterations, Cls is the vector of Nit Cls values, M is the array of target matrices ($K \times K \times J$), w ($1 \times J$) is the weight vector, TOL is the tolerance which was set to $1x10^{-16}$. The initial diagonalising matrix was not specified in the call; therefore it was automatically set to the identity matrix. The ACDC function call in Matlab specifying the initial guess for the diagonalising matrix A_0, was [A,D,Nit,Cls]=acdc(M,w,TOL,A0). The original ACDC algorithm written by Yeredor (2004) was changed slightly, as the maximum number of allowed full iterations was increased from 50 to 100,000. The MATLAB code used can be viewed in Appendix 6.

The weight vector plays a significant part in the ACDC algorithm as it contains the weights assigned to the corresponding target matrices. The weight vector was used to systematically reduce the number of semivariogram matrices used in the diagonalisation. The first weight vector ensured that all fifteen target matrices were included; the next weight vector was reduced to that the first fourteen matrices were approximately simultaneously diagonalised by making the weight of the last target matrix zero. For every subsequent ACDC performed the last non zero weight was set to zero until only the first target matrix remained. This process was carried out both for the normal scores subset and standardised subset. The weight vectors and resulting values of $\bar{\zeta}$, $\bar{\tau}$ and $\bar{\kappa}$ using the normal score subset and standardised subset are summarised in Table 11 and Table 13, respectively.

With respect to $\bar{\zeta}$ and $\bar{\tau}$, the best decorrelation for ACDC using the normal scores was obtained using the first eleven semivariogram matrices, while for $\bar{\kappa}$ the use of the first thirteen semivariogram matrices yielded the best result. These values are highlighted on Table 11 by having a border around them. The percentage difference between the values for $\bar{\zeta}$, $\bar{\tau}$ and $\bar{\kappa}$ using thirteen or eleven semivariogram matrices was 117.03%, 90.86%, 0.11%, respectively. Therefore using the first eleven semivariogram matrices yielded the best results for ACDC using the normal scores. A visual inspection of the cross

semivariogram factors and spatial decorrelation plots (see Appendix 5) confirmed the conclusion. The $\bar{\tau}$ value using the first eleven semivariogram matrices is lower than the corresponding MAF $\bar{\tau}$ value ($\leq$0.0907). The $\bar{\kappa}$ using the first thirteen semivariograms is higher than the corresponding MAF $\bar{\kappa}$ value ($\geq$0.9976).

Table 11- The ACDC weights and corresponding average spatial decorrelation values using the normal scores subset. The borders indicate the best spatial decorrelation values for that column.

Number of Exp. semivariogram matrices used	Weight vector	Average Spatial Decorrelation Values		
		$\bar{\zeta}$	$\bar{\tau}$	$\bar{\kappa}$
15	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]	0.0656	0.136	0.9893
14	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 0]	0.076	0.1548	0.9874
13	[1 1 1 1 1 1 1 1 1 1 1 1 1 0 0]	0.0726	0.1567	0.9981
12	[1 1 1 1 1 1 1 1 1 1 1 1 0 0 0]	0.1361	0.1559	0.9783
11	[1 1 1 1 1 1 1 1 1 1 1 0 0 0 0]	0.019	0.0588	0.997
10	[1 1 1 1 1 1 1 1 1 1 0 0 0 0 0]	0.0507	0.1099	0.9924
9	[1 1 1 1 1 1 1 1 1 0 0 0 0 0 0]	0.0578	0.112	0.9915
8	[1 1 1 1 1 1 1 1 0 0 0 0 0 0 0]	0.0592	0.1073	0.9913
7	[1 1 1 1 1 1 1 0 0 0 0 0 0 0 0]	0.0434	0.1377	0.9937
6	[1 1 1 1 1 1 0 0 0 0 0 0 0 0 0]	0.0461	0.1125	0.9933
5	[1 1 1 1 1 0 0 0 0 0 0 0 0 0 0]	0.1188	0.16	0.9829
4	[1 1 1 1 0 0 0 0 0 0 0 0 0 0 0]	0.0677	0.1476	0.9903
3	[1 1 1 0 0 0 0 0 0 0 0 0 0 0 0]	0.0938	0.1727	0.9865
2	[1 1 0 0 0 0 0 0 0 0 0 0 0 0 0]	0.3753	0.398	0.9458
1	[1 0 0 0 0 0 0 0 0 0 0 0 0 0 0]	0.2839	0.251	0.959

For ACDC the transformation matrix is the inverse of the diagonalising matrix A. The ACDC transformation matrix using the normal scores subset and including the first eleven matrices is given as

$$A_{NS}^{-1}=\begin{bmatrix} 1.584 & -0.4104 & -0.0845 & -1.025 & -0.5786 \\ 0.606 & 2.2174 & 1.3374 & 0.4762 & 0.3463 \\ -1.4133 & -3.0201 & -2.6701 & 0.8501 & 0.7002 \\ -2.5549 & -1.8318 & -1.5408 & 2.6954 & -0.9458 \\ -1.7193 & 1.9411 & 2.9292 & 1.6409 & 1.2326 \end{bmatrix}.$$

The histograms of the corresponding factors are displayed in Figure 16. The distributions of the factors do not appear to be normal. This is supported by Kolmogorov-Smirnov statistics with a Lilliefors significance level test of normality, in Table 12, showing that there is significant evidence that the factors are not normally distributed (sig.<0.05). The scatter plots and corresponding correlation coefficients between the factors, shown in Appendix 4.5, confirm that the factors are uncorrelated.

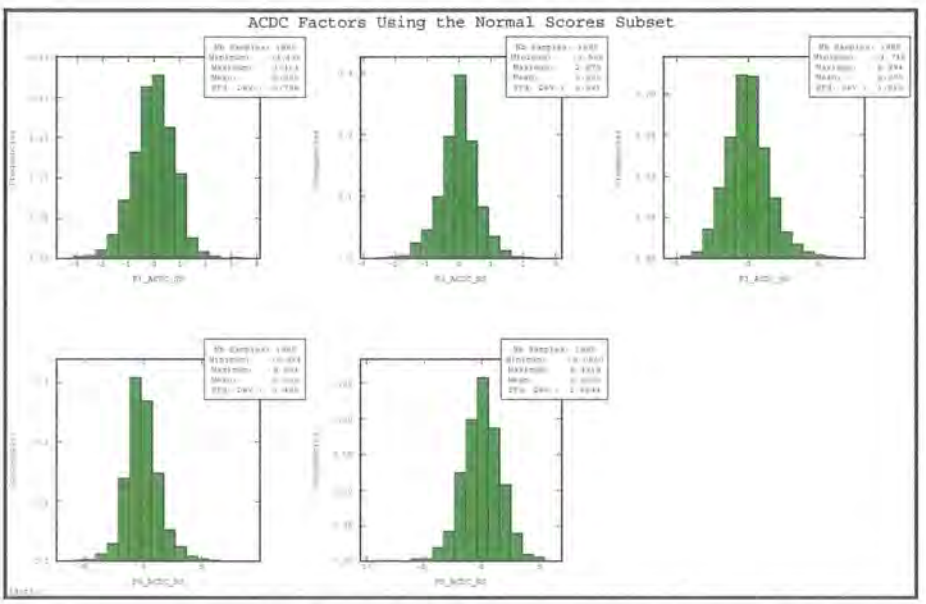

Figure 16- The histograms of the ACDC factors using the normal scores subset and first eleven experimental semivariogram matrices.

Table 12- The Kolmogorov-Smirnov statistics test of normality results for all the ACDC factors using the normal scores subset and first eleven experimental semivariogram matrices.

	Kolmogorov-Smirnov		
	Statistic	Df	Sig.
F1_ACDC_NS	0.025149	1885	0.008
F2_ACDC_NS	0.044756	1885	0
F3_ACDC_NS	0.044239	1885	0
F4_ACDC_NS	0.054831	1885	0
F5_ACDC_NS	0.022927	1885	0.022

With respect to $\bar{\zeta}$ and $\bar{\kappa}$, the best decorrelation for ACDC using the five standardised variables was obtained using the first seven semivariogram matrices, while for $\bar{\tau}$ the use of the first nine semivariograms yielded the best result. The percentage difference between the values for $\bar{\zeta}$, $\bar{\tau}$ and $\bar{\kappa}$ using seven or nine semivariogram matrices was 15.51%, 17.6% and 0.08%, respectively. A visual inspection of the experimental cross semivariogram factors and spatial decorrelation plots (see Appendix 5) between using seven or nine semivariogram matrices showed the decorrelation using seven semivariogram matrices to be better than that using nine semivariogram matrices. Therefore using the first seven semivariogram matrices yielded the best results for ACDC using the five standardised variables. None of three average spatial decorrelation values in Table 13 were better than the corresponding MAF average spatial

decorrelation values, therefore the MAF method is the better method when using just the standardised variables.

Table 13- The ACDC weights and corresponding average assessment values using the standardised subset. The borders indicate the best spatial decorrelation values for that column.

Number of Exp. semivariogram matrices used	Weight vector	Average Spatial Decorrelation Values		
		$\bar{\zeta}$	$\bar{\tau}$	$\bar{\kappa}$
15	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]	758480	1.8403	-100410
14	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 0]	11948000	0.8145	-1582100
13	[1 1 1 1 1 1 1 1 1 1 1 1 1 0 0]	105820000	0.7761	-14008000
12	[1 1 1 1 1 1 1 1 1 1 1 1 0 0 0]	21018000	0.7986	-2781900
11	[1 1 1 1 1 1 1 1 1 1 1 0 0 0 0]	0.4708	0.3566	0.9364
10	[1 1 1 1 1 1 1 1 1 1 0 0 0 0 0]	0.2866	0.2218	0.9618
9	[1 1 1 1 1 1 1 1 1 0 0 0 0 0 0]	0.0382	0.0793	0.9951
8	[1 1 1 1 1 1 1 1 0 0 0 0 0 0 0]	0.0394	0.0997	0.9952
7	[1 1 1 1 1 1 1 0 0 0 0 0 0 0 0]	0.0327	0.0946	0.9959
6	[1 1 1 1 1 1 0 0 0 0 0 0 0 0 0]	0.0379	0.1118	0.9954
5	[1 1 1 1 1 0 0 0 0 0 0 0 0 0 0]	0.0686	0.1083	0.992
4	[1 1 1 1 0 0 0 0 0 0 0 0 0 0 0]	0.1138	0.1738	0.9867
3	[1 1 1 0 0 0 0 0 0 0 0 0 0 0 0]	0.193	0.2137	0.977
2	[1 1 0 0 0 0 0 0 0 0 0 0 0 0 0]	0.2199	0.2534	0.974
1	[1 0 0 0 0 0 0 0 0 0 0 0 0 0 0]	0.3312	0.2716	0.9596

The ACDC transformation matrix

$$A_{St}^{-1}= \begin{bmatrix} 2.5068 & 4.3366 & 3.068 & -0.2417 & 0.5622 \\ -1.2471 & -7.5238 & -4.2105 & -1.7231 & -1.9398 \\ 2.7725 & 1.6742 & 0.1346 & -1.2494 & -0.326 \\ -1.2477 & -0.0761 & -0.3075 & 2.0621 & -0.6093 \\ -1.9128 & -4.9115 & -3.386 & 0.3537 & 0.0682 \end{bmatrix}$$

is the transformation matrix calculated when the ACDC method including the first seven experimental semivariogram matrices is used on the standardised subset. The histograms of the ACDC factors are displayed in Figure 17 and show all the distributions of the factors to be skewed. The scatter plots and corresponding correlation coefficients between the factors, shown in Appendix 4.6, confirm that the factors are uncorrelated.

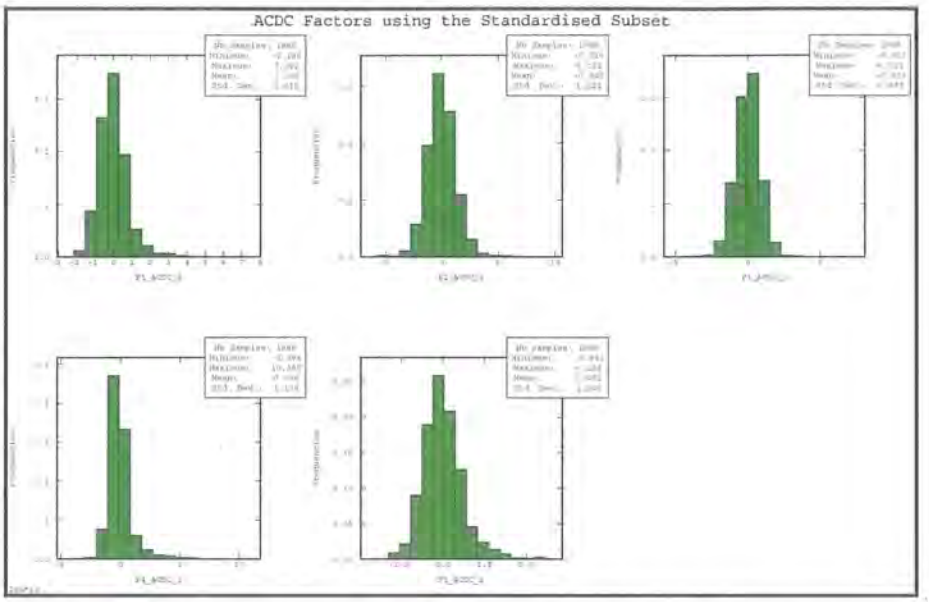

Figure 17- The histograms of the ACDC factors using the standardised subset.

The effect of using an initial guess for the diagonalising matrix A_0 with the ACDC algorithm was also explored in conjunction with changing the weights as done previously. The initial guess decided on was the eigenvector matrix obtained from the PCA using the normal scores and standardised subset. The PCA eigenvalue matrix was chosen because the transpose of the PCA already transforms the variables into approximately uncorrelated factors, therefore the ACDC method would improve on the PCA eigenvalue matrix. The PCA eigenvector matrix when using the normal score subset was calculated to be

$$A_{0_{NS}}=Q_{NS}=\begin{bmatrix} 0.4995 & -0.2914 & -0.3244 & 0.7085 & 0.2416 \\ -0.5131 & -0.3250 & -0.1737 & -0.1130 & 0.7670 \\ 0.3927 & 0.6743 & 0.2085 & -0.1020 & 0.5807 \\ 0.4789 & -0.2269 & -0.5185 & -0.6711 & 0.0079 \\ 0.3220 & -0.5507 & 0.7432 & -0.1566 & 0.1273 \end{bmatrix}.$$

The PCA eigenvector matrix using the standardised subset is

$$A_{0_{St}}=Q_{St}=\begin{bmatrix} 0.505 & 0.1385 & -0.3394 & -0.6989 & -0.3494 \\ -0.5197 & 0.1936 & -0.2077 & 0.1586 & -0.79 \\ 0.4069 & -0.5783 & 0.467 & 0.1988 & -0.4923 \\ 0.4688 & 0.0715 & -0.5987 & 0.6455 & -0.0038 \\ 0.2992 & 0.777 & 0.5149 & 0.1736 & -0.1069 \end{bmatrix}.$$

The results of the average spatial decorrelation measures using the ACDC method on either the normal scores subset or standardised subset while changing the weights, as

well as including the initial diagonalising matrix $A_{0_{NS}}$ or $A_{0_{St}}$ for the corresponding subset are shown in Table 14 and 16, respectively.

All three average spatial decorrelation results (Table 14) using the first ten, nine, six and five experimental semivariogram matrices are better than the corresponding average spatial decorelation results obtained for the MAF, shown in Table 10. In addition, the values $\bar{\zeta}$ and $\bar{\kappa}$ using thirteen, twelve, eleven and eight semivariogram matrices are better than the corresponding MAF $\bar{\zeta}$ ($\leq$0.0164) and $\bar{\kappa}$ values ($\geq$0.9976), but not for the values of $\bar{\tau}$, which was lowest using the first seven experimental semivariogram matrices. Overall, because there are so many options of good spatial decorrelations, the experimental cross semivariograms of the factors and spatial decorrelation plots were also examined to determine which number of included experimental semivariogram matrices gives the overall best ACDC spatial decorrelation using the normal scores and $A_{0_{NS}}$. The experimental cross semivariograms for every factor calculated with the corresponding spatial decorrelation plots are shown in Appendix 5. The experimental cross semivariogram factors and spatial decorrelation plots using the first ten, nine, six and five matrices were compared and the best decorrelated cross semivariogram factors resulted using the first nine semivariogram matrices. The reason for choosing the first nine experimental semivariogram matrices was because the experimental cross semivariograms of the factors appear to be more decorrelated for the first eight lags. For most of the ACDC experimental cross semivariogram factors using the matrix $A_{0_{NS}}$, there is a link between the number of experimental semivariogram matrices used for decorrelation and the number of lags showing excellent spatial decorrelation.

Table 14- The ACDC weights and corresponding average assessment values using the normal scores subset and the matrix $A_{0_{NS}}$. The borders indicate the best spatial decorrelation values for that column.

Number of Exp. semivariogram matrices used	Weight vector	Average Spatial Decorrelation Values		
		$\bar{\zeta}$	$\bar{\tau}$	$\bar{\kappa}$
15	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]	207230	1.9721	-31720
14	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 0]	0.0173	0.1633	0.9972
13	[1 1 1 1 1 1 1 1 1 1 1 1 1 0 0]	0.0139	0.1455	0.9978
12	[1 1 1 1 1 1 1 1 1 1 1 1 0 0 0]	0.013	0.1021	0.998
11	[1 1 1 1 1 1 1 1 1 1 1 0 0 0 0]	0.0117	0.0909	0.9982
10	[1 1 1 1 1 1 1 1 1 1 0 0 0 0 0]	0.0132	0.0894	0.9981
9	[1 1 1 1 1 1 1 1 1 0 0 0 0 0 0]	0.0147	0.0883	0.9979
8	[1 1 1 1 1 1 1 1 0 0 0 0 0 0 0]	0.0087	0.0934	0.9987
7	[1 1 1 1 1 1 1 0 0 0 0 0 0 0 0]	0.0172	0.0876	0.9975
6	[1 1 1 1 1 1 0 0 0 0 0 0 0 0 0]	0.0151	0.0813	0.9978
5	[1 1 1 1 1 0 0 0 0 0 0 0 0 0 0]	0.0144	0.0782	0.9979
4	[1 1 1 1 0 0 0 0 0 0 0 0 0 0 0]	0.0226	0.0933	0.9968
3	[1 1 1 0 0 0 0 0 0 0 0 0 0 0 0]	0.0338	0.1102	0.9951
2	[1 1 0 0 0 0 0 0 0 0 0 0 0 0 0]	0.0775	0.1974	0.9888
1	[1 0 0 0 0 0 0 0 0 0 0 0 0 0 0]	0.0282	0.1008	0.9959

The ACDC transformation matrix using the normal scores, $A_{0_{NS}}$ matrix and including the first nine experimental semivariogram matrices is

$$A^{-1}_{A_{0NS}\ NS} = \begin{bmatrix} 2.364 & 1.3825 & 1.5983 & -1.3335 & -0.4226 \\ 1.9548 & 3.012 & 1.2632 & -0.3682 & 0.4095 \\ -1.3222 & 0.418 & 0.1076 & 2.1648 & -0.4263 \\ -0.2409 & 0.6133 & 0.5944 & 0.3454 & 0.3787 \\ -0.003 & -1.4094 & -1.176 & -0.0893 & -0.1312 \end{bmatrix}.$$

The histograms of the factors using the normal scores subset and matrix $A_{0_{NS}}$ are shown in Figure 18. The distributions of the factors do not appear to be normal. This is supported by Kolmogorov-Smirnov statistics with a Lilliefors significance level test of normality, in Table 15, showing that there is significant evidence that the factors are not normally distributed (sig.<0.05). The scatter plots and corresponding correlation coefficients between the factors, shown in Appendix 4.7, confirm that the factors are uncorrelated.

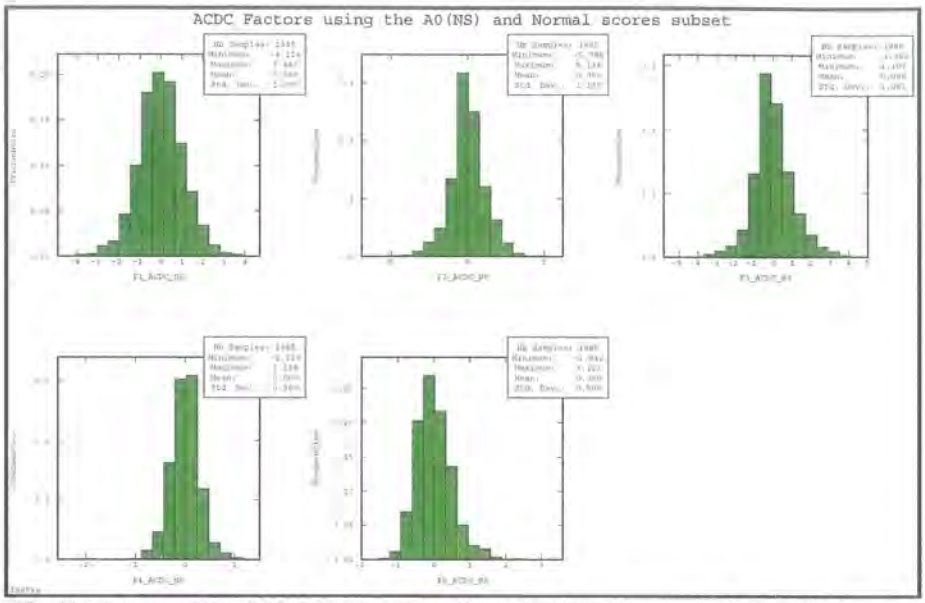

Figure 18- The histograms of the ACDC factors using the normal scores subset, the matrix $A_{0_{NS}}$ and first nine experimental semivariogram matrices.

Table 15- The Kolmogorov-Smirnov statistics test of normality results for all the ACDC factors using the normal scores subset, the matrix $A_{0_{NS}}$ and first nine experimental semivariogram matrices.

	Kolmogorov-Smirnov		
	Statistic	Df	Sig.
F1_ACDC_NS+A_0	0.024361	1885	0.011
F2_ACDC_NS+A_0	0.05146	1885	0
F3_ACDC_NS+A_0	0.063552	1885	0
F4_ACDC_NS+A_0	0.039039	1885	0
F5_ACDC_NS+A_0	0.052242	1885	0

The best spatial decorrelation measures for ACDC using the standardised variables and $A_{0_{St}}$ are obtained using the first four experimental semivariogram matrices (Table 16). The average spatial decorrelation resulting from using the first four experimental semivariogram matrices is also overall the best spatial decorrelation result achieved. The values of $\bar{\zeta}$ and $\bar{\kappa}$ using eight, six and one experimental semivariogram matrix are better than the value of $\bar{\zeta}$ ($\leq$0.0177) for MAF and the value of $\bar{\kappa}$ for MAF ($\geq$0.9978). The value of $\bar{\tau}$ using five semivariogram matrices was better than the corresponding PCA value of $\bar{\tau}$ ($\leq$0.0760).

When the matrix $A_{0_{St}}$ and the first experimental semivariogram matrix in the ACDC algorithm were used the average spatial decorrelation results were very similar to the results calculated from the MAF method used on the standardised variables.

Table 16- The ACDC weights and corresponding average assessment values using the standardised subset, the matrix A_{0St} and first four experimental semivariogram matrices. The borders indicate the best spatial decorrelation values for that column.

Number of Exp. semivariogram matrices used	Weight vector	Average Spatial Decorrelation Values		
		$\bar{\zeta}$	$\bar{\tau}$	$\bar{\kappa}$
15	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]	374650	1.8683	-49593
14	[1 1 1 1 1 1 1 1 1 1 1 1 1 1 0]	741010	1.6695	-98073
13	[1 1 1 1 1 1 1 1 1 1 1 1 1 0 0]	1250500	1.4464	-165470
12	[1 1 1 1 1 1 1 1 1 1 1 1 0 0 0]	1321300	1.0632	-174780
11	[1 1 1 1 1 1 1 1 1 1 1 0 0 0 0]	152240	1.1424	-20134
10	[1 1 1 1 1 1 1 1 1 1 0 0 0 0 0]	0.0432	0.2018	0.9943
9	[1 1 1 1 1 1 1 1 1 0 0 0 0 0 0]	0.0256	0.0916	0.9964
8	[1 1 1 1 1 1 1 1 0 0 0 0 0 0 0]	0.0103	0.0823	0.9986
7	[1 1 1 1 1 1 1 0 0 0 0 0 0 0 0]	0.0186	0.0922	0.9975
6	[1 1 1 1 1 1 0 0 0 0 0 0 0 0 0]	0.0153	0.0956	0.9981
5	[1 1 1 1 1 0 0 0 0 0 0 0 0 0 0]	0.0203	0.0729	0.9976
4	[1 1 1 1 0 0 0 0 0 0 0 0 0 0 0]	0.0076	0.0612	0.9991
3	[1 1 1 0 0 0 0 0 0 0 0 0 0 0 0]	0.0201	0.082	0.9976
2	[1 1 0 0 0 0 0 0 0 0 0 0 0 0 0]	0.0219	0.1077	0.9974
1	[1 0 0 0 0 0 0 0 0 0 0 0 0 0 0]	0.0177	0.0792	0.9978

The factors of the ACDC method using the standardised subset, A_{0St} matrix and including the first four experimental semivariogram matrices were calculated using the transformation matrix

$$A^{-1}_{A_{0St}} = \begin{bmatrix} 3.2673 & 4.9355 & 3.8439 & -0.1762 & 0.9583 \\ -0.5603 & -1.8103 & -1.8559 & 0.144 & 0.3372 \\ 2.3918 & 3.5799 & 1.6771 & -0.2971 & 0.0895 \\ -0.8222 & -0.481 & -0.3298 & 0.8346 & -0.1925 \\ 0.0178 & -1.654 & -1.1417 & -0.5042 & -0.4807 \end{bmatrix}.$$

The histograms of the ACDC factors are shown in Figure 19. The distributions of factors show all the factors to be skewed with factors 1, 3 and 4 being severely skewed. The scatter plots and corresponding correlation coefficients between the factors, shown in Appendix 4.8, confirm that the factors are uncorrelated.

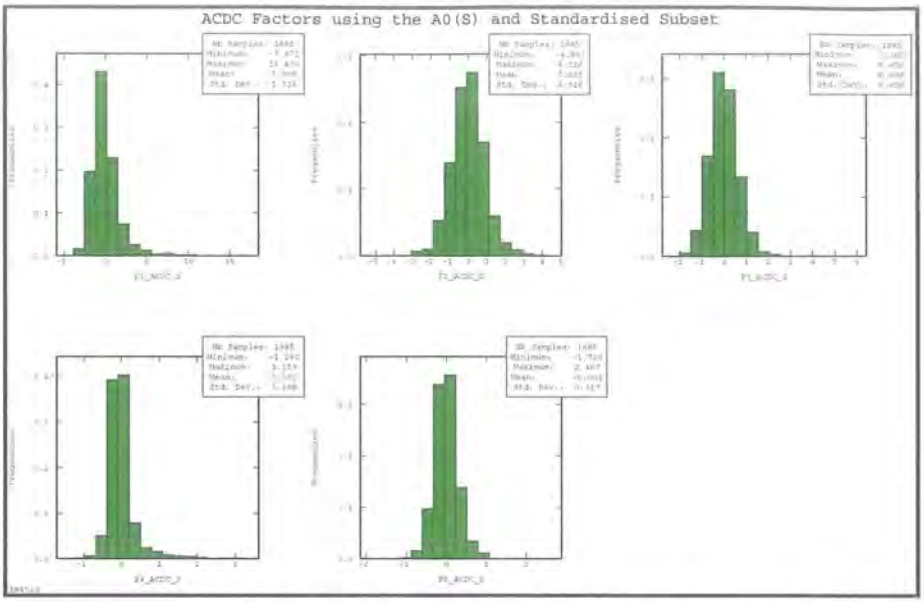

Figure 19- The histograms of the ACDC factors using the standardised subset and the matrix A_{0St}.

4.2 Comparison of Results

Graphs of all the values $\bar{\zeta}, \bar{\tau}$ and $\bar{\kappa}$ calculated from the factor semivariogram matrices that were produced by the three methods using the normal scores subset and standardised subset are shown in Figure 20. Here the values $\bar{\zeta}, \bar{\tau}$ and $\bar{\kappa}$ are treated as functions of the number of zeros in the weight vector. The three graphs on the left correspond to the normal scores, those to the right corresponds to standardised variables. The graphs in Figure 20 further illustrate the best spatial decorrelation discussed in the previous section for each different ACDC method performed.

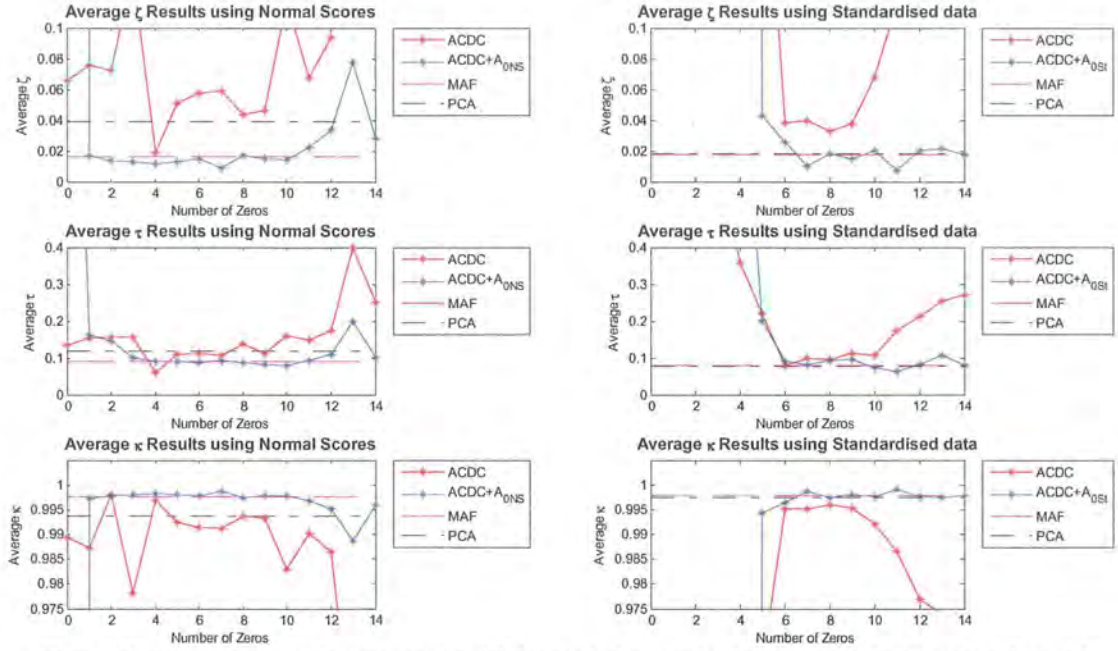

Figure 20- The plots of all the average spatial decorrelation results. The x axes title 'Number of Zeros' represent the number of zeros present in the weight vector, as shown in Tables 11, 13, 14 and 16.

In general, the decorrelation results for ACDC are better when the data are transformed to normal scores prior to the the application of the algorithm. For both approaches, ACDC with the use of the diagonalising matrix of the correlation matrix as the initial guess outperforms ACDC with the identity matrix as the intial diagonaliser. For the normal scores variables the ACDC method performs at least as well as MAF, as long as more than the first four experimental semivariogram matrices are used. For the standardised variables, the ACDC method shows worse decorrelation than MAF when the ACDC algorithm is initialised with the identity matrix. The performance is comparable to MAF, when the initialising matrix is the diagonalising matrix of the correlation matrix and no more than eleven experimental semivariogram matrices are used for calculating the transformation matrix. At eleven lags, most of the semivariograms and cross-variograms of most of the variables have reached the sill. The experimental cross semivariograms of the PCA and MAF factors as well as the factors of the ACDC methods which produced the best decorrelation measures are shown in Figure 21.

Perfect spatial decorrelation occurs when the experimental cross semivariogram factors are equal to zero for all lags. For PCA the spatial decorrelation is good for the majority of the factors except for two or three factor pairs which still exhibit correlation. For MAF, the spatial decorrelation is perfect at the second lag with the other lags showing slight correlation between the factor pairs. The ACDC factors which included an initial diagonalising matrix showed the best spatial decorrelation for both the normal scores and standardised scores. The best overall spatial decorrelation was obtained by the ACDC factors including the $A_{0_{St}}$ using the standardised subset, while the worst spatial decorrelation was shown by the experimental cross semivariogram factors for the ACDC factors pairs using the standardised subset.

The plots of the corresponding measures of spatial decorrelation ($\zeta(\mathbf{h}), \tau(\mathbf{h})$ and $\kappa(\mathbf{h})$) are displayed in Figure 22. The plots of $\kappa(\mathbf{h})$ appear to be very similar for all the plots. The MAF spatial decorrelation plot for $\zeta(\mathbf{h})$ and $\tau(\mathbf{h})$ is perfect at the second lag with a slight increase occurring after the eleventh lag. For all the MAF and ACDC $\zeta(\mathbf{h})$ and $\tau(\mathbf{h})$ plots, the values of $\zeta(\mathbf{h})$ and $\tau(\mathbf{h})$ increase after the eleventh lag and eighth lag for the ACDC using the normal scores and the matrix $A_{0_{NS}}$, with varying severity of increase. The best decorrelation plot is the ACDC transformation on the standardised subset which included the matrix $A_{0_{St}}$.

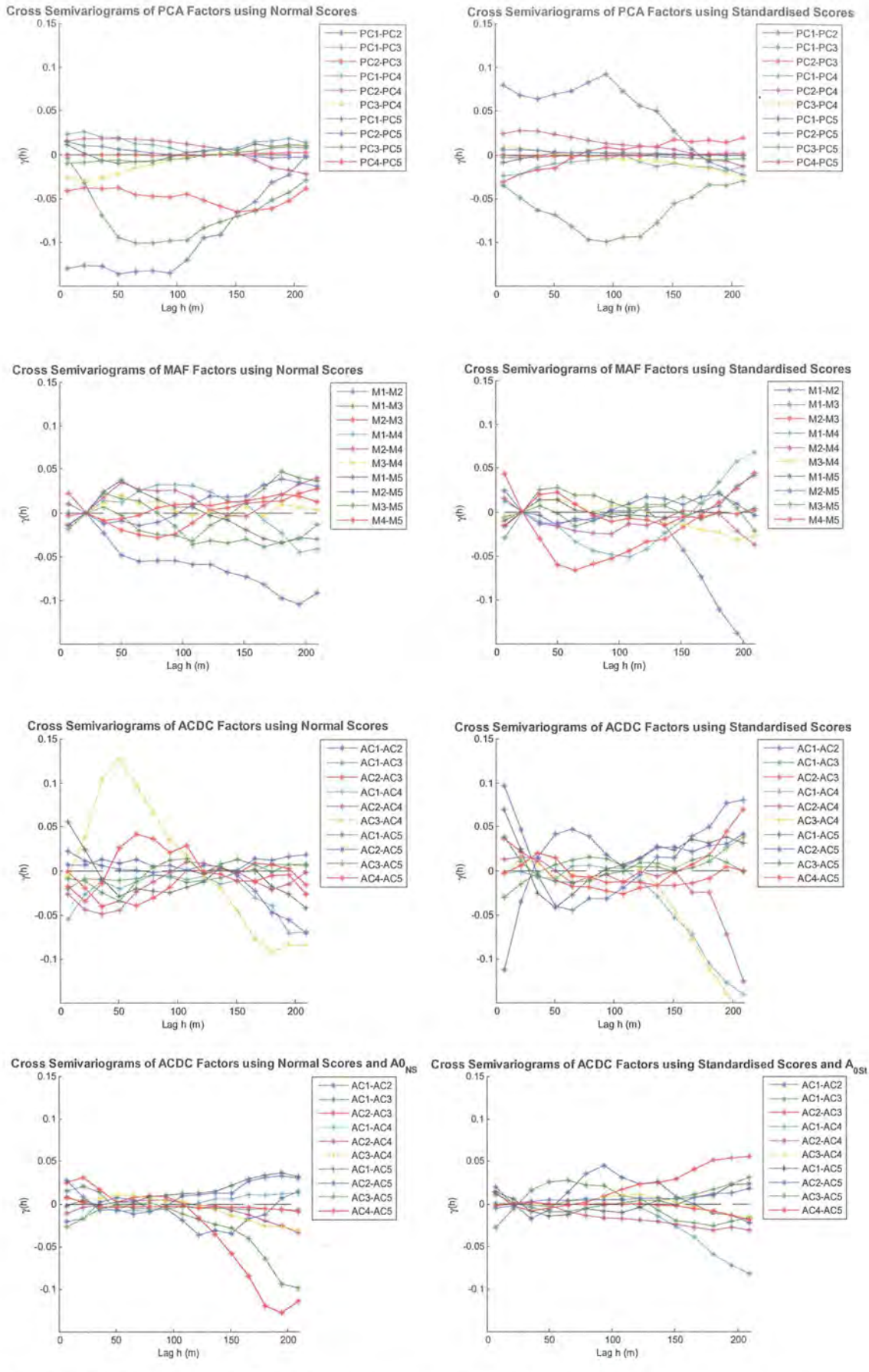

Figure 21- The experimental cross semivariograms of the factors obtained for each of the methods

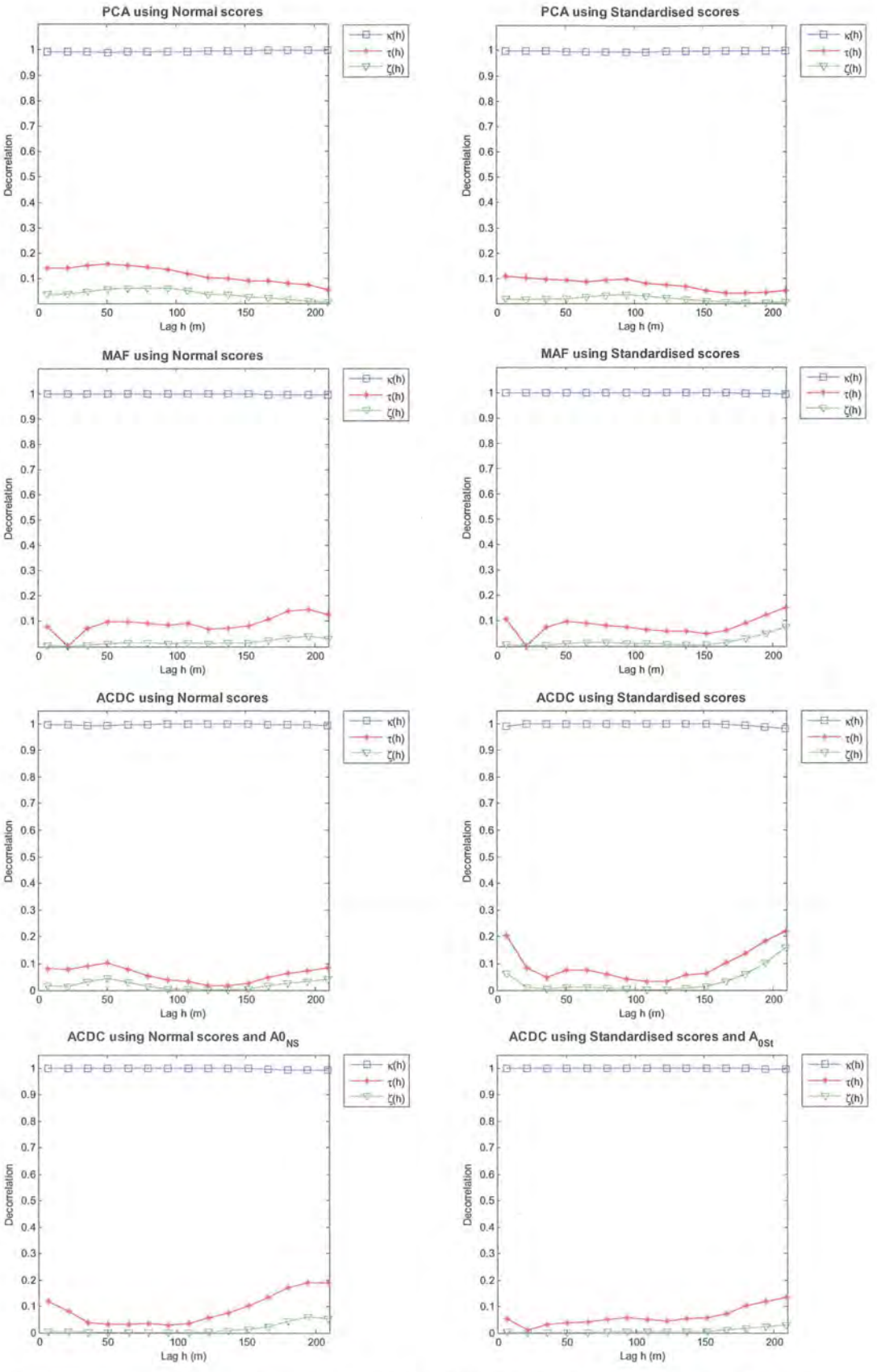

Figure 22- The plots of the spatial decorrelation ($\zeta(\mathrm{h}), \tau(\mathrm{h})$ and $\kappa(\mathrm{h})$) for every lag for all the factors.

5. Discussion and Conclusion

In this chapter the various transformation methods and effectiveness for spatial decorrelation will be reviewed, and a conclusion will be made on which of the methods seemed to be the most effective for the data set.

Linear transformation methods can be used to transform spatially correlated variables into spatially decorrelated factors which can then be modelled and simulated using univariate geostatistical techniques, which have less complexity than multivariate techniques. Linear transformation methods, such as PCA and MAF, are established techniques used for spatial decorrelation in geostatistics; however these methods have limitations, such as not performing well with poorly correlated data, which has led to the exploration of other linear transformation methods. In this thesis we looked at whether a more general and recent approach for spatial decorrelation using the ACDC method is able to decorrelate a multivariate data set of more than four variables better than the currently used MAF method. The ACDC method is appealing as it has no distributional requirements and there is no joint modelling required. In addition, we also explored whether it is beneficial to transform the variables into normal scores rather than standardised scores before decorrelating the variables.

PCA is very convenient and easy to implement, yet it is very limited as spatial decorrelation is only guaranteed when the spatial dependence of the variables under consideration can be modelled by an intrinsic model of co-regionalisation. Although, the method still provided reasonable spatial decorrelation, it may be more suited to performing multivariate data analysis prior to decorrelation via other methods (e.g. MAF or ACDC).For example, PCA was used to select the variable subset to be decorrelated, and to provide an initial guess for a diagonalising matrix in the ACDC method. The spatial decorrelation was acceptable, considering that the data are not intrinsically correlated, with only a few factor pairs showing correlation. The factors obtained from applying the PCA method on the standardised variable appeared to have better spatial decorrelation than those obtained from the PCA method using the transformed normal scores.

The MAF method has been shown to overcome the limitations of the PCA provided that the covariance function of the variables is fully characterised by a 2SLMC. In this thesis the MAF method involved an experimental variance/covariance matrix and the correlation matrix in which the factors were derived via two successive PCAs. The

spatial decorrelation obtained using MAF achieved better decorrelation results than PCA and the ACDC using the standardised variables. The MAF using the standardised variables achieved slightly better decorrelation results than the MAF using the normal scores.

The MAF method does not cope well with poor correlation and non linear correlations between variables. Poor correlation was exhibited between LOI and the other four variables; this may have affected the efficiency of the MAF method. However, the spatial decorrelation was good overall, so the impact of LOI on the results cannot have been that strong.

The ACDC method is a more general approach to the spatial decorrelation of a set of variables, and is not constrained to determining an orthogonal transformation matrix. The ACDC method was used to simultaneously approximately diagonalise a set of up to fifteen experimental semivariogram matrices calculated for lag spacings in multiples of 15m. The ACDC method showed the best and worst spatial decorrelation in comparison to PCA and MAF. The spatial decorrelation for the ACDC factors using the standardised variables showed the worst spatial decorrelation, regardless of how many experimental semivariogram matrices were included in the joint-daigonalisation. On the other hand, the ACDC factors using normal scores and including the first eleven experimental semivariogram matrices achieved better decorrelation results than the PCA and MAF factors. The best spatial decorrelation results using the standardised variables and normal scores were obtained when the initial diagonalising matrix $A_{0_{St}}$ and $A_{0_{NS}}$ were included in the ACDC method. The overall best spatial decorrelation was achieved between the ACDC factors that were calculated using the standardised variables using the ACDC method which used the diagonalising matrix $A_{0_{St}}$ of the correlation matrix and the first four experimental semivariogram matrices.

The ACDC decorrelation results using the matrix $A_{0_{St}}$ and first experimental semivariogram matrix on the standardised data set was similar to the decorrelation results obtained when the MAF method was used on the standardised variables. This is not a surprise as the matrices used in the ACDC method are similar to the matrices used in the MAF method, suggesting consistency between the ACDC method and the MAF method.

Overall, the ACDC method has been the best method to use on either transformed subsets. However, the choice of the number of experimental semivariogram matrices to include may need to be explored further, as there was no distinct pattern for the exact number of experimental semivariogram matrices that need to be included. The ACDC method is still relatively new and therefore it is unknown how the ACDC method may decorrelate large multivariate data sets consisting of a variety of variables with different statistically and spatial features.

With regard to transforming the variables before applying the transformation methods, the results for the standardised data were superior to those for the normalised data, with the exception of the ACDC method using only the standardised data. The transformation methods applied to the standardised variables achieved better spatial decorrelation than the transformation methods applied to the normal scores. This was also observed by Bandarian (2008) who applied MAF and ACDC to a subset of the Jura data set. Another reason not to transform the variables to normal scores is that the variables that were transformed to normal scores before being decorrelated, for the exception of MAF factor 2, did not yield normally distributed factors following the decorrelation. If a Gaussian algorithm is used for simulating the factors, the factors would still need to be further transformed to normal scores. Therefore the factors would have to be back-transformed three times.

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Appendices

Appendix 1 – Standardised Variables

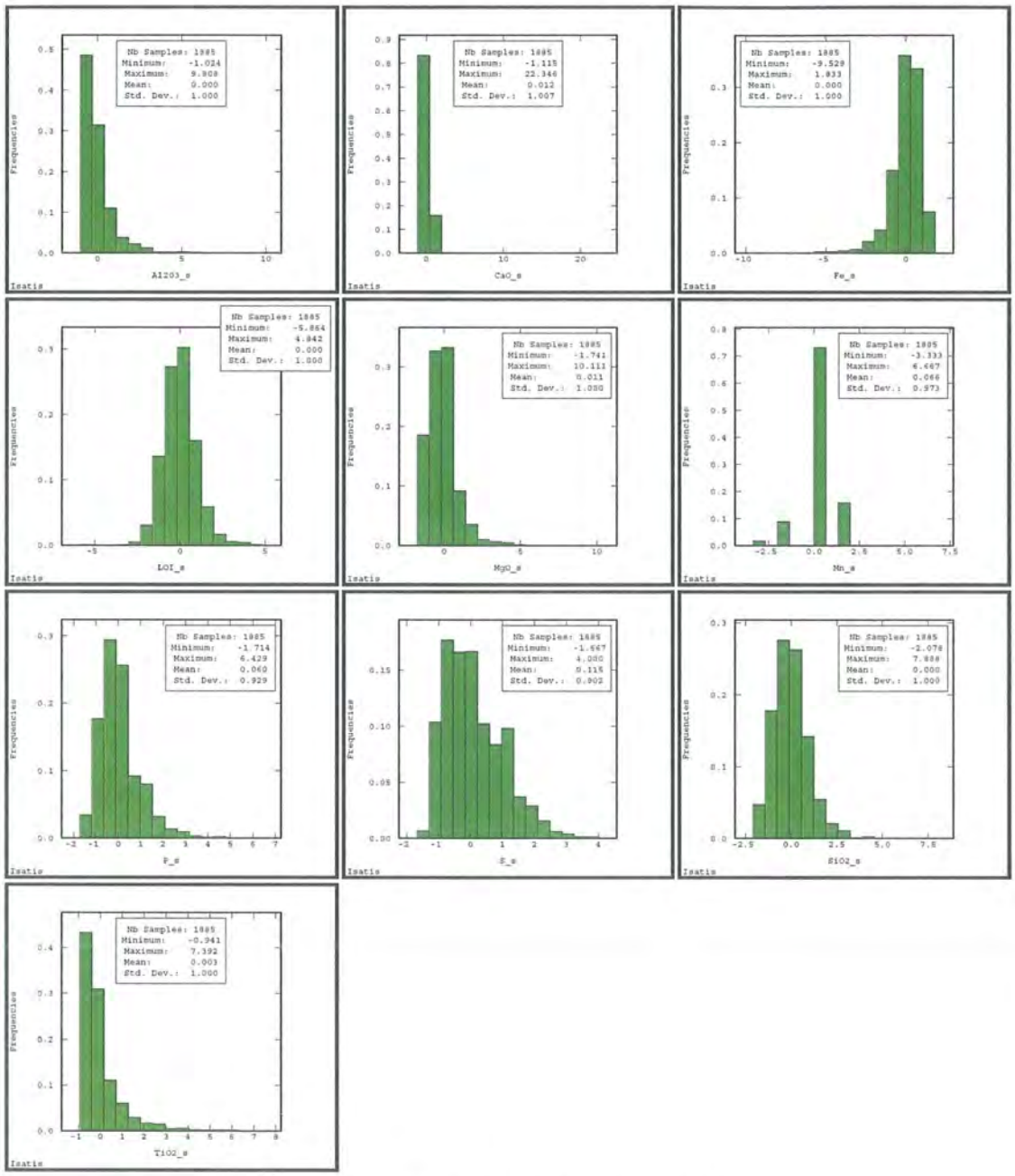


Figure A1- The histograms for the standardised variables in alphabetical order.

Appendix 2- Normal Scores

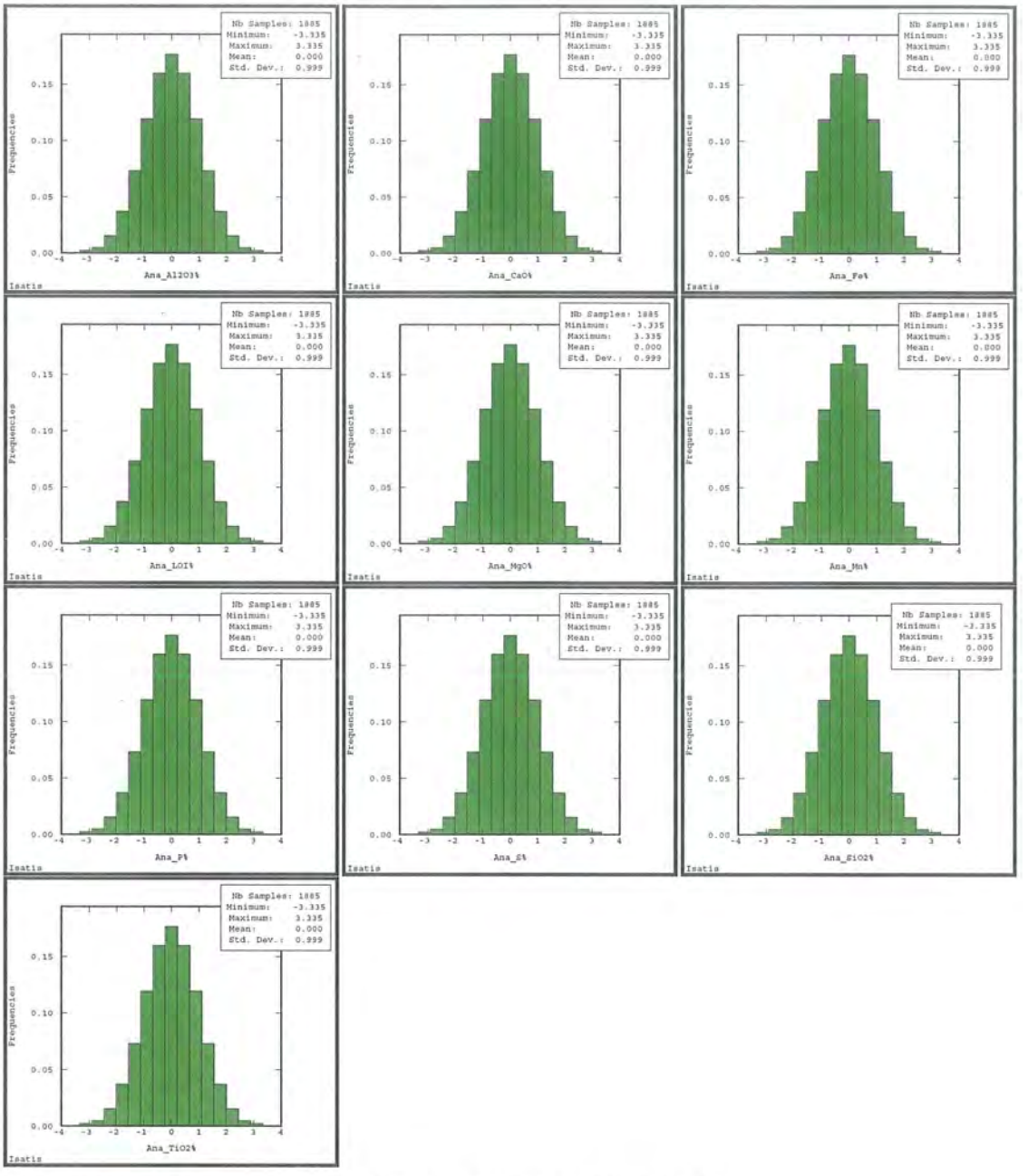


Figure A2- The histograms of the normal score variables in alphabetical order.

2.1 Anamorphosis Parameters Files

========== Parameter File Print ==========
Point Anamorphosis
==========
Number of variables = 1
Number of Polynomials = 60
Raw Variable %Al2O3 :

Distribution Type = Standard
Dispersion Law used = None
Raw Variable Format = Decimal, Length = 10, Digits = 2 (Unit: "%")
Mean (model) = 1.56%
Mean (Exp.) = 1.56%
Point Variance (model) = 1.445088
Point Variance (Exp.) = 1.445984
Gaussian Variable Name = Ana_Al2O3%
Gaussian Mean (Exp.) = 0.000
Gaussian Variance (Exp.)= 0.999
Interval of Definition:
Zmin = 0.00%
Zmax = 14.00%
Ymin = -4.645223
Ymax = 4.354389
Lower Left Control Point Y = -4.000000
Upper Right Control Point Y = 4.000000
Lower Left Control Point Z = 0.00%
Upper Right Control Point Z = 14.00%
Normalized coefficients for the Hermite polynomials:

	0	1	2	3	4
0+	1.562	-1.021	0.576	-0.248	0.045
5+	0.046	-0.054	0.017	0.016	-0.019
10+	-0.001	0.013	-0.002	-0.008	0.005
15+	0.005	-0.007	0	0.007	-0.004
20+	-0.005	0.007	0	-0.007	0.004
25+	0.004	-0.008	0	0.008	-0.005
30+	-0.006	0.009	0.002	-0.011	0.003
35+	0.01	-0.008	-0.007	0.011	0.003
40+	-0.012	0.002	0.011	-0.007	-0.009
45+	0.01	0.005	-0.012	-0.001	0.012
50+	-0.003	-0.01	0.006	0.008	-0.008
55+	-0.005	0.009	0.002	-0.008	0.001

========== End of Parameter File Print ==========

========== Parameter File Print ==========
Point Anamorphosis
==========
Number of variables = 1
Number of Polynomials = 40

Raw Variable %CaO :

Distribution Type = Standard
Dispersion Law used = None
Raw Variable Format = Decimal, Length = 10, Digits = 2 (Unit: "%")
Mean (model) = 0.06%
Mean (Exp.) = 0.06%
Point Variance (model) = 0.000673
Point Variance (Exp.) = 0.000685

Gaussian Variable Name = Ana_CaO%
Gaussian Mean (Exp.) = 0.000
Gaussian Variance (Exp.)= 0.999

Interval of Definition:
Zmin = 0.00%
Zmax = 0.70%
Ymin = -4.257693
Ymax = 4.596678

Lower Left Control Point Y = -4.000000
Upper Right Control Point Y = 4.000000
Lower Left Control Point Z = 0.00%
Upper Right Control Point Z = 0.70%
Normalized coefficients for the Hermite polynomials:

	0	1	2	3	4
0+	0.059	-0.02	0.008	-0.008	0.009
5+	-0.006	0	0.004	-0.003	0
10+	0.002	-0.002	0	0.001	-0.001
15+	0	0.001	-0.001	-0.001	0.001
20+	0	-0.001	0	0	0
25+	0	0	0	0	0
30+	0	0	0	0	0
35+	0	0	0	0	0

========== End of Parameter File Print ==========

========== Parameter File Print ==========
Point Anamorphosis
==========
Number of variables = 1
Number of Polynomials = 60

Raw Variable %Fe :

Distribution Type = Standard
Dispersion Law used = None
Raw Variable Format = Decimal, Length = 10, Digits = 2 (Unit: "%")
Mean (model) = 56.89%
Mean (Exp.) = 56.89%
Point Variance (model) = 3.836169
Point Variance (Exp.) = 3.840118

Gaussian Variable Name = Ana_Fe%
Gaussian Mean (Exp.) = 0.000
Gaussian Variance (Exp.)= 0.999
Interval of Definition:
Zmin = 37.00%
Zmax = 62.00%
Ymin = -3.776427
Ymax = 4.402786

Lower Left Control Point Y = -4.000000
Upper Right Control Point Y = 4.000000
Lower Left Control Point Z = 37.00%
Upper Right Control Point Z = 62.00%
Normalized coefficients for the Hermite polynomials:

	0	1	2	3	4
0+	56.887	-1.812	-0.628	-0.349	-0.137
5+	0.049	0.09	0.024	-0.022	-0.024
10+	0.004	0.021	-0.002	-0.021	-0.002
15+	0.017	0.009	-0.008	-0.012	-0.002
20+	0.009	0.009	-0.002	-0.012	-0.006
25+	0.009	0.011	-0.004	-0.012	-0.002
30+	0.007	0.007	0	-0.008	-0.007
35+	0.007	0.012	-0.002	-0.014	-0.003
40+	0.012	0.008	-0.007	-0.012	0
45+	0.013	0.006	-0.012	-0.012	0.008
50+	0.015	-0.003	-0.016	-0.003	0.015
55+	0.009	-0.011	-0.013	0.007	0.015

========== End of Parameter File Print ==========

========== Parameter File Print ==========
Point Anamorphosis
==========
Number of variables = 1
Number of Polynomials = 50

Raw Variable %LOI :

Distribution Type = Standard
Dispersion Law used = None
Raw Variable Format = Decimal, Length = 10, Digits = 2 (Unit: "%")
Mean (model) = 9.75%
Mean (Exp.) = 9.75%
Point Variance (model) = 0.168793
Point Variance (Exp.) = 0.168805

Gaussian Variable Name = Ana_LOI%
Gaussian Mean (Exp.) = 0.000
Gaussian Variance (Exp.)= 0.999

Interval of Definition:
Zmin = 7.00%
Zmax = 12.00%
Ymin = -4.306025
Ymax = 4.499673

Lower Left Control Point Y = -4.000000
Upper Right Control Point Y = 4.000000
Lower Left Control Point Z = 7.00%
Upper Right Control Point Z = 12.00%
Normalized coefficients for the Hermite polynomials:

	0	1	2	3	4
0+	9.75	-0.406	0.027	-0.051	-0.01
5+	-0.004	-0.011	0.013	0.012	-0.004
10+	-0.003	-0.003	-0.005	0.004	0.008
15+	-0.002	-0.006	0	0.002	0.002
20+	0.002	-0.002	-0.004	0.001	0.005
25+	0	-0.004	-0.001	0.002	0.002
30+	0	-0.001	-0.002	0	0.003
35+	0	-0.003	-0.001	0.002	0.002
40+	-0.002	-0.002	0.001	0.001	0
45+	-0.001	-0.001	0	0.001	0.001

========== End of Parameter File Print ==========

========== Parameter File Print ==========
Point Anamorphosis
==========
Number of variables = 1
Number of Polynomials = 40

Raw Variable %MgO :

Distribution Type = Standard
Dispersion Law used = None
Raw Variable Format = Decimal, Length = 10, Digits = 2 (Unit: "ppm")
Mean (model) = 0.08ppm
Mean (Exp.) = 0.08ppm
Point Variance (model) = 0.000722
Point Variance (Exp.) = 0.000730

Gaussian Variable Name = Ana_MgO%
Gaussian Mean (Exp.) = 0.000
Gaussian Variance (Exp.)= 0.999

Interval of Definition:
Zmin = 0.00ppm
Zmax = 0.40ppm
Ymin = -4.306025
Ymax = 4.402786

Lower Left Control Point Y = -4.000000
Upper Right Control Point Y = 4.000000
Lower Left Control Point Z = 0.00ppm
Upper Right Control Point Z = 0.40ppm
Normalized coefficients for the Hermite polynomials:

	0	1	2	3	4
0+	0.077	-0.024	0.009	-0.005	0.004
5+	0	-0.002	0.001	0	-0.001
10+	0	0	0	0	0
15+	0	0	0	0	0
20+	0	0	0	0	0
25+	0	0	0	0	0
30+	0	0	0	0	0
35+	0	0	0	0	0

========== End of Parameter File Print ==========

========== Parameter File Print ==========
Point Anamorphosis
==========
Number of variables = 1
Number of Polynomials = 50

Raw Variable %Mn :

Distribution Type = Standard
Dispersion Law used = None
Raw Variable Format = Decimal, Length = 10, Digits = 2 (Unit: "%")
Mean (model) = 0.02%
Mean (Exp.) = 0.02%
Point Variance (model) = 0.000032
Point Variance (Exp.) = 0.000034

Gaussian Variable Name = Ana_Mn%
Gaussian Mean (Exp.) = 0.000
Gaussian Variance (Exp.)= 0.999

Interval of Definition:
Zmin = 0.00%
Zmax = 0.07%
Ymin = -2.597642
Ymax = 4.209395

Lower Left Control Point Y = -4.000000
Upper Right Control Point Y = 4.000000
Lower Left Control Point Z = 0.00%
Upper Right Control Point Z = 0.07%
Normalized coefficients for the Hermite polynomials:

	0	1	2	3	4
0+	0.02	-0.005	0	-0.001	0
5+	0.001	0.001	-0.001	-0.001	0.001
10+	0	-0.001	0	0.001	0
15+	0	0	0	0	0
20+	0	0	0	0	0
25+	0	0	0	0	0
30+	0	0	0	0	0
35+	0	0	0	0	0
40+	0	0	0	0	0
45+	0	0	0	0	0

========== End of Parameter File Print ==========

========== Parameter File Print ==========
Point Anamorphosis
==========
Number of variables = 1
Number of Polynomials = 50

Raw Variable %P :

Distribution Type = Standard
Dispersion Law used = None
Raw Variable Format = Decimal, Length = 10, Digits = 2 (Unit: "%")
Mean (model) = 0.03%
Mean (Exp.) = 0.03%
Point Variance (model) = 0.000042
Point Variance (Exp.) = 0.000042

Gaussian Variable Name = Ana_P%
Gaussian Mean (Exp.) = 0.000
Gaussian Variance (Exp.)= 0.999

Interval of Definition:
Zmin = 0.00%
Zmax = 0.08%
Ymin = -4.354389
Ymax = 4.354389

Lower Left Control Point Y = -4.000000
Upper Right Control Point Y = 4.000000
Lower Left Control Point Z = 0.00%
Upper Right Control Point Z = 0.08%
Normalized coefficients for the Hermite polynomials:

	0	1	2	3	4
0+	0.034	-0.006	0.002	-0.001	0
5+	0	0	0	0	0
10+	0	0	0	0	0
15+	0	0	0	0	0
20+	0	0	0	0	0
25+	0	0	0	0	0
30+	0	0	0	0	0
35+	0	0	0	0	0
40+	0	0	0	0	0
45+	0	0	0	0	0

========== End of Parameter File Print ==========

========== Parameter File Print ==========
Point Anamorphosis
==========
Number of variables = 1
Number of Polynomials = 40

Raw Variable %S :

Distribution Type = Standard
Dispersion Law used = None
Raw Variable Format = Decimal, Length = 10, Digits = 2 (Unit: "%")
Mean (model) = 0.01%
Mean (Exp.) = 0.01%
Point Variance (model) = 0.000007
Point Variance (Exp.) = 0.000007

Gaussian Variable Name = Ana_S%
Gaussian Mean (Exp.) = 0.000
Gaussian Variance (Exp.)= 0.999

Interval of Definition:
Zmin = 0.00%
Zmax = 0.02%
Ymin = -4.742394
Ymax = 4.354389

Lower Left Control Point Y = -4.000000
Upper Right Control Point Y = 4.000000
Lower Left Control Point Z = 0.00%
Upper Right Control Point Z = 0.02%
Normalized coefficients for the Hermite polynomials:

	0	1	2	3	4
0+	0.007	-0.003	0.001	0	0
5+	0	0	0	0	0
10+	0	0	0	0	0
15+	0	0	0	0	0
20+	0	0	0	0	0
25+	0	0	0	0	0
30+	0	0	0	0	0
35+	0	0	0	0	0

========== End of Parameter File Print ==========

========== Parameter File Print ==========
Point Anamorphosis
==========
Number of variables = 1
Number of Polynomials = 40

Raw Variable %SiO2 :

Distribution Type = Standard
Dispersion Law used = None
Raw Variable Format = Decimal, Length = 10, Digits = 2 (Unit: "%")
Mean (model) = 7.13%
Mean (Exp.) = 7.13%
Point Variance (model) = 3.066877
Point Variance (Exp.) = 3.068877

Gaussian Variable Name = Ana_SiO2%
Gaussian Mean (Exp.) = 0.000
Gaussian Variance (Exp.)= 0.999

Interval of Definition:
Zmin = 3.00%
Zmax = 22.00%
Ymin = -4.451214
Ymax = 4.645223

Lower Left Control Point Y = -4.000000
Upper Right Control Point Y = 4.000000
Lower Left Control Point Z = 3.00%
Upper Right Control Point Z = 22.00%
Normalized coefficients for the Hermite polynomials:

	0	1	2	3	4
0+	7.131	-1.707	0.346	-0.137	0.106
5+	-0.013	-0.035	0.029	-0.009	-0.007
10+	0.005	-0.001	0.007	-0.004	-0.01
15+	0.01	0.005	-0.01	0.003	0.006
20+	-0.008	0	0.007	-0.005	-0.004
25+	0.007	-0.001	-0.006	0.004	0.003
30+	-0.006	0	0.005	-0.002	-0.003
35+	0.004	0.001	-0.003	0.001	0.002

========== End of Parameter File Print ==========

========== Parameter File Print ==========
Point Anamorphosis
==========
Number of variables = 1
Number of Polynomials = 50

Raw Variable %TiO2 :

Distribution Type = Standard
Dispersion Law used = None
Raw Variable Format = Decimal, Length = 10, Digits = 2 (Unit: "%")
Mean (model) = 0.11%
Mean (Exp.) = 0.11%
Point Variance (model) = 0.010400
Point Variance (Exp.) = 0.010412

Gaussian Variable Name = Ana_TiO2%
Gaussian Mean (Exp.) = 0.000
Gaussian Variance (Exp.)= 0.999

Interval of Definition:
Zmin = 0.00%
Zmax = 0.88%
Ymin = -4.306025
Ymax = 4.402786

Lower Left Control Point Y = -4.000000
Upper Right Control Point Y = 4.000000
Lower Left Control Point Z = 0.00%
Upper Right Control Point Z = 0.88%
Normalized coefficients for the Hermite polynomials:

	0	1	2	3	4
0+	0.106	-0.085	0.051	-0.02	0
5+	0.007	-0.005	0	0.003	-0.002
10+	0	0.001	-0.001	0	0.001
15+	0	0	0	0	0
20+	0	0	0	0	0
25+	0	0	0	0	0
30+	0	0	0	0	0
35+	0	0	0	0	0
40+	0	0	0	0	0
45+	0	0	0	0	0

========== End of Parameter File Print ==========

Appendix 3 – Average Distances, Experimental Semivariogram Matrices and Eigenvalues

Table A1- The average distance, experimental semivariogram matrices using the normal scores and corresponding eigenvalues.

Average Distance	Matrix					Eigenvalues
6.959		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.8517	-0.6108	0.3467	0.7624	0.5083	0.0188
	Fe	-0.6108	0.7558	-0.6458	-0.5632	-0.3632	0.04
	SiO_2	0.3467	-0.6458	0.7283	0.3322	0.0739	0.3217
	TiO_2	0.7624	-0.5632	0.3322	0.7568	0.4439	0.7916
	LOI	0.5083	-0.3632	0.0739	0.4439	0.782	2.7024
16.721		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.9073	-0.6464	0.3615	0.8164	0.5184	0.0222
	Fe	-0.6464	0.8083	-0.6841	-0.5992	-0.369	0.0431
	SiO_2	0.3615	-0.6841	0.7652	0.3476	0.0718	0.3577
	TiO_2	0.8164	-0.5992	0.3476	0.8147	0.4544	0.8385
	LOI	0.5184	-0.369	0.0718	0.4544	0.8145	2.8486
30.822		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.9416	-0.6642	0.3649	0.8559	0.5165	0.0252
	Fe	-0.6642	0.8345	-0.7007	-0.6238	-0.3656	0.0489
	SiO_2	0.3649	-0.7007	0.784	0.3563	0.0626	0.3959
	TiO_2	0.8559	-0.6238	0.3563	0.8722	0.449	0.8709
	LOI	0.5165	-0.3656	0.0626	0.449	0.8382	2.9296
45.331		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.9719	-0.6753	0.3637	0.8859	0.5243	0.0264
	Fe	-0.6753	0.8512	-0.7134	-0.6367	-0.3607	0.0548
	SiO_2	0.3637	-0.7134	0.7998	0.3578	0.0499	0.4208
	TiO_2	0.8859	-0.6367	0.3578	0.9154	0.4486	0.9099
	LOI	0.5243	-0.3607	0.0499	0.4486	0.8616	2.988
60.155		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.9941	-0.6928	0.3775	0.9137	0.5333	0.0271
	Fe	-0.6928	0.8779	-0.7367	-0.6559	-0.3732	0.0577
	SiO_2	0.3775	-0.7367	0.8221	0.3748	0.0551	0.4569
	TiO_2	0.9137	-0.6559	0.3748	0.9578	0.4462	0.9317
	LOI	0.5333	-0.3732	0.0551	0.4462	0.8991	3.0779

Table A1 continued- The average distance, experimental semivariogram matrices using the normal scores and corresponding eigenvalues.

		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
75.159	Al_2O_3	1.0116	-0.7026	0.3821	0.9323	0.5407	0.0271
	Fe	-0.7026	0.8968	-0.7546	-0.6651	-0.3804	0.0595
	SiO_2	0.3821	-0.7546	0.8404	0.3804	0.0584	0.487
	TiO_2	0.9323	-0.6651	0.3804	0.9834	0.4441	0.955
	LOI	0.5407	-0.3804	0.0584	0.4441	0.9297	3.1333
90.052		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0163	-0.6996	0.3805	0.9387	0.543	0.0272
	Fe	-0.6996	0.8976	-0.7602	-0.6621	-0.383	0.0611
	SiO_2	0.3805	-0.7602	0.8491	0.3796	0.0626	0.5159
	TiO_2	0.9387	-0.6621	0.3796	0.9984	0.4357	0.9674
	LOI	0.543	-0.383	0.0626	0.4357	0.9536	3.1434
104.986		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0223	-0.7013	0.3836	0.9473	0.5453	0.0267
	Fe	-0.7013	0.9099	-0.7809	-0.6665	-0.384	0.063
	SiO_2	0.3836	-0.7809	0.8772	0.3859	0.0652	0.536
	TiO_2	0.9473	-0.6665	0.3859	1.0158	0.432	0.9914
	LOI	0.5453	-0.384	0.0652	0.432	0.9677	3.1758
120.005		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0201	-0.7085	0.393	0.9437	0.5445	0.0269
	Fe	-0.7085	0.9268	-0.802	-0.6722	-0.389	0.0638
	SiO_2	0.393	-0.802	0.9035	0.3954	0.0722	0.5551
	TiO_2	0.9437	-0.6722	0.3954	1.0151	0.421	1.0047
	LOI	0.5445	-0.389	0.0722	0.421	0.9875	3.2025
135.021		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0314	-0.7222	0.4063	0.9518	0.5556	0.0268
	Fe	-0.7222	0.9402	-0.815	-0.6851	-0.3995	0.0641
	SiO_2	0.4063	-0.815	0.9156	0.4086	0.0807	0.5591
	TiO_2	0.9518	-0.6851	0.4086	1.0233	0.4243	1.0069
	LOI	0.5556	-0.3995	0.0807	0.4243	1.0026	3.2562
149.904		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0275	-0.7256	0.4122	0.9445	0.5469	0.0264
	Fe	-0.7256	0.9514	-0.8276	-0.6883	-0.4005	0.0648
	SiO_2	0.4122	-0.8276	0.9272	0.4164	0.087	0.5758
	TiO_2	0.9445	-0.6883	0.4164	1.017	0.4056	1.005
	LOI	0.5469	-0.4005	0.087	0.4056	1.0097	3.2607

Table A1 continued- The average distance, experimental semivariogram matrices using the normal scores and corresponding eigenvalues.

		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
164.941	Al_2O_3	1.0312	-0.7219	0.4127	0.9387	0.5472	0.0256
	Fe	-0.7219	0.9497	-0.8343	-0.6832	-0.3988	0.0653
	SiO_2	0.4127	-0.8343	0.9372	0.418	0.0918	0.5829
	TiO_2	0.9387	-0.6832	0.418	1.0064	0.3944	1.0059
	LOI	0.5472	-0.3988	0.0918	0.3944	1.008	3.2529
179.968		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0228	-0.7128	0.403	0.9254	0.54	0.0254
	Fe	-0.7128	0.9575	-0.8464	-0.6765	-0.3968	0.0677
	SiO_2	0.403	-0.8464	0.9537	0.4136	0.0943	0.6091
	TiO_2	0.9254	-0.6765	0.4136	0.9985	0.3726	1.0195
	LOI	0.54	-0.3968	0.0943	0.3726	1.0186	3.2295
194.881		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0297	-0.716	0.4067	0.9269	0.5411	0.0255
	Fe	-0.716	0.9671	-0.8579	-0.6764	-0.4069	0.071
	SiO_2	0.4067	-0.8579	0.9665	0.4149	0.1081	0.6289
	TiO_2	0.9269	-0.6764	0.4149	1.0045	0.3656	1.0142
	LOI	0.5411	-0.4069	0.1081	0.3656	1.0226	3.2508
209.877		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0196	-0.7049	0.3985	0.9197	0.5273	0.0262
	Fe	-0.7049	0.9753	-0.8704	-0.6671	-0.4137	0.0722
	SiO_2	0.3985	-0.8704	0.984	0.4089	0.1208	0.6653
	TiO_2	0.9197	-0.6671	0.4089	1.0052	0.3468	1.0128
	LOI	0.5273	-0.4137	0.1208	0.3468	1.0266	3.2342

Table A2- The average distance, experimental semivariogram matrices using the standardised and corresponding eigenvalues.

Average Lag	Matrix					Eigenvalues
		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
6.959	Al_2O_3	0.8678	-0.7567	0.4924	0.7814	0.4993	0.0045
	Fe	-0.7567	0.8199	-0.6951	-0.6676	-0.3898	0.0363
	SiO_2	0.4924	-0.6951	0.7645	0.4234	0.0984	0.2661
	TiO_2	0.7814	-0.6676	0.4234	0.7797	0.4296	0.7292
	LOI	0.4993	-0.3898	0.0984	0.4296	0.7858	2.9816
16.721		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.8951	-0.7778	0.5033	0.8127	0.4962	0.0059
	Fe	-0.7778	0.8492	-0.7184	-0.6877	-0.3948	0.0393
	SiO_2	0.5033	-0.7184	0.7908	0.4309	0.0986	0.3092
	TiO_2	0.8127	-0.6877	0.4309	0.8229	0.4232	0.76
	LOI	0.4962	-0.3948	0.0986	0.4232	0.8211	3.0649
30.822		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.8865	-0.7614	0.4835	0.8128	0.4794	0.007
	Fe	-0.7614	0.8397	-0.7115	-0.678	-0.3825	0.0436
	SiO_2	0.4835	-0.7115	0.7941	0.416	0.0856	0.3479
	TiO_2	0.8128	-0.678	0.416	0.8425	0.4025	0.7851
	LOI	0.4794	-0.3825	0.0856	0.4025	0.8399	3.0191
45.331		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.8807	-0.7511	0.4693	0.8108	0.478	0.0077
	Fe	-0.7511	0.8353	-0.7074	-0.6712	-0.3776	0.0469
	SiO_2	0.4693	-0.7074	0.7951	0.4064	0.0751	0.3672
	TiO_2	0.8108	-0.6712	0.4064	0.8534	0.3941	0.8088
	LOI	0.478	-0.3776	0.0751	0.3941	0.8596	2.9935
60.155		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.917	-0.7776	0.4838	0.8477	0.4914	0.0078
	Fe	-0.7776	0.8638	-0.7291	-0.6968	-0.3928	0.0496
	SiO_2	0.4838	-0.7291	0.8155	0.4229	0.0811	0.3997
	TiO_2	0.8477	-0.6968	0.4229	0.8996	0.3953	0.8334
	LOI	0.4914	-0.3928	0.0811	0.3953	0.8989	3.1042
75.159		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.9524	-0.8032	0.4959	0.8835	0.5068	0.0077
	Fe	-0.8032	0.8882	-0.7457	-0.7233	-0.4089	0.0517
	SiO_2	0.4959	-0.7457	0.831	0.4376	0.0881	0.4256
	TiO_2	0.8835	-0.7233	0.4376	0.9435	0.3999	0.8514
	LOI	0.5068	-0.4089	0.0881	0.3999	0.9315	3.21

Table A2 continues- The average distance, experimental semivariogram matrices using the standardised and corresponding eigenvalues.

90.052		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.9694	-0.812	0.4982	0.902	0.5157	0.0076
	Fe	-0.812	0.8978	-0.7548	-0.7317	-0.4193	0.0523
	SiO_2	0.4982	-0.7548	0.8436	0.4395	0.0942	0.4527
	TiO_2	0.902	-0.7317	0.4395	0.9679	0.3996	0.8664
	LOI	0.5157	-0.4193	0.0942	0.3996	0.9582	3.2578
104.986		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	0.9855	-0.8283	0.513	0.9191	0.5203	0.0076
	Fe	-0.8283	0.9234	-0.7842	-0.7473	-0.426	0.054
	SiO_2	0.513	-0.7842	0.88	0.4535	0.0991	0.473
	TiO_2	0.9191	-0.7473	0.4535	0.9917	0.3992	0.8866
	LOI	0.5203	-0.426	0.0991	0.3992	0.973	3.3323
120.005		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0235	-0.8623	0.5385	0.9495	0.5306	0.0077
	Fe	-0.8623	0.9622	-0.8201	-0.7731	-0.4386	0.0562
	SiO_2	0.5385	-0.8201	0.9184	0.4724	0.1091	0.4977
	TiO_2	0.9495	-0.7731	0.4724	1.0216	0.3995	0.9071
	LOI	0.5306	-0.4386	0.1091	0.3995	0.9966	3.4537
135.021		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0458	-0.89	0.562	0.9628	0.5479	0.0077
	Fe	-0.89	0.995	-0.8484	-0.7929	-0.4555	0.0581
	SiO_2	0.562	-0.8484	0.9434	0.4905	0.1218	0.4971
	TiO_2	0.9628	-0.7929	0.4905	1.0323	0.4098	0.9124
	LOI	0.5479	-0.4555	0.1218	0.4098	1.0088	3.5501
149.904		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0238	-0.8783	0.5616	0.9392	0.5349	0.0077
	Fe	-0.8783	0.9926	-0.8548	-0.7819	-0.4491	0.0614
	SiO_2	0.5616	-0.8548	0.9536	0.4918	0.1245	0.5016
	TiO_2	0.9392	-0.7819	0.4918	1.0156	0.3922	0.9117
	LOI	0.5349	-0.4491	0.1245	0.3922	1.007	3.5102
164.941		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
	Al_2O_3	1.0364	-0.8917	0.5753	0.9443	0.5382	0.0075
	Fe	-0.8917	1.0111	-0.8761	-0.79	-0.4526	0.0655
	SiO_2	0.5753	-0.8761	0.9772	0.5027	0.131	0.5105
	TiO_2	0.9443	-0.79	0.5027	1.0263	0.386	0.9116
	LOI	0.5382	-0.4526	0.131	0.386	1.002	3.5579

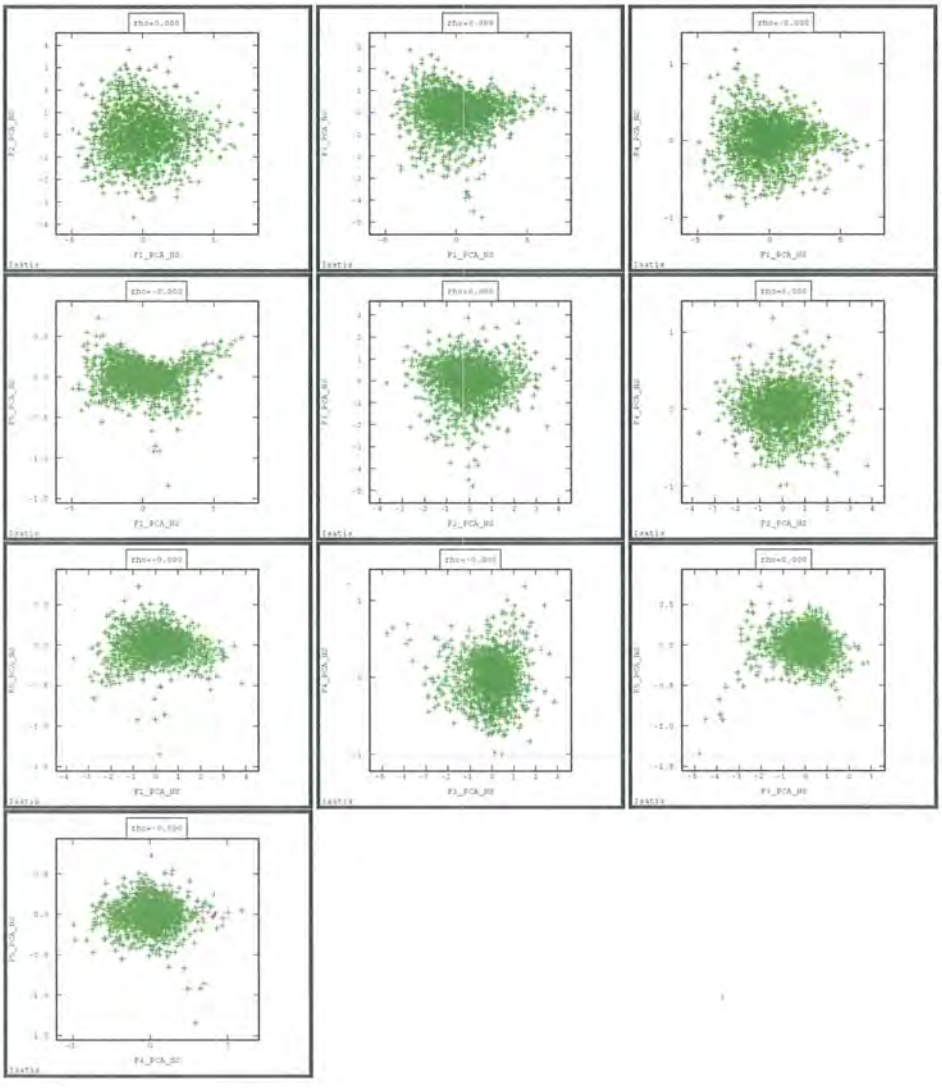
Table A2 continued- The average distance, experimental semivariogram matrices using the standardised and corresponding eigenvalues.

		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
179.968	Al_2O_3	1.0284	-0.8837	0.5693	0.9307	0.5313	0.0075
	Fe	-0.8837	1.0109	-0.8821	-0.7804	-0.4504	0.0704
	SiO_2	0.5693	-0.8821	0.9905	0.4982	0.1345	0.5308
	TiO_2	0.9307	-0.7804	0.4982	1.0221	0.3665	0.9133
	LOI	0.5313	-0.4504	0.1345	0.3665	1.0025	3.5323
		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
194.881	Al_2O_3	1.0581	-0.9078	0.5867	0.9522	0.5393	0.0075
	Fe	-0.9078	1.0374	-0.9053	-0.7969	-0.465	0.0771
	SiO_2	0.5867	-0.9053	1.0122	0.5088	0.1512	0.5548
	TiO_2	0.9522	-0.7969	0.5088	1.0537	0.3676	0.9073
	LOI	0.5393	-0.465	0.1512	0.3676	1.0066	3.6213
		Al_2O_3	Fe	SiO_2	TiO_2	LOI	
209.877	Al_2O_3	1.0559	-0.9007	0.5804	0.9486	0.5301	0.0076
	Fe	-0.9007	1.0368	-0.9086	-0.7897	-0.4698	0.0843
	SiO_2	0.5804	-0.9086	1.0193	0.5048	0.1633	0.5911
	TiO_2	0.9486	-0.7897	0.5048	1.0695	0.3472	0.8981
	LOI	0.5301	-0.4698	0.1633	0.3472	1.0093	3.6097

Appendix 4 – Scatter Plots and Correlation Coefficients of Factors

4.1 PCA Factors using Normal Scores

Scatter plots

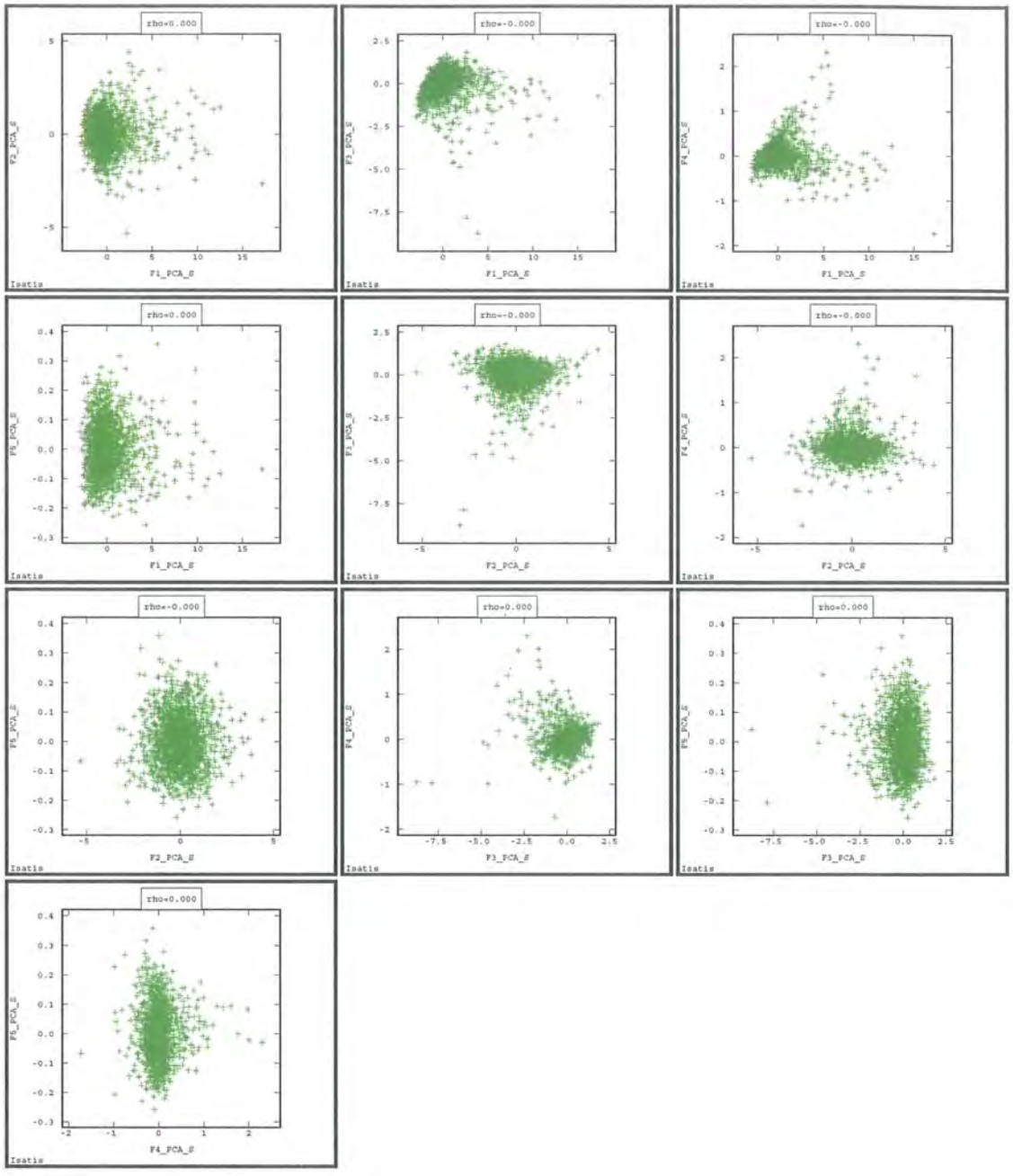


Correlation Matrix:

VARIABLES	F1_PCA_NS	F2_PCA_NS	F3_PCA_NS	F4_PCA_NS	F5_PCA_NS
F1_PCA_NS	1	0	0	0	0
F2_PCA_NS	0	1	0	0	0
F3_PCA_NS	0	0	1	0	0
F4_PCA_NS	0	0	0	1	0
F5_PCA_NS	0	0	0	0	1

4.2 PCA Factors using Standardised Variables

Scatter plots

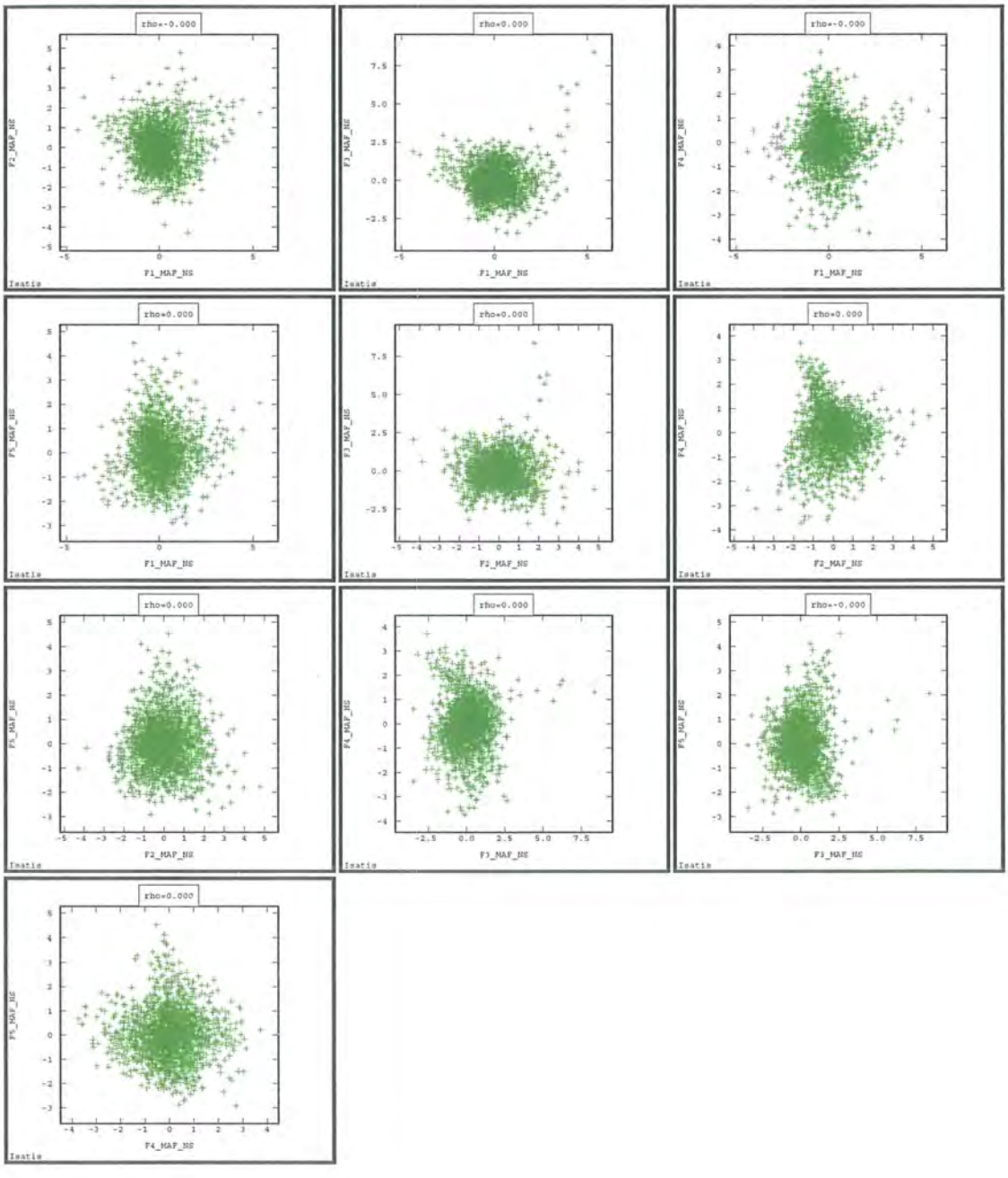


Correlation Matrix:

VARIABLES	F1_PCA_S	F2_PCA_S	F3_PCA_S	F4_PCA_S	F5_PCA_S
F1_PCA_S	1	0	0	0	0
F2_PCA_S	0	1	0	0	0
F3_PCA_S	0	0	1	0	0
F4_PCA_S	0	0	0	1	0
F5_PCA_S	0	0	0	0	1

4.3 MAF Factors using Normal Scores

Scatter plots

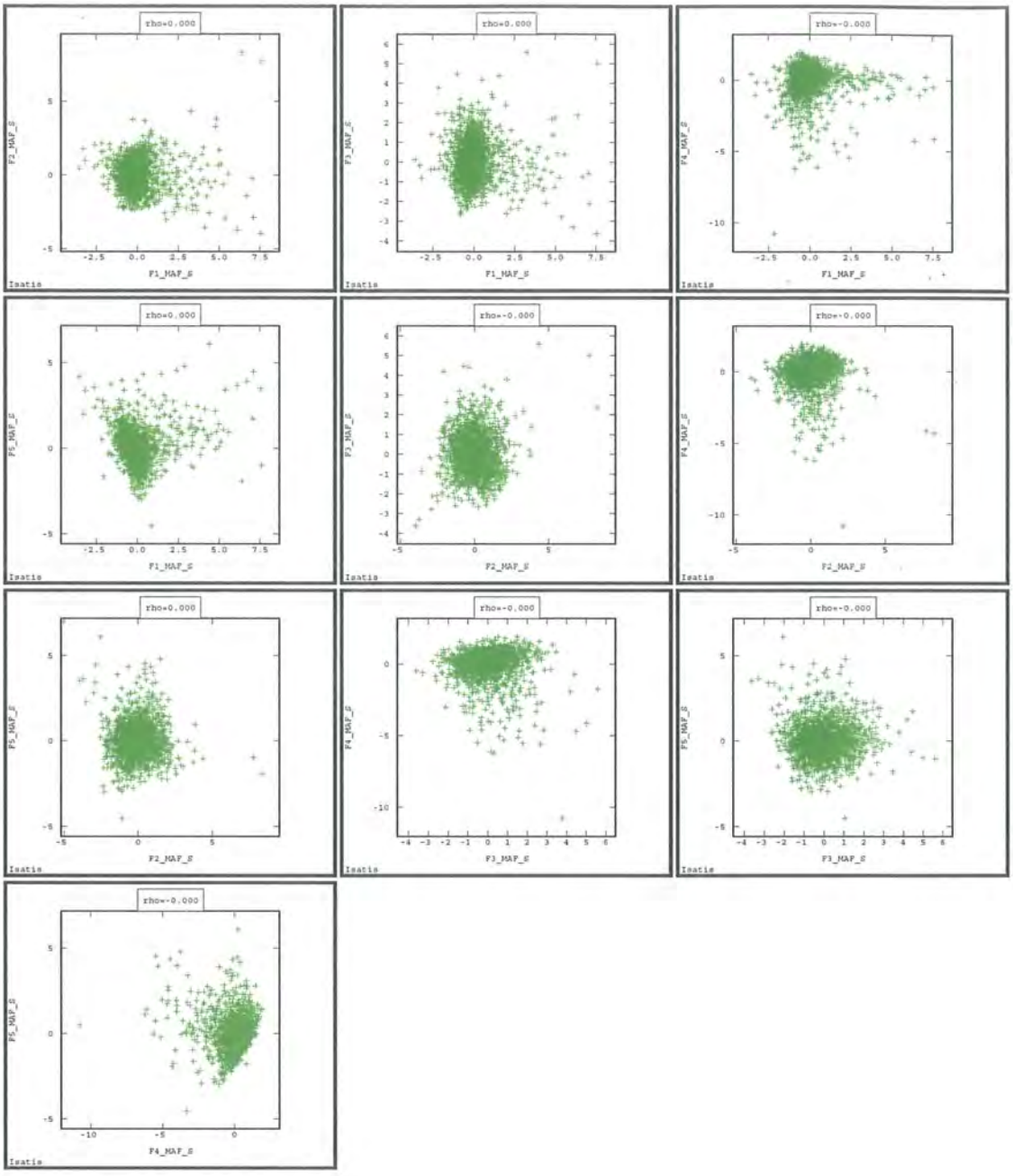


Correlation Matrix:

VARIABLES	F1_PCA_NS	F2_PCA_NS	F3_PCA_NS	F4_PCA_NS	F5_PCA_NS
F1_PCA_NS	1	0	0	0	0
F2_PCA_NS	0	1	0	0	0
F3_PCA_NS	0	0	1	0	0
F4_PCA_NS	0	0	0	1	0
F5_PCA_NS	0	0	0	0	1

4.4 MAF Factors using Standardised Variables

Scatter plots

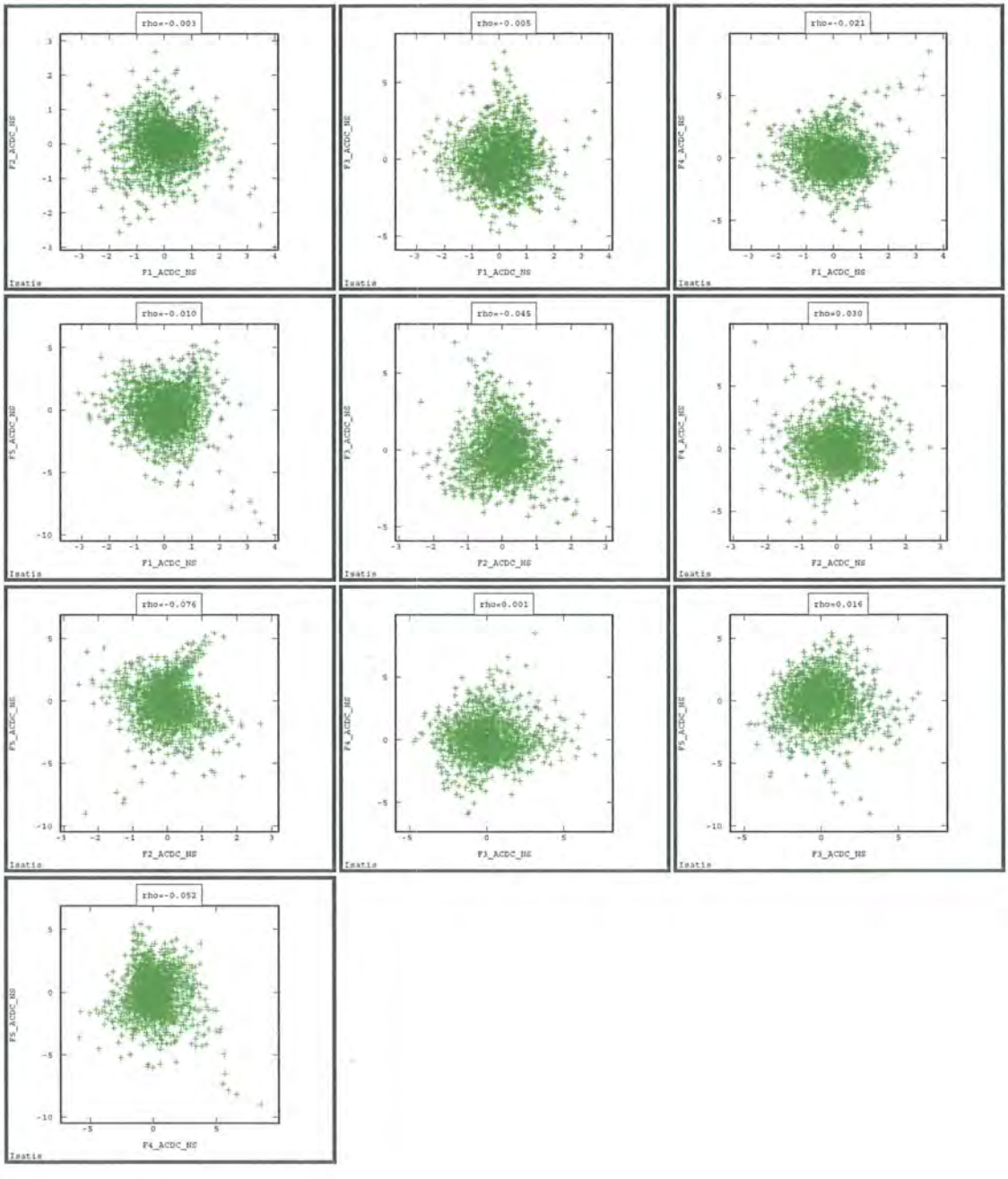


Correlation Matrix:

VARIABLES	F1_MAF_S	F2_MAF_S	F3_MAF_S	F4_MAF_S	F5_MAF_S
F1_MAF_S	1	0	0	0	0
F2_MAF_S	0	1	0	0	0
F3_MAF_S	0	0	1	0	0
F4_MAF_S	0	0	0	1	0
F5_MAF_S	0	0	0	0	1

4.5 ACDC Factors using Normal Scores

Scatter plots

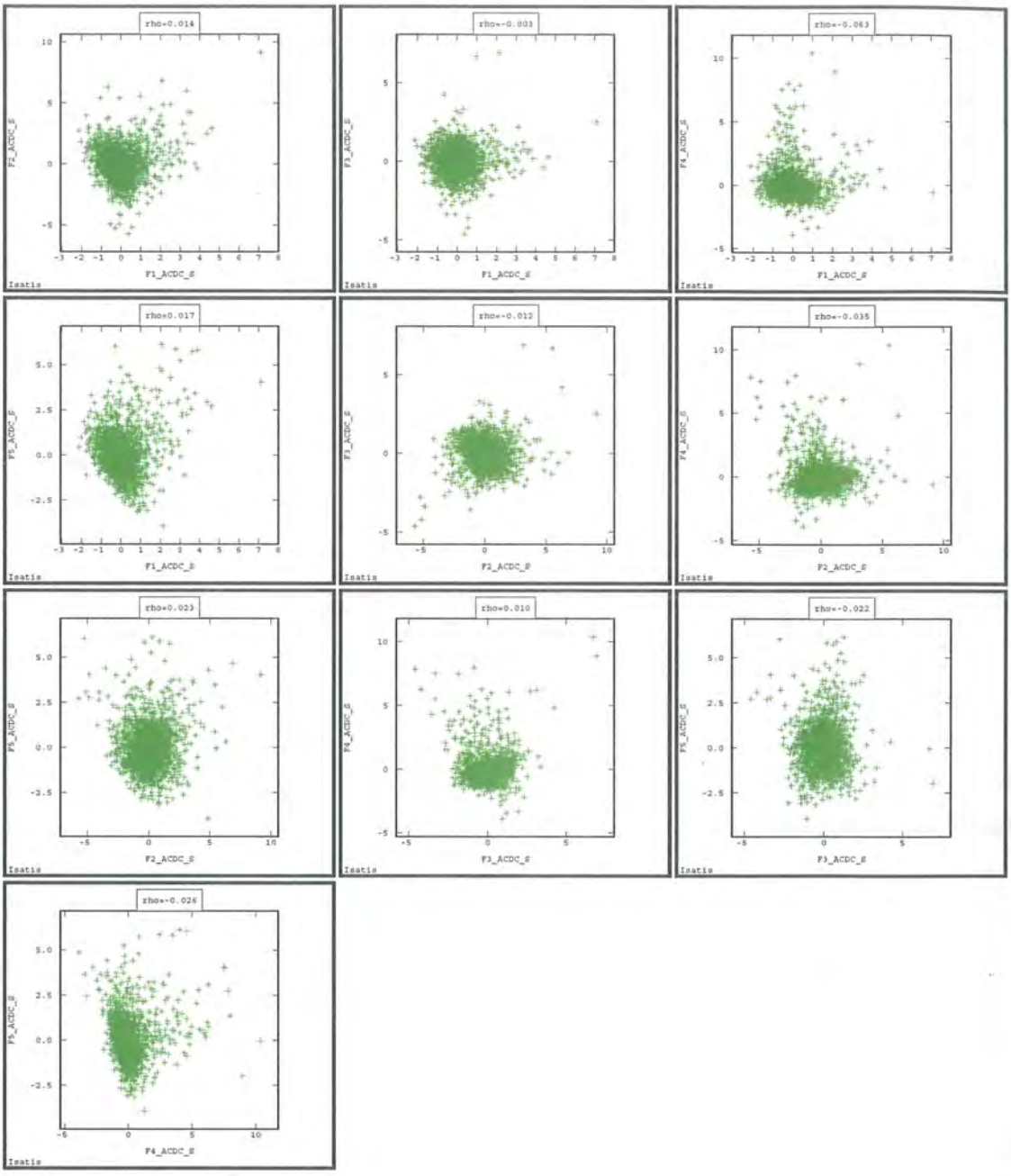


Correlation Matrix:

VARIABLES	F1_ACDC_NS	F2_ACDC_NS	F3_ACDC_NS	F4_ACDC_NS	F5_ACDC_NS
F1_ACDC_NS	1	0	-0.01	-0.02	-0.01
F2_ACDC_NS	0	1	-0.05	0.03	-0.08
F3_ACDC_NS	-0.01	-0.05	1	0	0.02
F4_ACDC_NS	-0.02	0.03	0	1	-0.05
F5_ACDC_NS	-0.01	-0.08	0.02	-0.05	1

4.6 ACDC Factors using Standardised Variables

Scatter plots

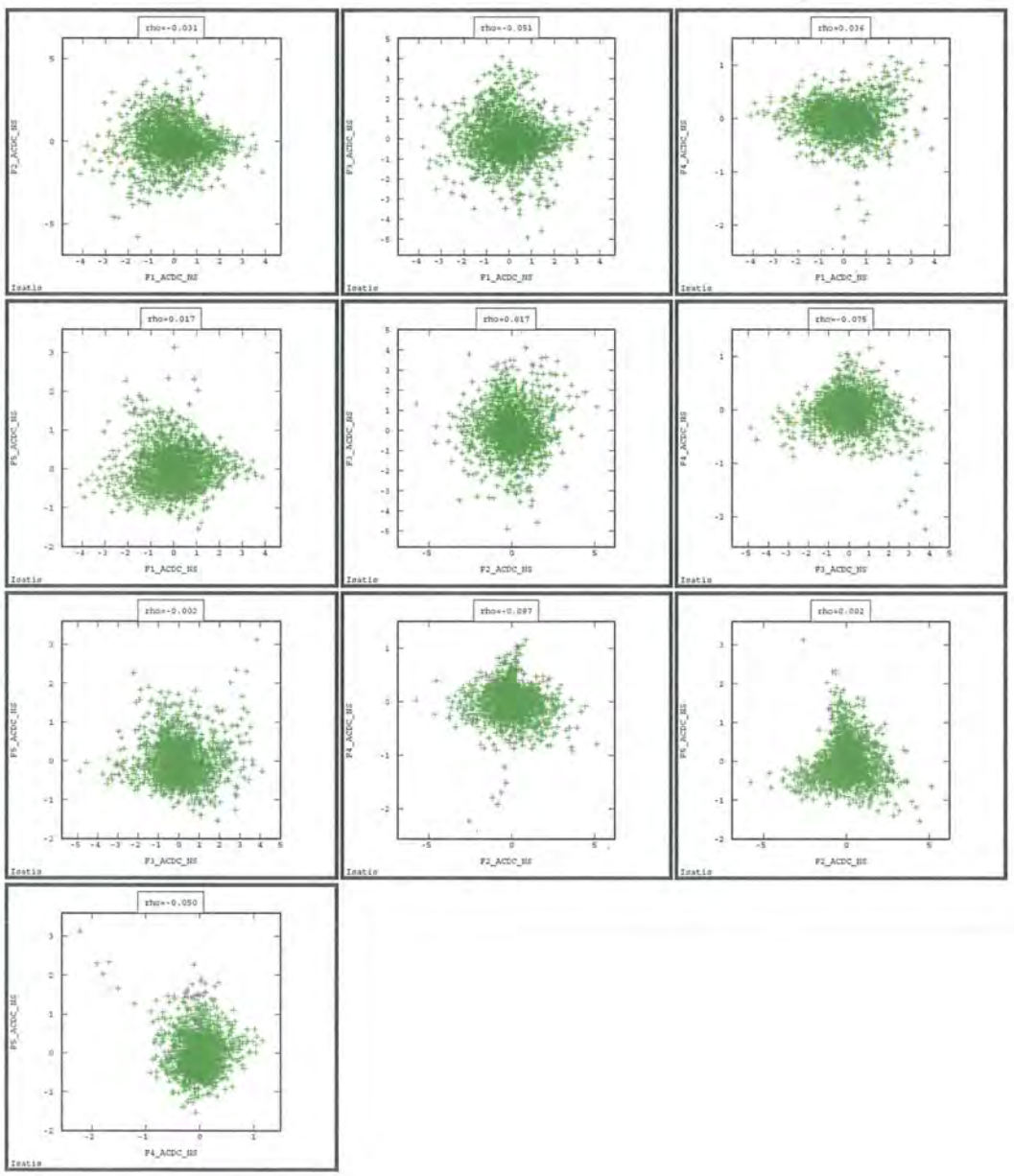


Correlation Matrix:

VARIABLES	F1_ACDC_S	F2_ACDC_S	F3_ACDC_S	F4_ACDC_S	F5_ACDC_S
F1_ACDC_S	1	0.01	0	-0.06	0.02
F2_ACDC_S	0.01	1	-0.01	-0.03	0.02
F3_ACDC_S	0	-0.01	1	0.01	-0.02
F4_ACDC_S	-0.06	-0.03	0.01	1	-0.03
F5_ACDC_S	0.02	0.02	-0.02	-0.03	1

4.7 ACDC Factors using Normal Scores and Matrix $A_{0_{NS}}$

Scatter plots

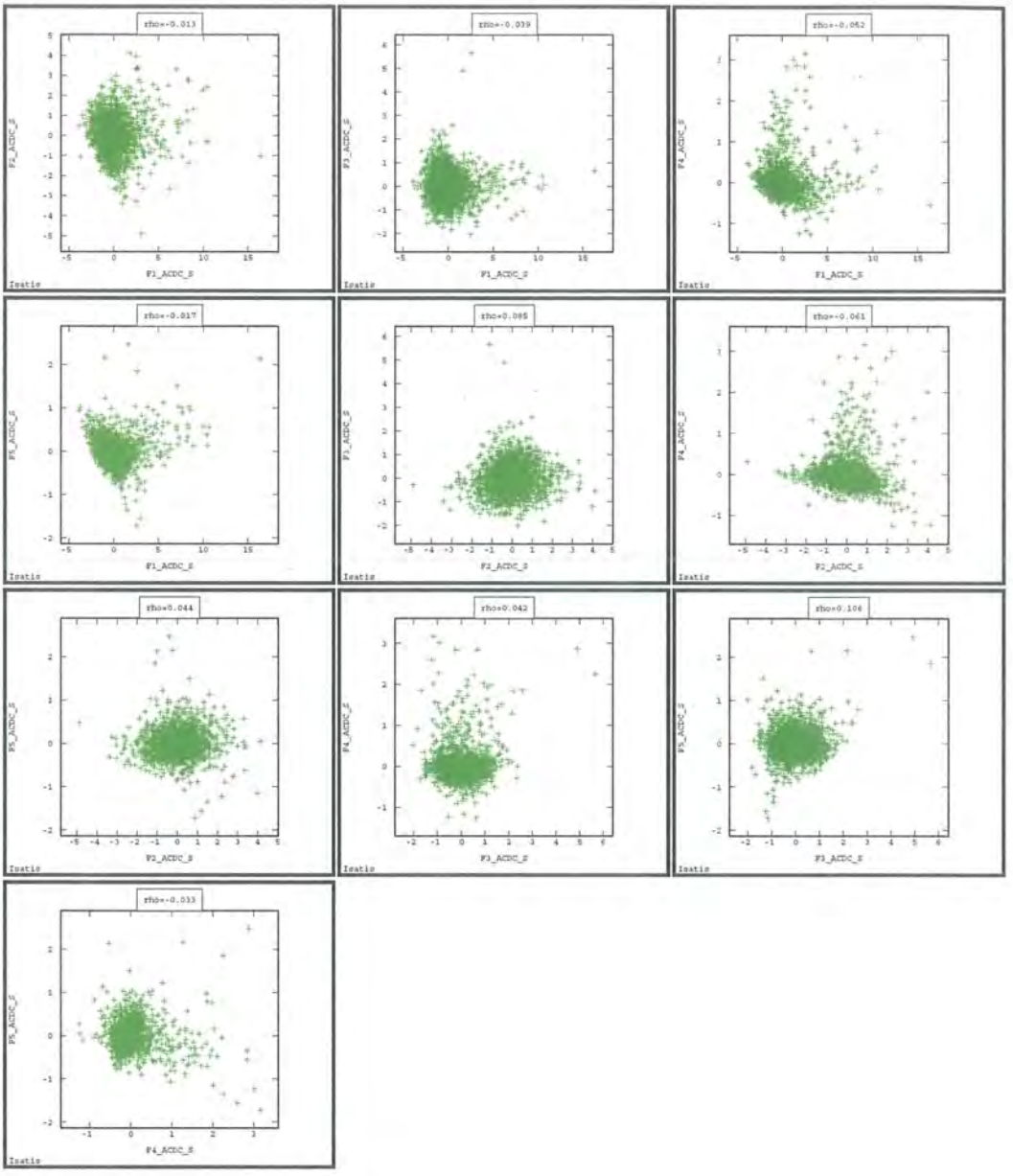


CorrelationMatrix:

VARIABLES	F1_ACDC_NS+A0	F2_ACDC_NS+A0	F3_ACDC_NS+A0	F4_ACDC_NS+A0	F5_ACDC_NS+A0
F1_ACDC_NS+A0	1	-0.03	-0.05	0.04	0.02
F2_ACDC_NS+A0	-0.03	1	0.02	-0.1	0
F3_ACDC_NS+A0	-0.05	0.02	1	-0.07	0
F4_ACDC_NS+A0	0.04	-0.1	-0.07	1	-0.05
F5_ACDC_NS+A0	0.02	0	0	-0.05	1

4.8 ACDC Factors using Standardised Variables and Matrix A_{0St}

Scatter plots

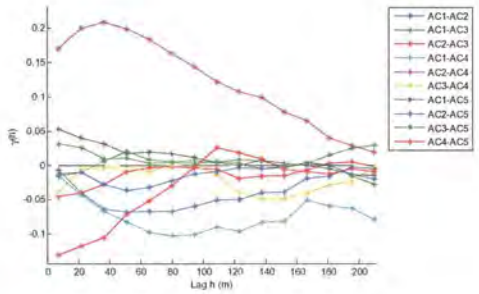


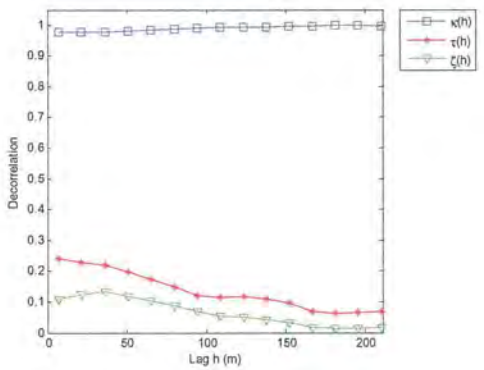
Correlation matrix:

VARIABLES	F1_ACDC_S +A0	F2_ACDC_S +A0	F3_ACDC_S +A0	F4_ACDC_S +A0	F5_ACDC_S +A0
F1_ACDC_S +A0	1	-0.01	-0.04	-0.05	-0.02
F2_ACDC_S +A0	-0.01	1	0.09	-0.06	0.04
F3_ACDC_S +A0	-0.04	0.09	1	0.04	0.11
F4_ACDC_S +A0	-0.05	-0.06	0.04	1	-0.03
F5_ACDC_S +A0	-0.02	0.04	0.11	-0.03	1

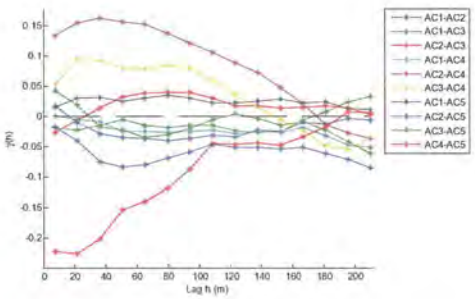
Appendix 5- Experimental Cross Semivariograms and Spatial Decorrelation Plots of the ACDC Factors

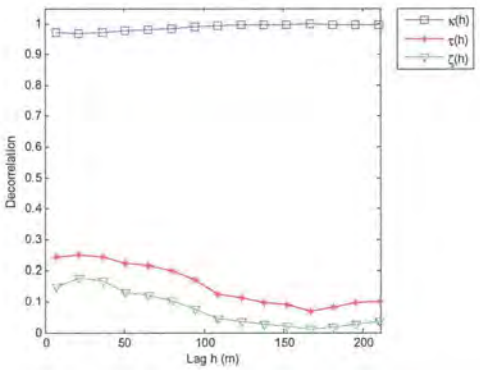
ACDC using Normal scores, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]



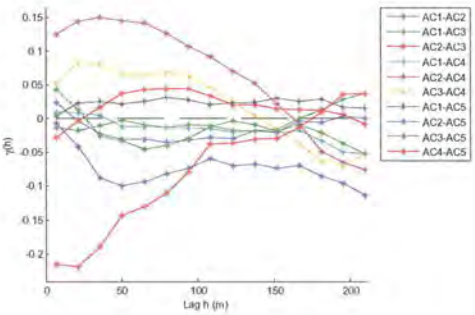


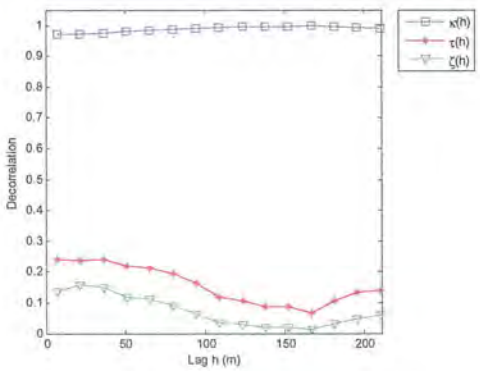
ACDC using Normal scores, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 1 1 0]



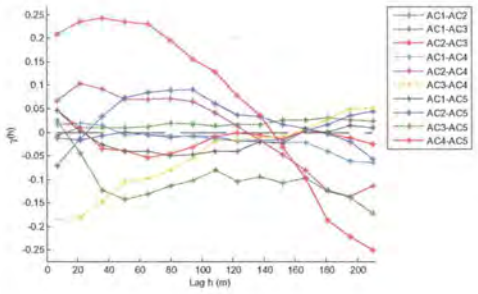


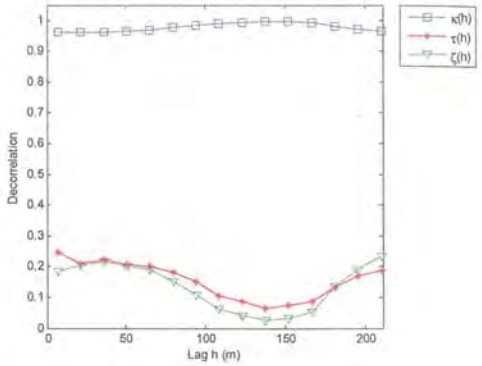
ACDC using Normal scores, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 1 0 0]



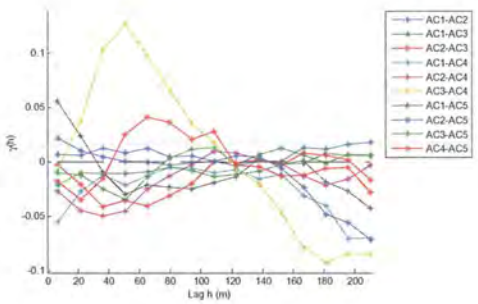


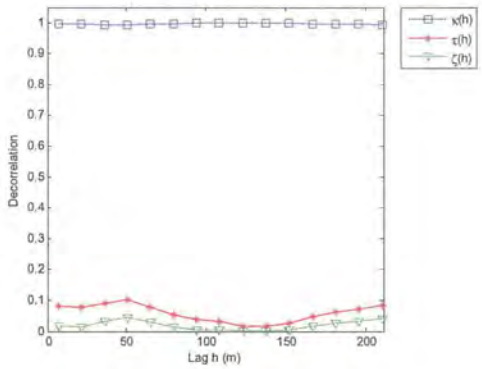
ACDC using Normal scores, weight vector [1 1 1 1 1 1 1 1 1 1 1 0 0 0]



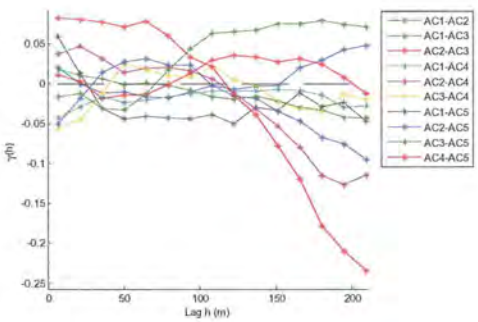


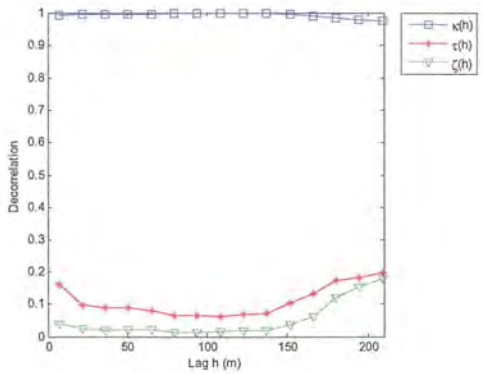
ACDC using Normal scores, weight vector [1 1 1 1 1 1 1 1 1 1 1 0 0 0 0]



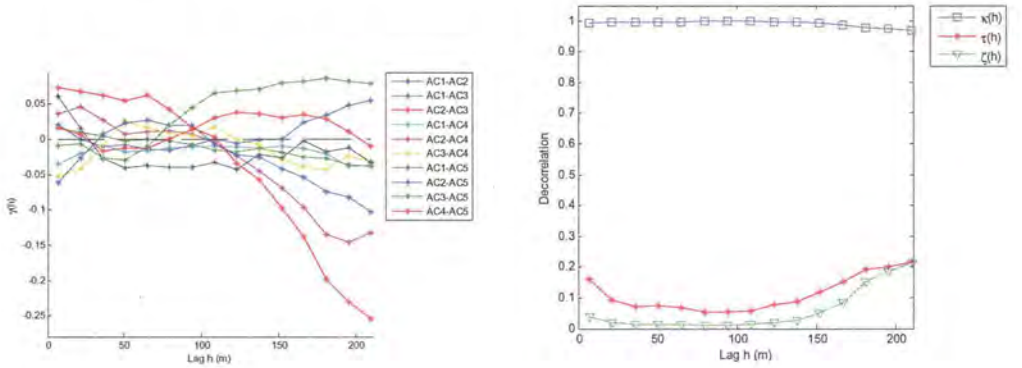


ACDC using Normal scores, weight vector [1 1 1 1 1 1 1 1 1 1 0 0 0 0 0]

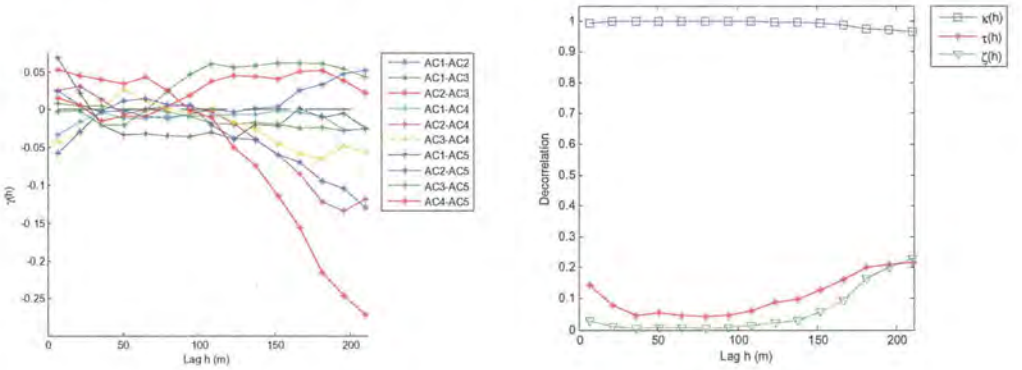




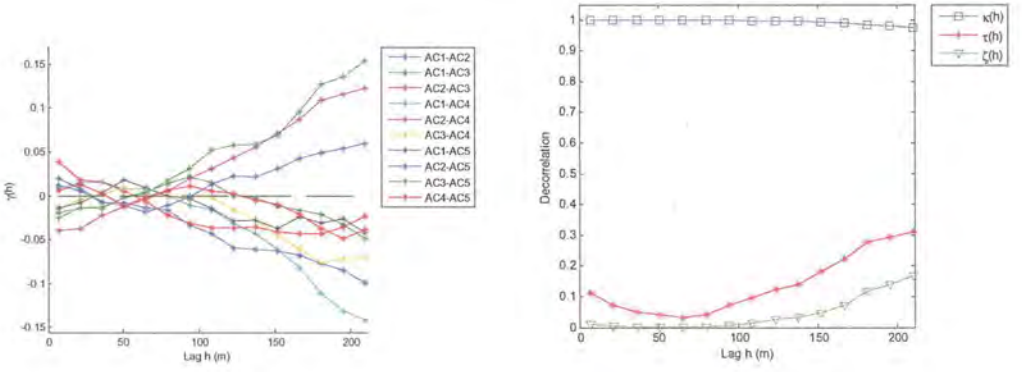
ACDC using Normal scores, weight vector [1 1 1 1 1 1 1 1 0 0 0 0 0 0]



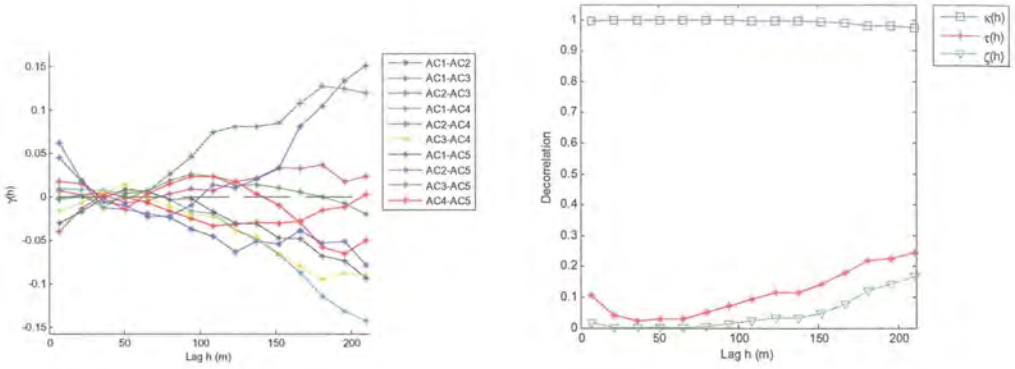
ACDC using Normal scores, weight vector [1 1 1 1 1 1 1 1 0 0 0 0 0 0 0]



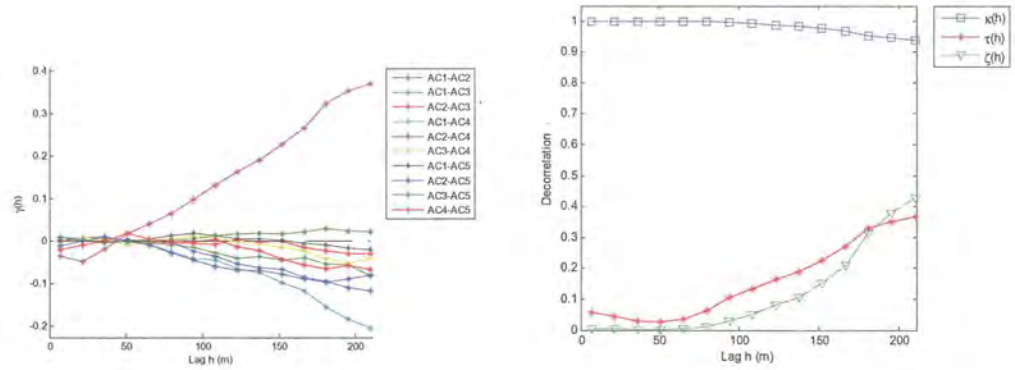
ACDC using Normal scores, weight vector [1 1 1 1 1 1 1 0 0 0 0 0 0 0 0]



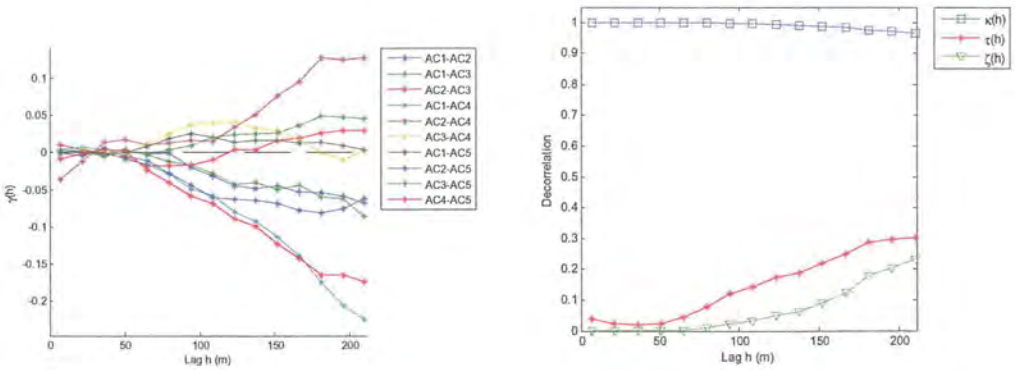
ACDC using Normal scores, weight vector [1 1 1 1 1 1 0 0 0 0 0 0 0 0 0]



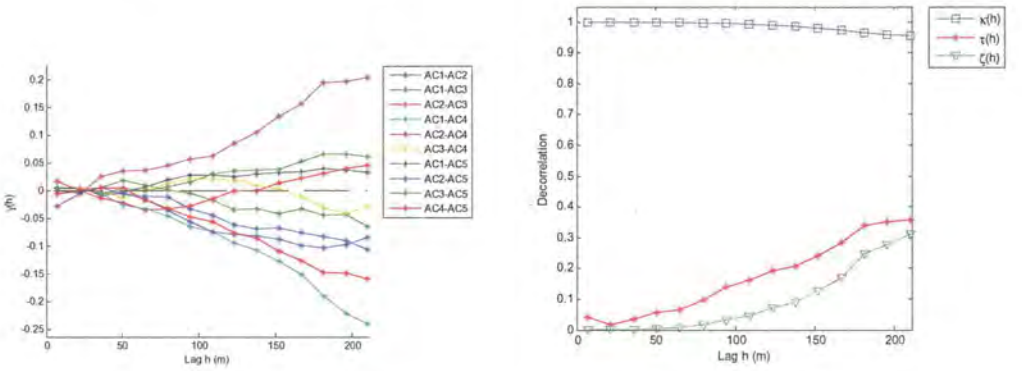
ACDC using Normal scores, weight vector [1 1 1 1 1 0 0 0 0 0 0 0 0 0 0]



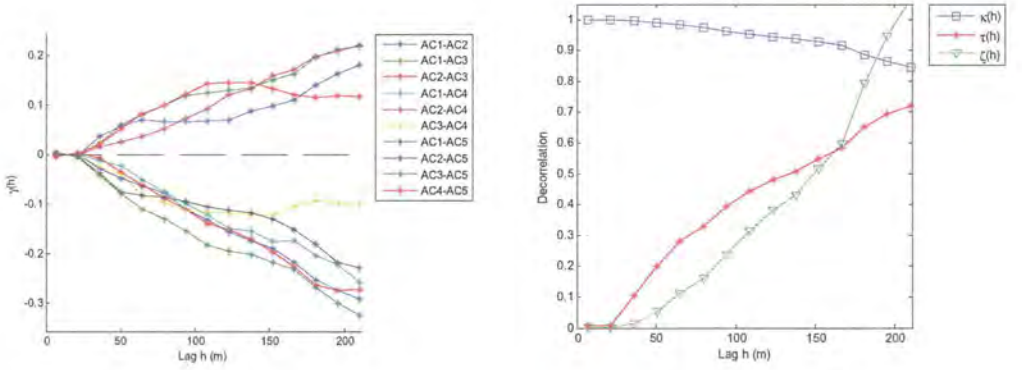
ACDC using Normal scores, weight vector [1 1 1 1 0 0 0 0 0 0 0 0 0 0 0]



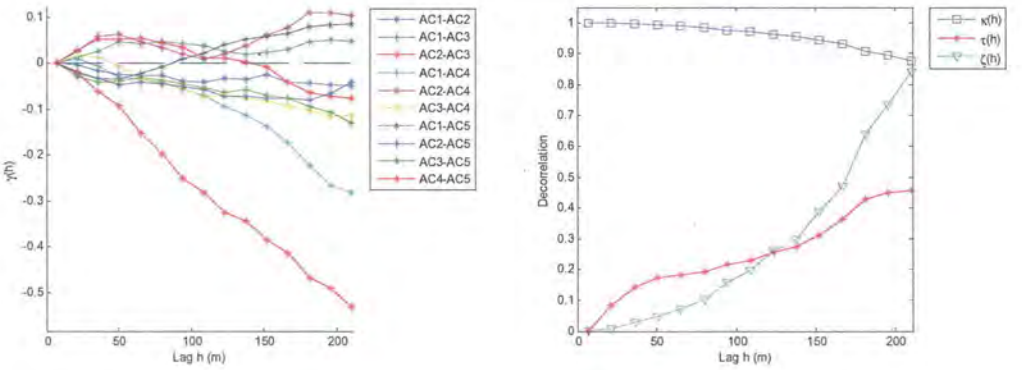
ACDC using Normal scores, weight vector [1 1 1 0 0 0 0 0 0 0 0 0 0 0 0]



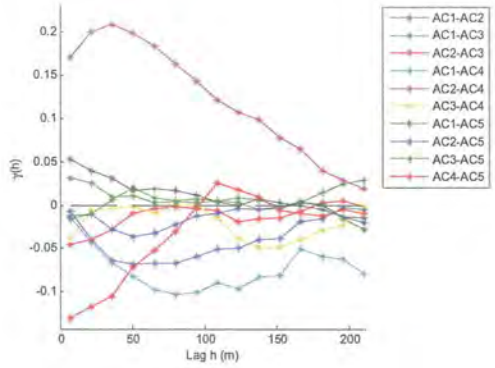
ACDC using Normal scores, weight vector [1 1 0 0 0 0 0 0 0 0 0 0 0 0 0]

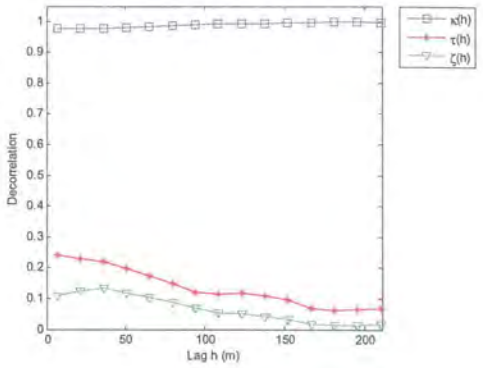


ACDC using Normal scores, weight vector [1 0 0 0 0 0 0 0 0 0 0 0 0 0 0]



ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 1 1]





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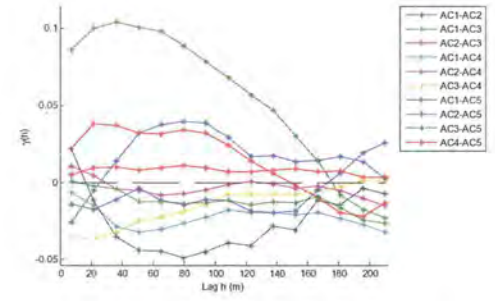
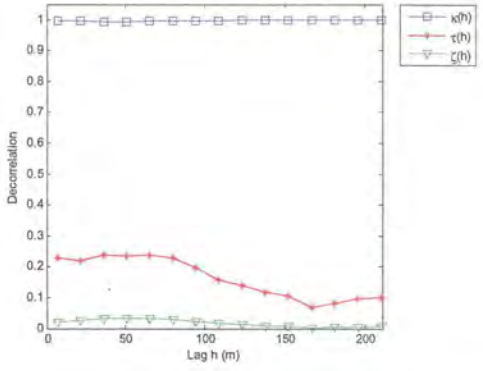
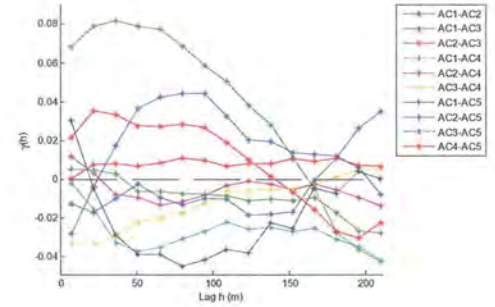
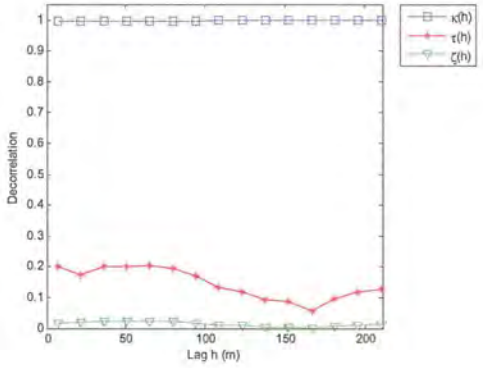


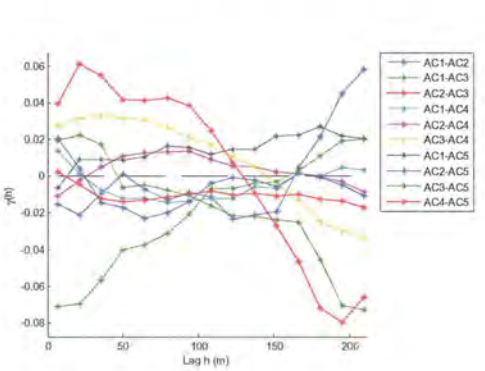


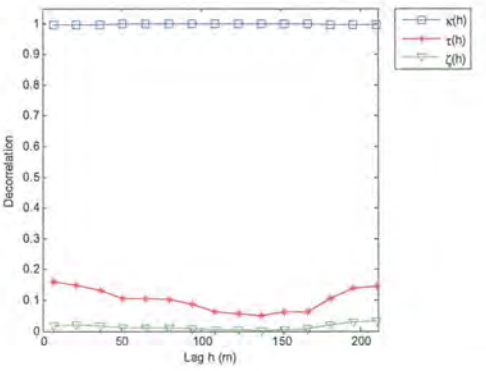
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 0 0]



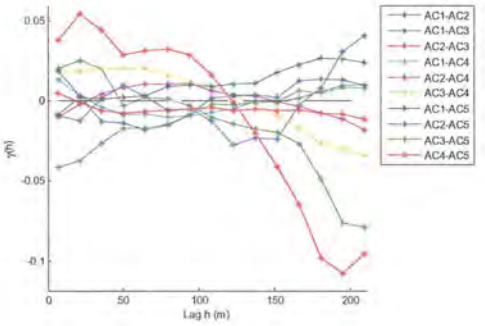


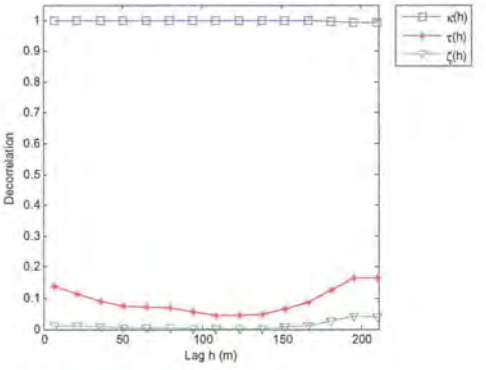
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 1 0 0 0]



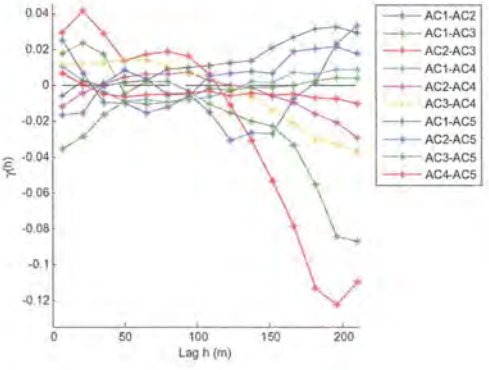


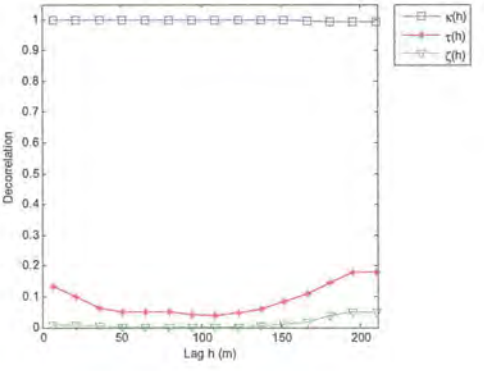
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 1 0 0 0 0]



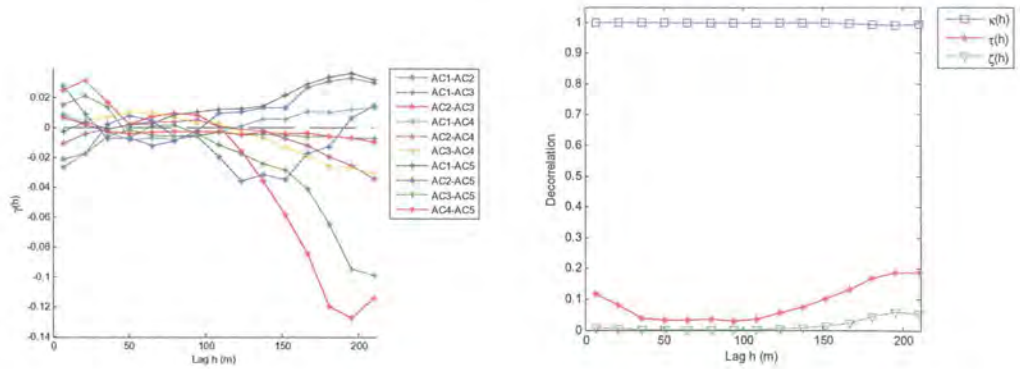


ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 0 0 0 0 0]

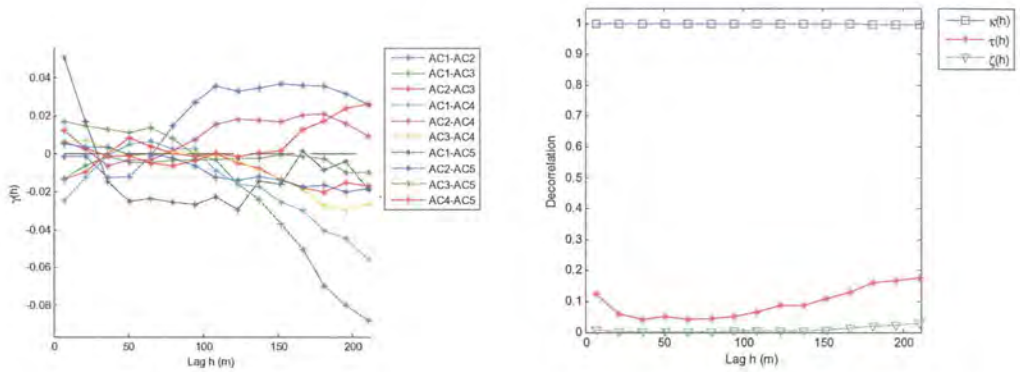




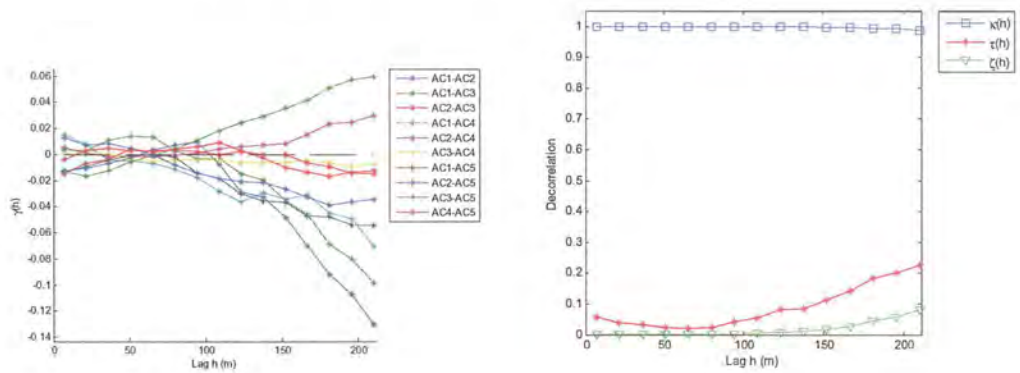
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 1 1 1 1 0 0 0 0 0 0]



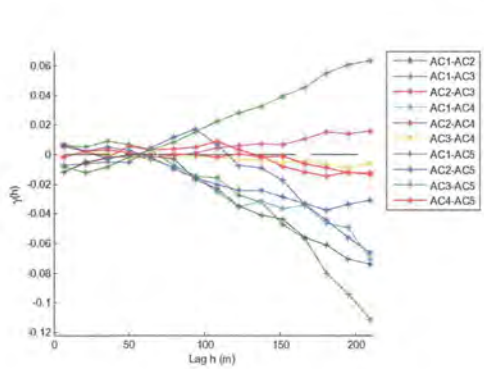
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 1 1 1 0 0 0 0 0 0 0]

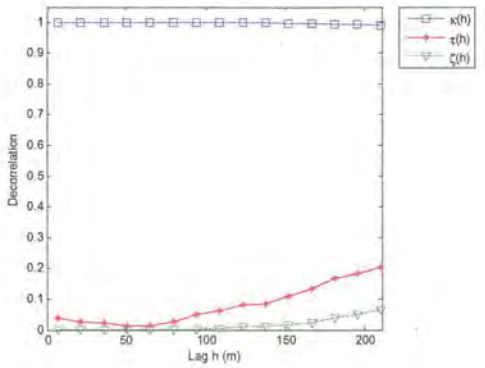


ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 1 1 0 0 0 0 0 0 0 0]

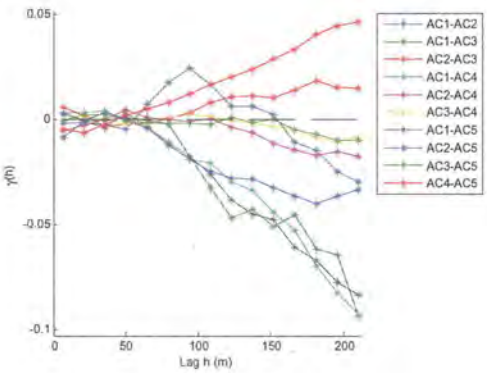


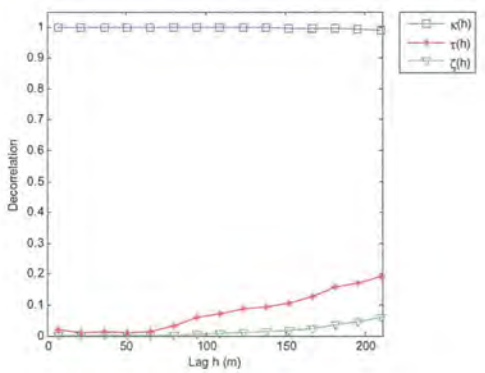
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 1 1 0 0 0 0 0 0 0 0 0]



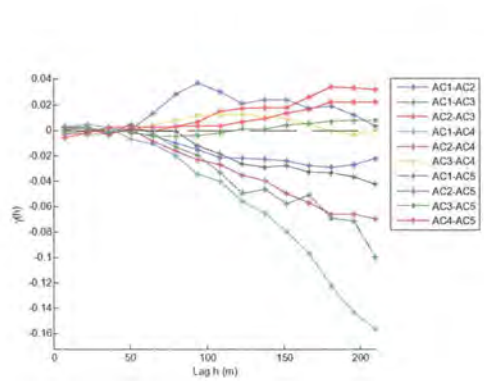


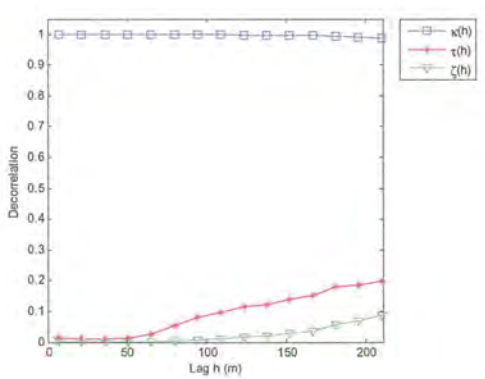
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 1 0 0 0 0 0 0 0 0 0 0]



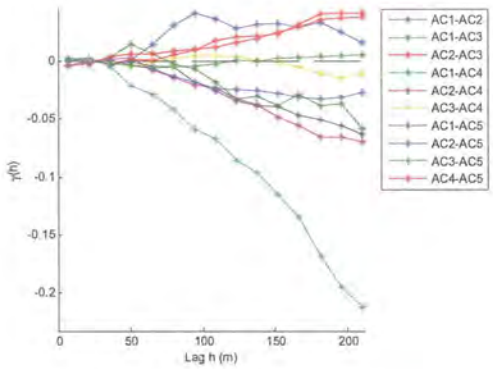


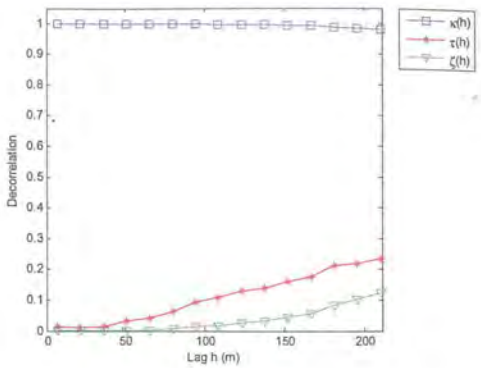
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 1 0 0 0 0 0 0 0 0 0 0 0]



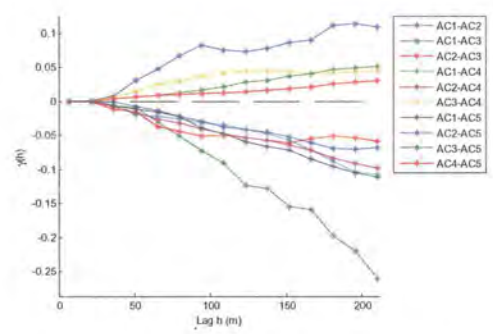


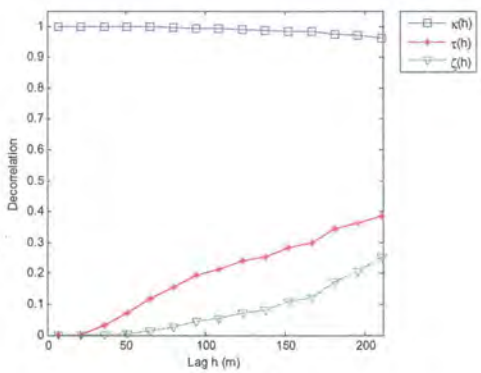
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 1 0 0 0 0 0 0 0 0 0 0 0 0]



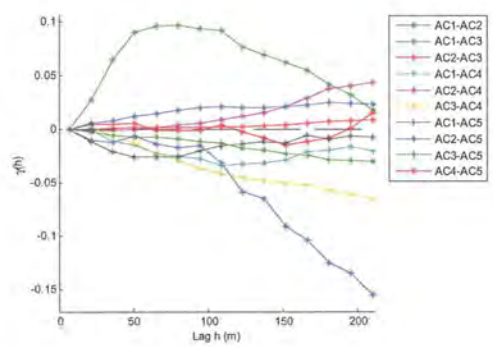


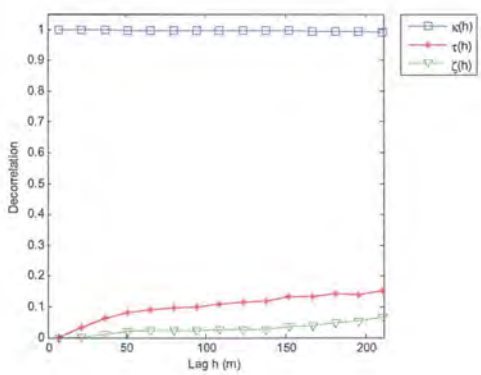
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 1 0 0 0 0 0 0 0 0 0 0 0 0 0]



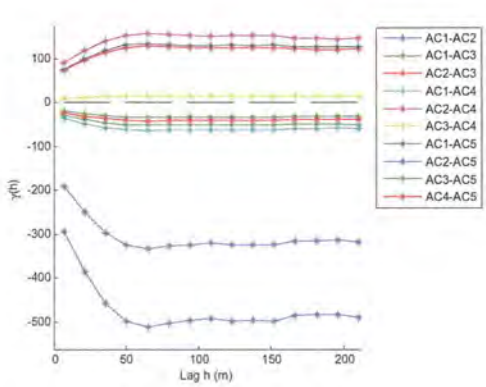


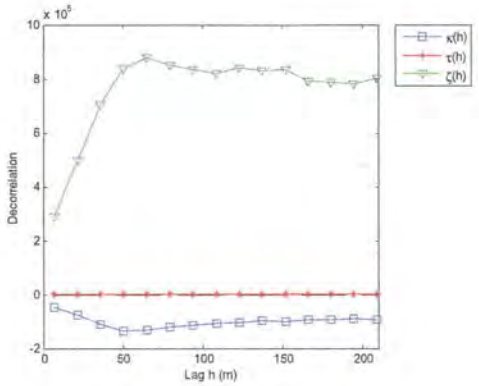
ACDC using Normal scores and $A_{0_{NS}}$ matrix, weight vector [1 0 0 0 0 0 0 0 0 0 0 0 0 0 0]



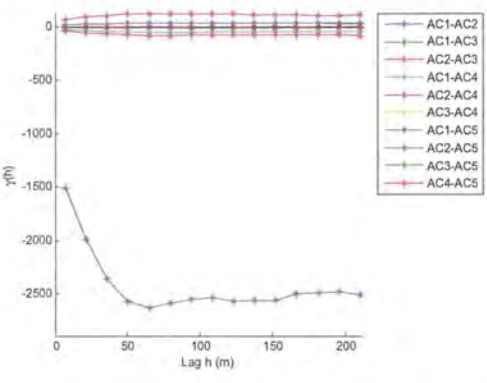


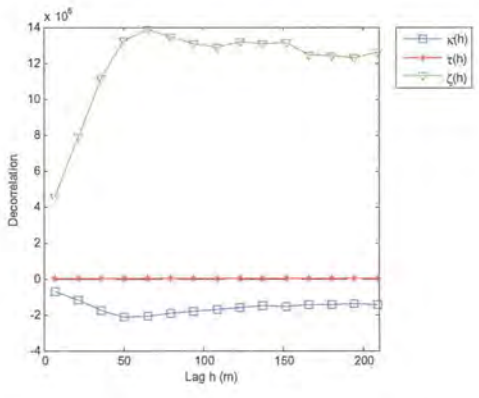
ACDC using Standardised scores, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 1 1]



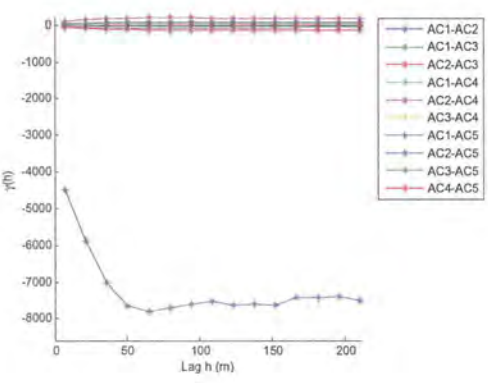


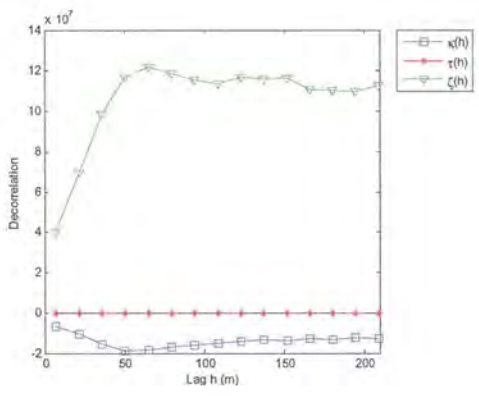
ACDC using Standardised scores, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 1 0]



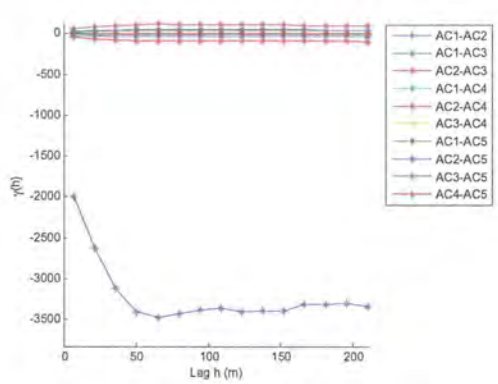


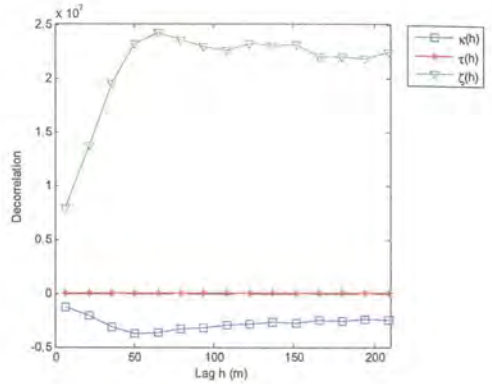
ACDC using Standardised scores, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 0 0]



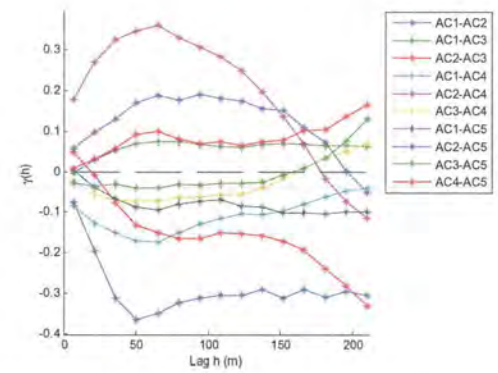


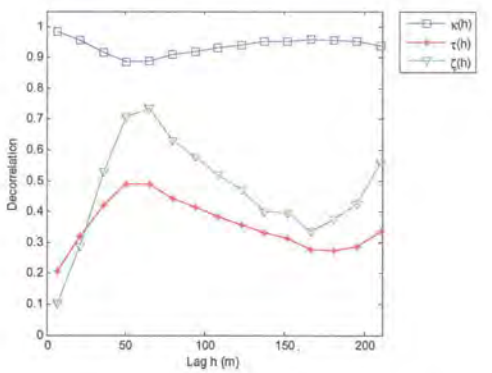
ACDC using Standardised scores, weight vector [1 1 1 1 1 1 1 1 1 1 1 0 0 0]



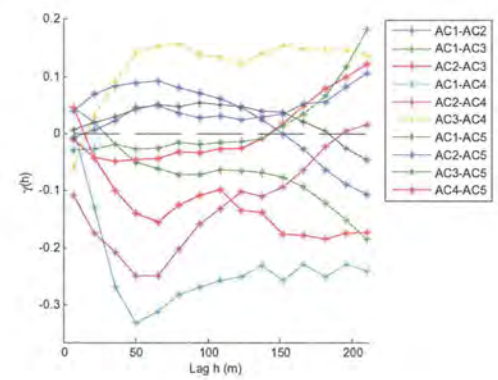


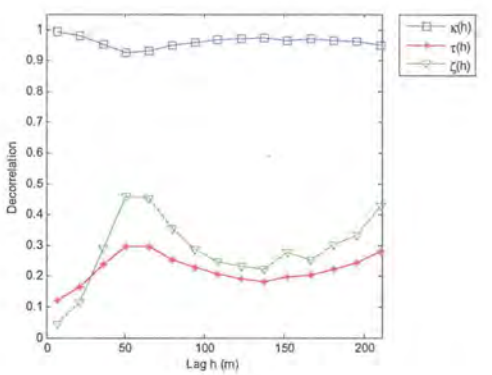
ACDC using Standardised scores, weight vector [1 1 1 1 1 1 1 1 1 1 1 0 0 0 0]



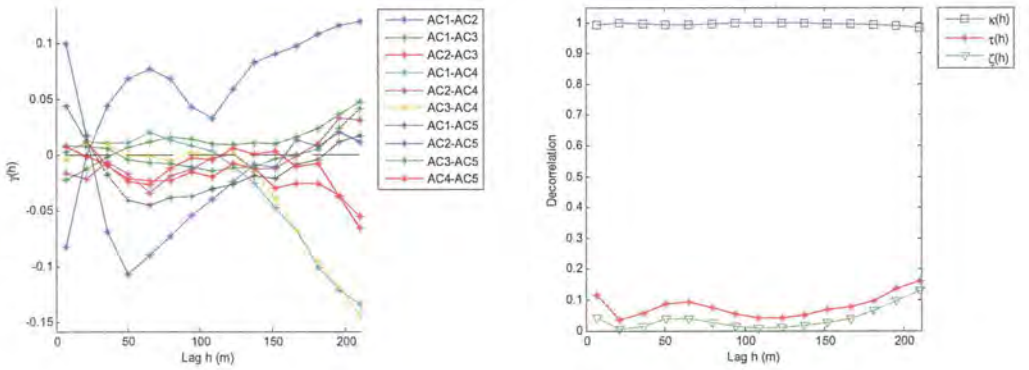


ACDC using Standardised scores, weight vector [1 1 1 1 1 1 1 1 1 1 0 0 0 0 0]

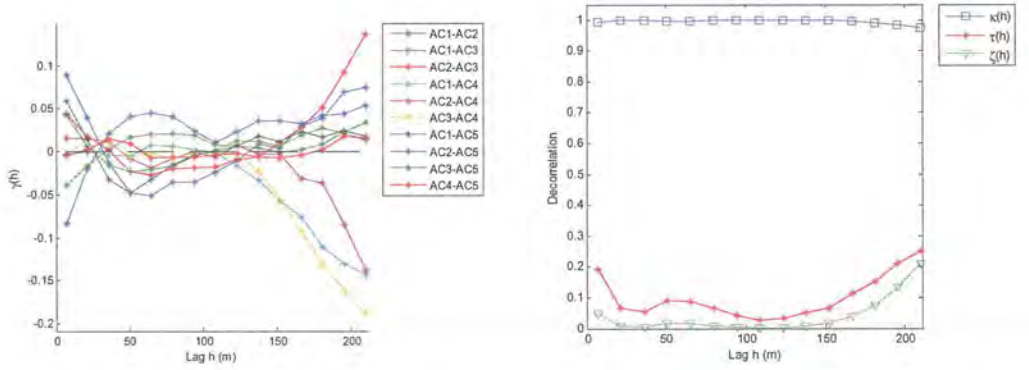




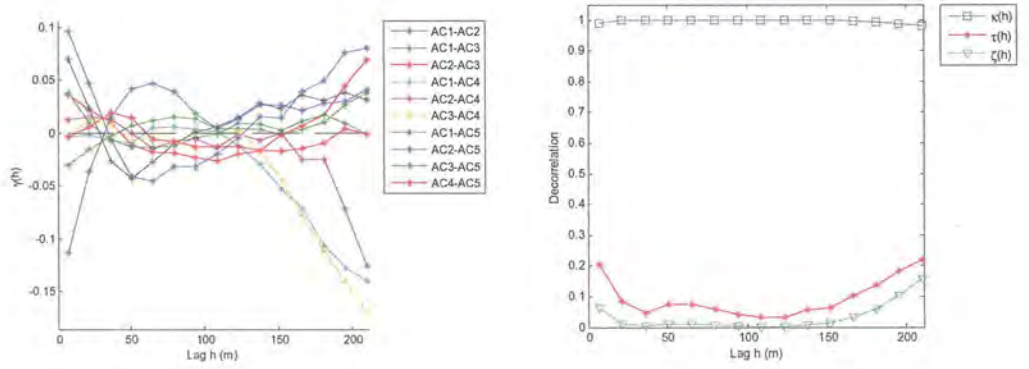
ACDC using Standardised scores, weight vector [1 1 1 1 1 1 1 1 0 0 0 0 0 0]



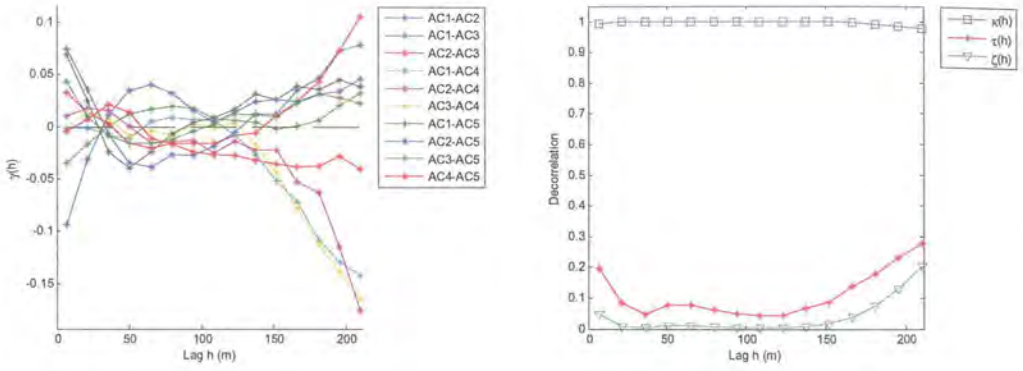
ACDC using Standardised scores, weight vector [1 1 1 1 1 1 1 1 0 0 0 0 0 0 0]



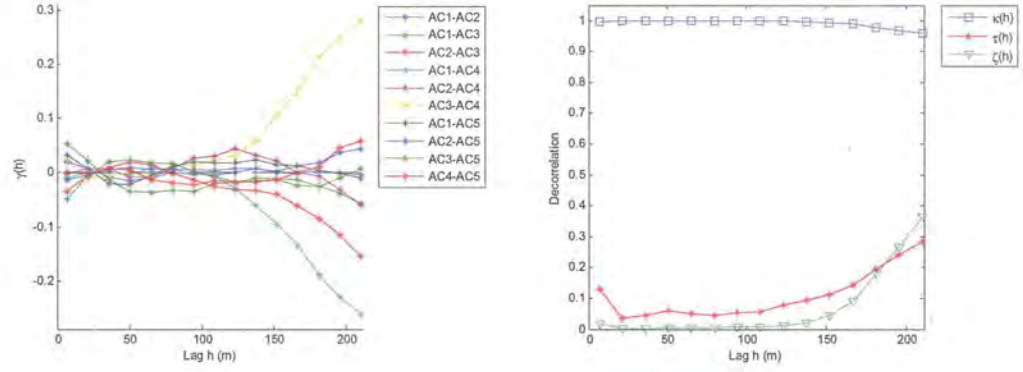
ACDC using Standardised scores, weight vector [1 1 1 1 1 1 1 0 0 0 0 0 0 0 0]



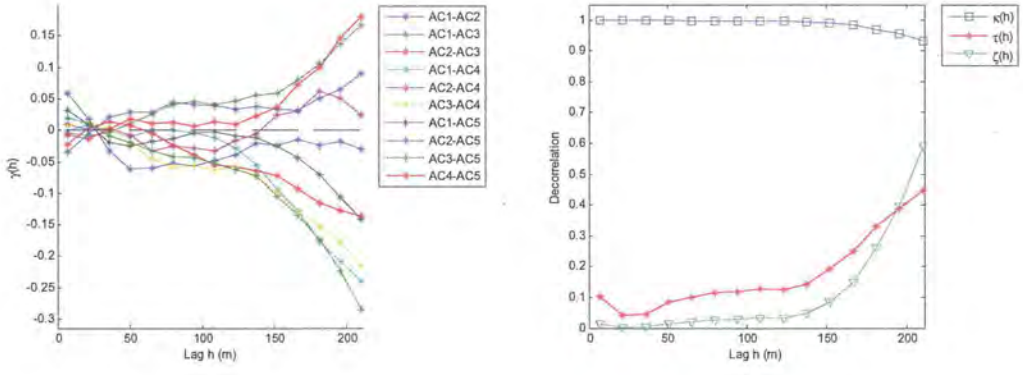
ACDC using Standardised scores, weight vector [1 1 1 1 1 1 0 0 0 0 0 0 0 0 0]



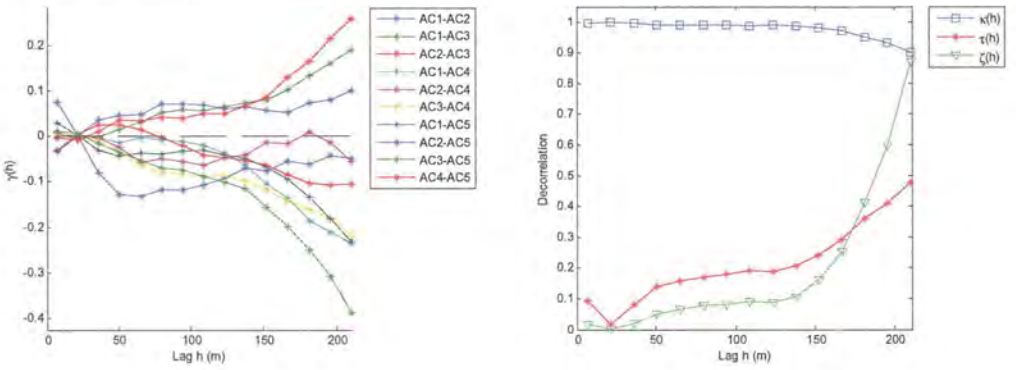
ACDC using Standardised scores, weight vector [1 1 1 1 1 0 0 0 0 0 0 0 0 0 0]



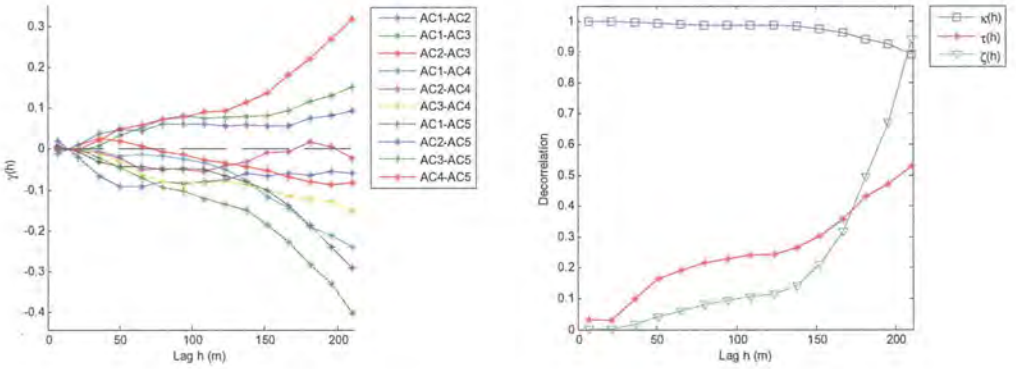
ACDC using Standardised scores, weight vector [1 1 1 1 0 0 0 0 0 0 0 0 0 0 0]



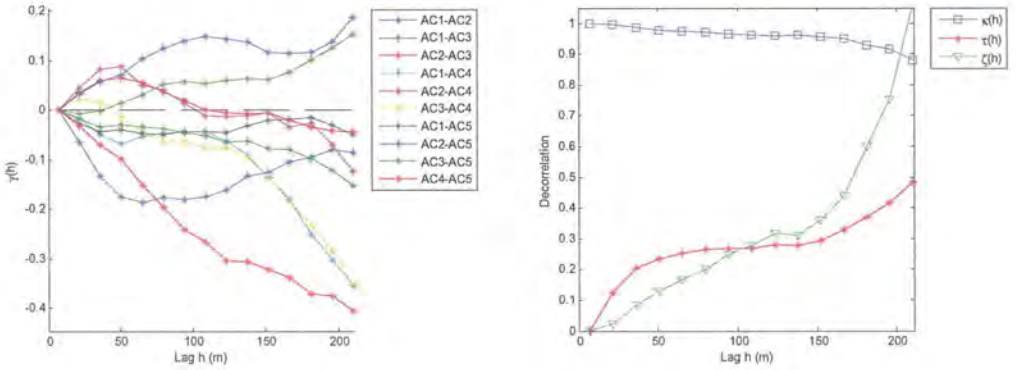
ACDC using Standardised scores, weight vector [1 1 1 0 0 0 0 0 0 0 0 0 0 0 0]



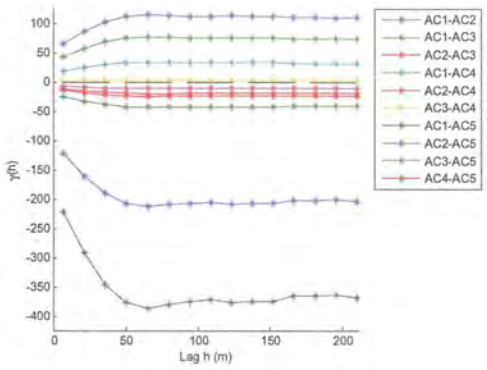
ACDC using Standardised scores, weight vector [1 1 0 0 0 0 0 0 0 0 0 0 0 0 0]

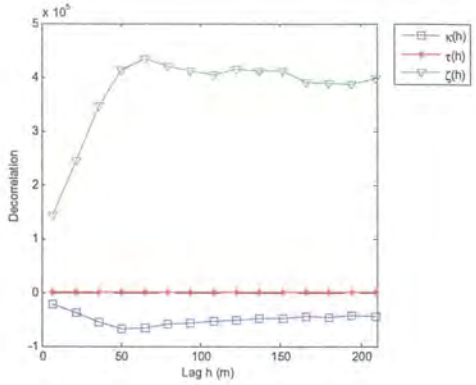


ACDC using Standardised scores, weight vector [1 0 0 0 0 0 0 0 0 0 0 0 0 0 0]

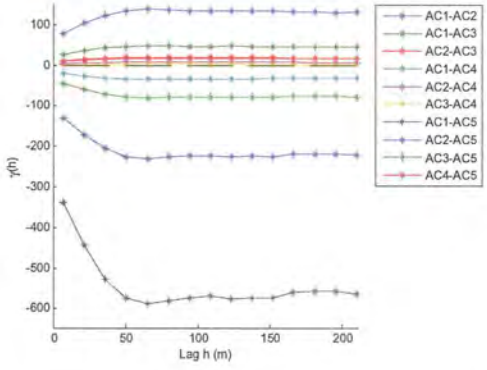


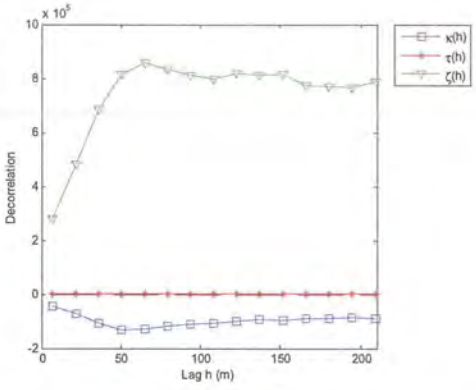
ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 1 1]



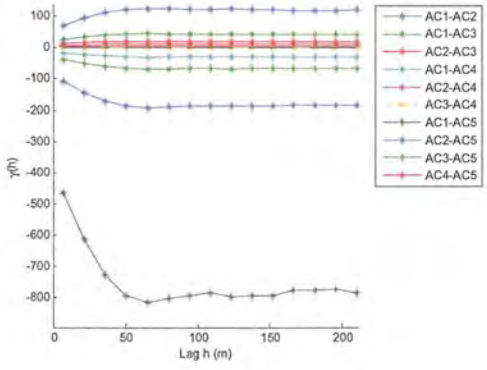


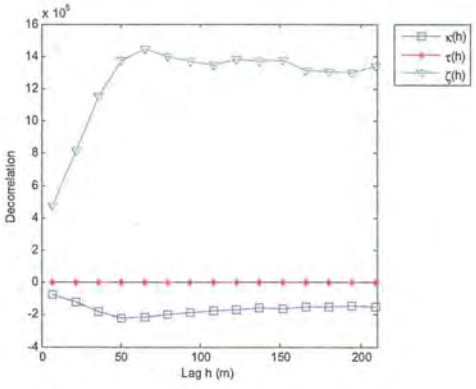
ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 1 0]



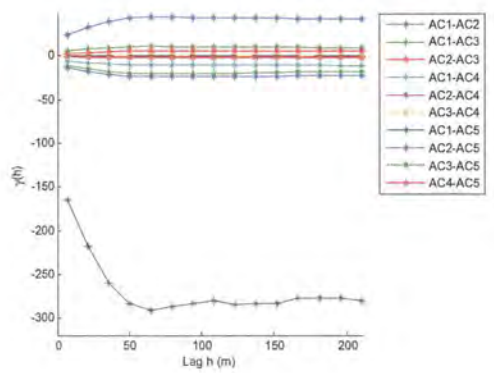


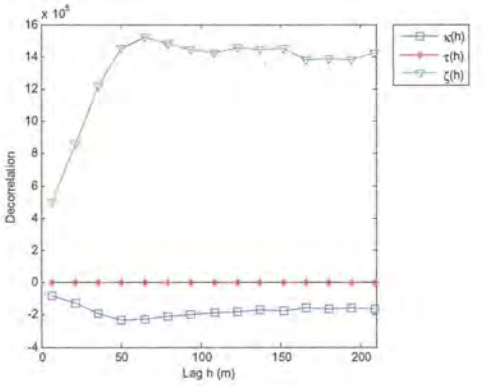
ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 1 1 0 0]



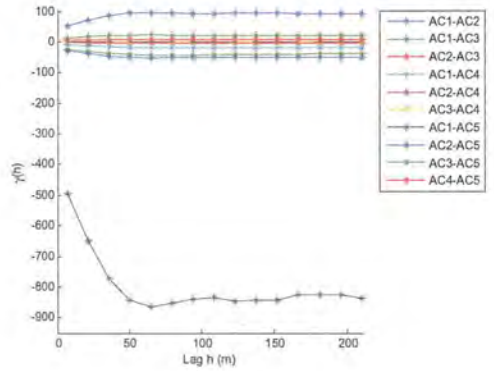


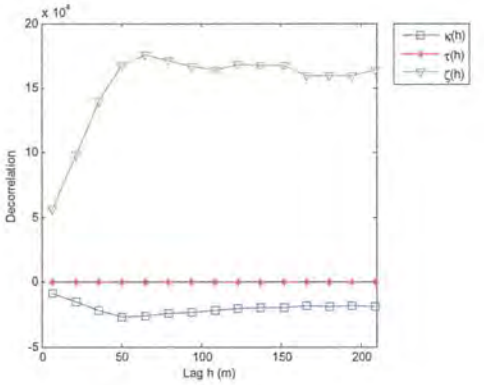
ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 1 0 0 0]



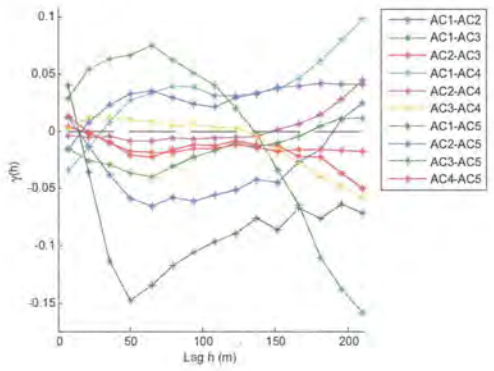


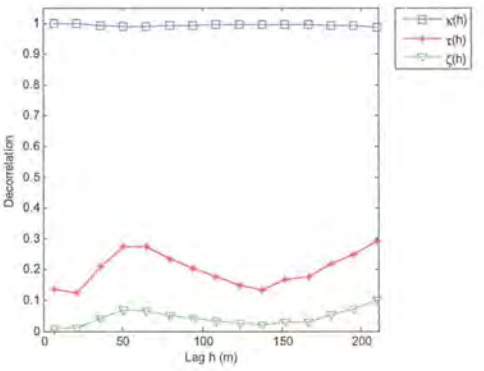
ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 1 0 0 0 0]



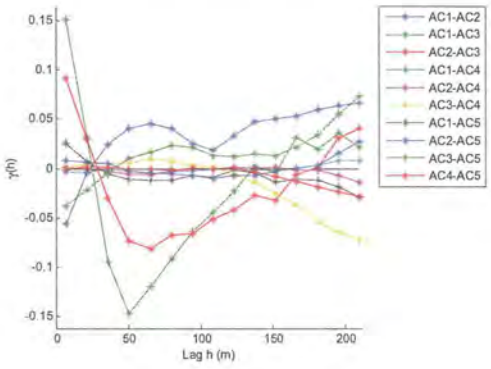


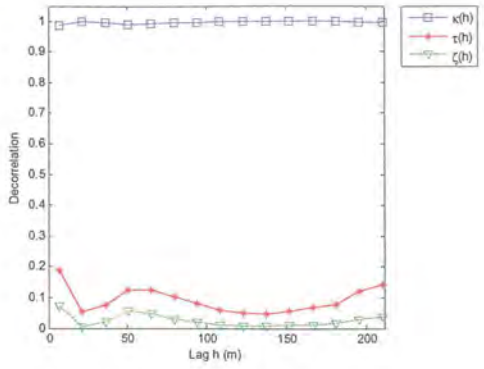
ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 1 1 1 1 1 1 1 1 0 0 0 0 0]



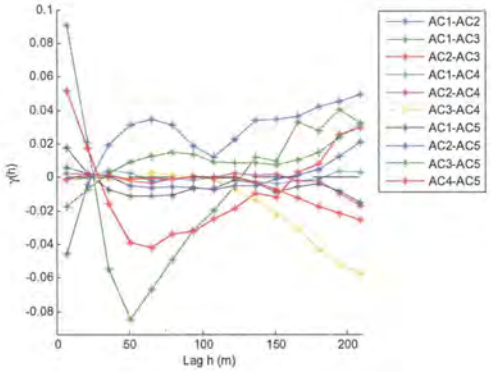


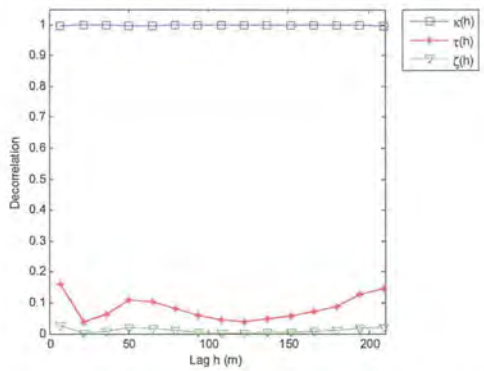
ACDC using Standardised scores and A_{0St} matrix, weight vector [1 1 1 1 1 1 1 1 0 0 0 0 0 0]



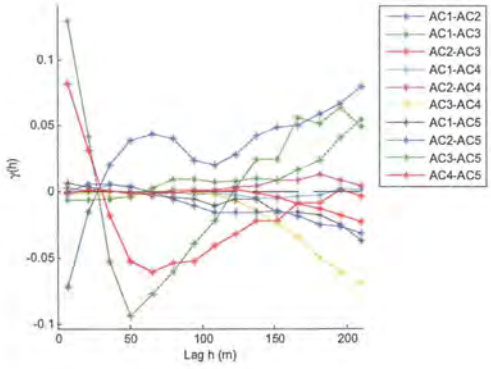


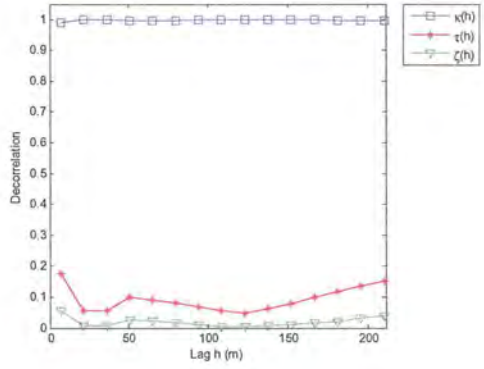
ACDC using Standardised scores and A_{0St} matrix, weight vector [1 1 1 1 1 1 1 1 0 0 0 0 0 0 0]



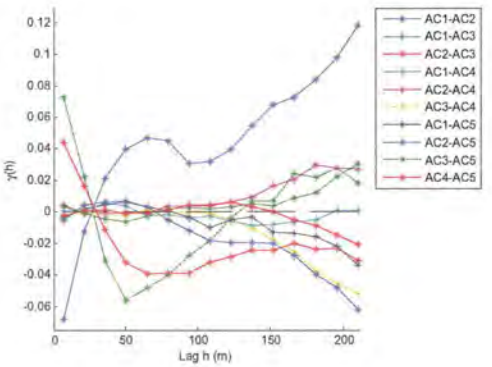


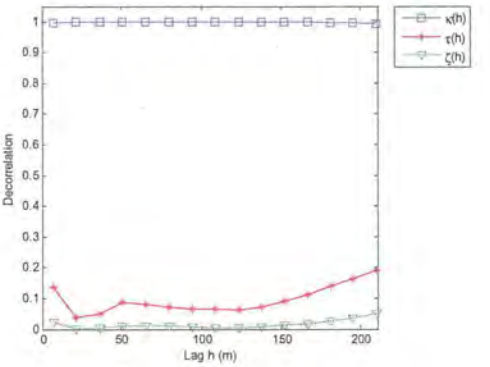
ACDC using Standardised scores and A_{0St} matrix, weight vector [1 1 1 1 1 1 1 0 0 0 0 0 0 0 0]



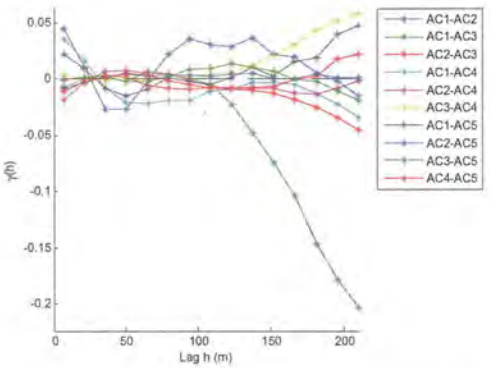


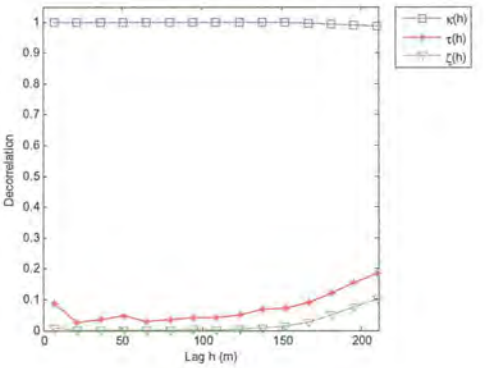
ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 1 1 1 1 0 0 0 0 0 0 0 0 0]



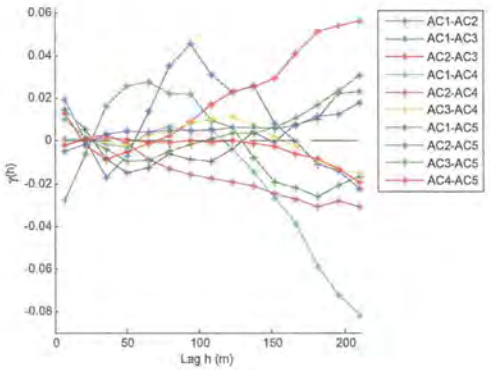


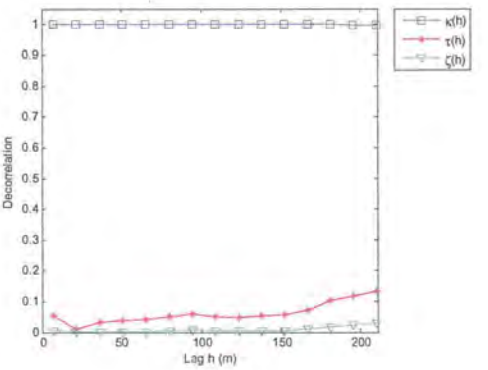
ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 1 1 1 0 0 0 0 0 0 0 0 0 0]



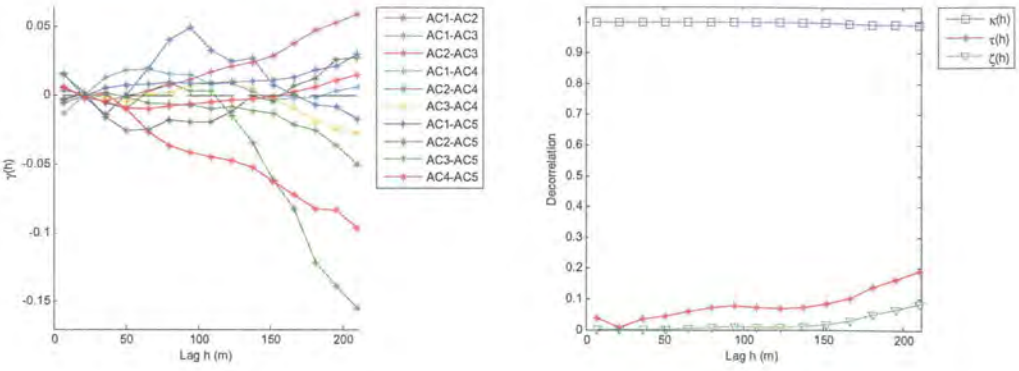


ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 1 1 0 0 0 0 0 0 0 0 0 0 0]

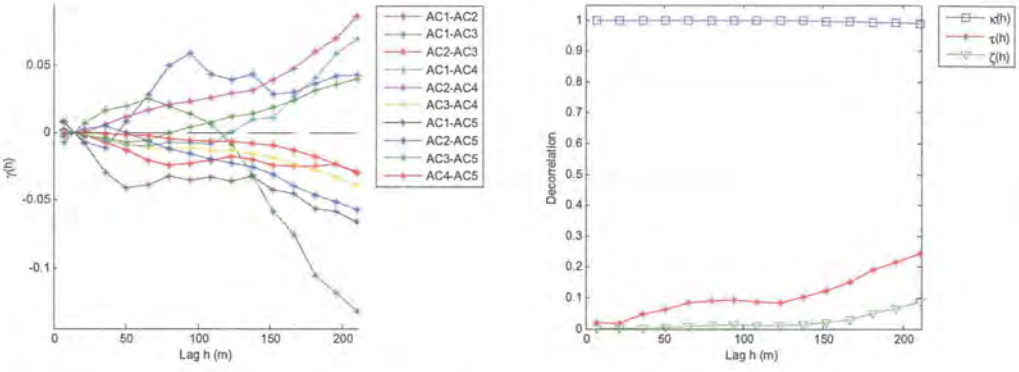




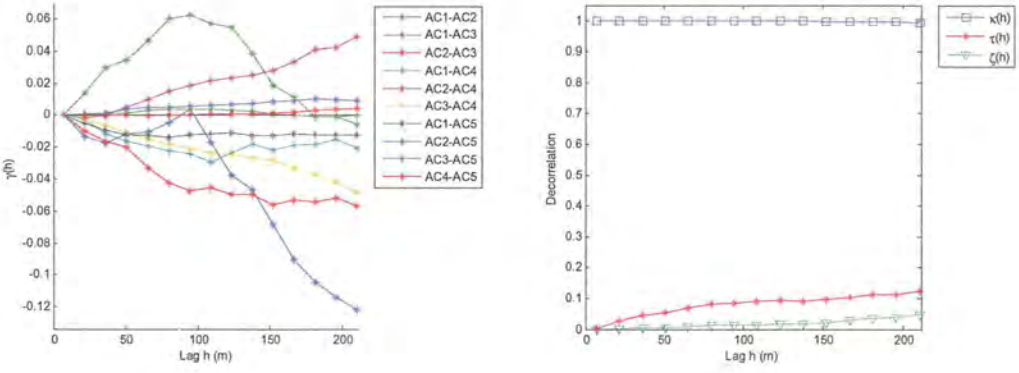
ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 1 0 0 0 0 0 0 0 0 0 0 0 0]



ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 1 0 0 0 0 0 0 0 0 0 0 0 0 0]



ACDC using Standardised scores and $A_{0_{St}}$ matrix, weight vector [1 0 0 0 0 0 0 0 0 0 0 0 0 0 0]



Appendix 6 – MATLAB CODES

6.1 ACDC code

```
function [A,Lam,Nit,Cls]=...
    acdc(M,w,TOL,A0,Lam0);

%acdc: appoximate joint diagonalization
%(in the direct Least-Squares sense) of
%a set of Hermitian matrices, using the
%iterative AC-DC algorithm.
%
%the basic call:
%[A,Lam]=acdc(M);
%
%Inputs:
%
%M(N,N,K) - the input set of K NxN
%           "target matrices". Note that
%           all matrices must be
%           Hermitian (but need not be
%           positive-definite). If they
%           are not Hermitian, an
%           equivalent problem can always
%           be formulated using Hermitian
%           matrices.
%
%Outputs:
%
%A(N,N)   - the diagonalizing matrix.
%
%Lam(N,K) - the diagonal values of the K
%           diagonal matrices.
%
%The algorithm finds an NxN matrix A and
%K diagonal matrices
%         L(:,:,k)=diag(Lam(:,k))
%such that
% C_{LS}=
% \sum_k\|M(:,:,k)-A*L(:,:,k)*A'\|_F^2
%is minimized.
%
%-----------------------------------------
%   Optional additional input/output
%   parameters:
%-----------------------------------------
%
%[A,Lam,Nit,Cls]=
%   acdc(M,w,A0,Lam0);
%
%(additional) Inputs:
%
%w(K) - a set of positive weights such that
%       C_{LS}=
%       \sum_k\w(k)|M(:,:,k)-A*L(:,:,k)*A'\|_F^2
%       Default: w=ones(K,1);
%
%A0 - an initial guess for A
%     default: eye(N);
%
```

```
%Lam0 - an initial guess for the values of
%       Lam. If specified, an AC phase is
%       run first; otherwise, a DC phase is
%       run first.
%
%(additional) Outputs:
%
%Nit - number of full iterations
%
%Cls - vector of Nit Cls values
%
%----------------------------------------
% Additional fixed processing parameters
%----------------------------------------
%
%TOL - a tolerance value on the change of
%      C_{LS}. AC-DC stops when the
%      decrease of C_{LS} is below tol.
%      Originally set to:
%            10^-3/(N*N*sum(w));
%
%MAXIT - maximum number of allowed full
%        iterations.
%        Originally set to: 50;
%
%INTLC - number of AC sweeps to interlace
%        dc sweeps.
%        Originally set to: 1.
%
%----------------------------------------
%
%Note that the implementation here is
%somewhat wasteful (computationally),
%mainly in performing a full eigenvalue
%decomposition at each AC iteration,
%where in fact only the largest eigenvalue
%(and associated eigenvector) are needed,
%and could be extracted e.g. using the
%power method. However, for small N (<10),
%the matlab eig function runs faster than
%the power method, so we stick to it.

%----------------------------------------
%version R1.0, June 2000.
%By Arie Yeredor  arie@eng.tau.ac.il
%
%rev. R1.1, December 2001
%forced s=real(diag(S)) rather than just s=diag(S)
%in the AC phase. S is always real anyway; however,
%it may be set to a complex number with a zero
%imaginary part, in which case the following
%max operation yields the max abs value, rather
%than the true max. This fixes that problem. -AY
%
%Permission is granted to use and
%distribute this code unaltered. You may
%also alter it for your own needs, but you
%may not distribute the altered code
%without obtaining the author's explicit
%consent.
%comments, bug reports, questions
%and suggestions are welcome.
%
```

```
%References:
%[1] Yeredor, A., Approximate Joint
%Diagonalization Using Non-Orthogonal
%Matrices, Proceedings of ICA2000,
%pp.33-38, Helsinki, June 2000.
%[2] Yeredor, A., Non-Orthogonal Joint
%Diagonalization in the Least-Squares
%Sense with Application in Blind Source
%Separation, IEEE Trans. On Signal Processing,
%vol. 50 no. 7 pp. 1545-1553, July 2002.


[N N1 K]=size(M);
if N~=N1
    error('input matrices must be square');
end
if K<2
    error('at least two input matrices are required');
end

if exist('w','var') & ~isempty(w)
    w=w(:);
    if length(w)~=K
        error('length of w must equal K')
    end
    if any(w<0)
        error('all weights must be positive');
    end
else
    w=ones(K,1);
end

if exist('A0','var') & ~isempty(A0)
    [NA0,Nc]=size(A0);
    if NA0~=N
        error('A0 must have the same number of rows as the target
matrices')
    end
else
    A0=eye(N);
    Nc=N;
end

if exist('Lam0','var') & ~isempty(Lam0)
    [NL0,KL0]=size(Lam0);
    if NL0~=Nc
        error('each vector in Lam0 must have M elements')
    end
    if KL0~=K
        error('Lam0 must have K vectors')
    end
    if ~isreal(Lam0)
        error('Lam0 must be real')
    end
    skipAC=0;
else
    skipAC=1;
end

%----------------------------------------
%  here's where the fixed processing-
%  parameters are set (and may be
```

```
%  modified):
%-----------------------------------------
%TOL=1e-3/(N*N*sum(w));
%MAXIT=50;
MAXIT=100000;
%MAXIT=1000000;
INTLC=1;

%-----------------------------------------
%  and this is where we start working
%-----------------------------------------

Cls=zeros(MAXIT,1);
Lam=zeros(N,K);
A=A0;
for Nit=1:MAXIT

    if ~skipAC

        %AC phase
        for nsw=1:INTLC
            for l=1:Nc
                P=zeros(N);
                for k=1:K
                    D=M(:,:,k);
                    for nc=[1:l-1 l+1:Nc]
                        a=A(:,nc);
                        D=D-Lam(nc,k)*a*a';
                    end
                    P=P+w(k)*Lam(l,k)*D;
                end
                [V S]=eig(P);
                s=real(diag(S));     %R1.1 - ay
                [vix,mix]=max(s);
                if vix>0
                    al=V(:,mix);
                    %this makes sure the 1st nonzero
                    %element is positive, to avoid
                    %hopping between sign changes:
                    fnz=find(al~=0);
                    al=al*sign(al(fnz(1)));
                    lam=Lam(l,:);
                    f=vix/((lam.*lam)*w);
                    a=al*sqrt(f);
                else
                    a=zeros(N,1);
                end
                A(:,l)=a;
            end %sweep
        end     %interlaces
    end         %skip AC
    skipAC=0;

    %DC phase
    AtA=A'*A;
    AtA2=AtA.*conj(AtA);
    G=inv(AtA2);
    for k=1:K
        Lam(:,k)=G*diag(A'*M(:,:,k)*A);
        L=diag(Lam(:,k));
        D=M(:,:,k)-A*L*A';
        Cls(Nit)=Cls(Nit)+w(k)*sum(sum(D.*conj(D)));
```

```
    end

    if Nit>1
        if abs(Cls(Nit)-Cls(Nit-1))<TOL
            break
        end
    end

end
Cls=Cls(1:Nit);
```

6.2 Spatial Decorrelation Code Using ACDC method.

```
%Start of Spatial Decorrelation ACDC m file -
%%%%%Getting the matrices into MATLAB
clear
X=xlsread('F:\ACDC_Standardised.xls','5v'); %%% excel spreadsheets
%X=xlsread('F:\ACDC3V.xls','3v_loi+TiO2');

m=size(X,1);

% Inputs
dim=5; % Number of compunds
lag=15; % Number of lags/matrices.
StartH=6.959; % start of H
EndH=209.877;  % last H
Xmin=0;    % min x axis value
Xmax=211;  % max x axis value


p=0;
for i=1:dim
    p=p+i;
end

counter=1;
B=zeros(p*lag,1);
for i=1:m
    if isnan(X(i,2)) || isnan(X(i,3))

    else
        B(counter)=X(i,3);
        counter=counter+1;
    end
end
display(counter)
display(counter-p*lag)

Fred=zeros(dim,dim,lag);

counter=1;
for c=1:dim
    for r=1:c
        for j=1:lag
            Fred(r,c,j)=B(counter);
            Fred(c,r,j)=Fred(r,c,j);
            counter=counter+1;
        end
```

```
    end
end

display(counter-1)
M=Fred

%Getting the off diagonal values from the expeimental semivariogram
matrices
m=zeros(0.5*dim*(dim+1),lag);
figure
counter=1;
for counter1=1:dim
    for counter2=1:counter1
        for i=1:lag
            m(counter,i)=M(counter2,counter1,i);
        end
        counter=counter+1;
    end
end
%%%%%%%%%%%%%%%%%%Experimental Cross semivariograms
counter=1;
mr=zeros(0.5*dim*(dim-1),lag); % mr=off diagonal values of exp
semivariogram
md=zeros(dim,lag);             % md=diagonal values of exp.
semivariograms
for i=1:0.5*dim*(dim+1)
    if i==0.5*counter*(counter+1)
        md(counter,:)=m(i,:);
        counter=counter+1;
    else
        mr(i+1-counter,:)=m(i,:);
    end
end
hold on
l=linspace(StartH,EndH,lag);
z=zeros(lag,1);
plot(l,mr,'-*')
plot(l,z,'k--')
xlabel('Lag h (m)')
ylabel('\gamma(h)')
hold off
Ymin=(min(min(mr)))*1.1;
Ymax=(max(max(mr)))*1.1;
axis([Xmin Xmax  Ymin Ymax])

%%%%%%%%%%Legends for variables
legend5 = legend('Fe & Al_2O_3','SiO_2 & Al_2O_3','SiO_2 & Fe','TiO_2
& Al_2O_3','TiO_2 & Fe','TiO_2 & SiO_2','Al_2O_3 & LOI','LOI &
Fe','LOI & SiO_2','LOI & TiO_2','Location','NEO');

%%%%%%%%Titles
    h=Title('Cross Semivariograms of Standardised Variables')
    %h=Title('Cross Semivariograms of Normal Score Variables')
    set(h,'FontSize',12,'FontWeight','bold');

%%%%%%%%%%%%% ACDC Algorithms

A0=[0.505   0.1385  -0.3394 -0.6989 -0.3494;        %PCA eigenvectors
matrix using standardised data
    -0.5197 0.1936  -0.2077 0.1586  -0.79;
    0.4069  -0.5783 0.467   0.1988  -0.4923;
    0.4688  0.0715  -0.5987 0.6455  -0.0038;
```

```
    0.2992   0.777    0.5149   0.1736   -0.1069];

%A0=[ 0.4995   -0.2914   -0.3244    0.7085    0.2416 ;    %PCA eigenvector
matrix using normal scores data
%     -0.5131   -0.3250   -0.1737   -0.1130    0.7670 ;
%     0.3927    0.6743    0.2085   -0.1020    0.5807 ;
%     0.4789   -0.2269   -0.5185   -0.6711    0.0079;
%     0.3220   -0.5507    0.7432   -0.1566    0.1273 ];

        w=[1,0,0,0,0,0,0,0,0,0,0,0,0,0,0];    %%% weigh vector
        NitTemp=1;
        TOL=1e-16;
    [A,D,Nit,Cls]=acdc(M,w,TOL);       %%%%%%%%%% ACDC with no AO
    [A,D,Nit,Cls]=acdc(M,w,TOL,A0);    %%%%%%%%%%ACDC with an AO

%%%%%%%%%%End of ACDC

inv(A) %%%% transformation matrix

display(M) % matrices of experimental semivariogram matrices
b3=zeros(dim,dim,lag);
for i=1:lag
      b3(:,:,i)=inv(A)*M(:,:,i)*inv(A'); %% Obtaining the Factor
      matrices
end
display(b3) % decorrelated factor matrices

%%%%%%Getting the cross validation decorrelated Factor values from the
matrices into vectors for plotting )

b=zeros(0.5*dim*(dim+1),lag);

counter=1;
for counter1=1:dim
    for counter2=1:counter1
        for i=1:lag
            b(counter,i)=b3(counter2,counter1,i);
        end
        counter=counter+1;
    end
end

figure
counter=1;
br=zeros(0.5*dim*(dim-1),lag);    % br=off diagonal factor values
bd=zeros(dim,lag);                % bd=diagonal factor values
for i=1:0.5*dim*(dim+1)
    if i==0.5*counter*(counter+1)
        bd(counter,:)=b(i,:);
        counter=counter+1;
    else
        br(i+1-counter,:)=b(i,:);
    end
end
hold on
l=linspace(StartH,EndH,lag);
z=zeros(lag,1);
plot(l,br,'*-')
plot(l,z,'k--')
xlabel('Lag h (m)')
ylabel('\gamma(h)')
```

```
hold off
Ymin=(min(min(br)))*1.1;
Ymax=(max(max(br)))*1.1;
axis([Xmin Xmax  Ymin Ymax])
legend5 = legend('AC1-AC2','AC1-AC3','AC2-AC3','AC1-AC4','AC2-
AC4','AC3-AC4','AC1-AC5','AC2-AC5','AC3-AC5','AC4-
AC5','Location','NEO');
br;

% Zeta values and plot
yy=(br).^2;
zeta=sum(yy)*2
figure
l=linspace(StartH,EndH,lag);%*****????
z=zeros(lag,1);
plot(l,zeta,'g-v',l,z,'k--')
xlabel('Lag h (m)')
ylabel('\zeta(h)')
z1=min(zeta)
z2=max(zeta);
Ymin=z1-(z1*0.1);
Ymax=z2+(z2*0.1);
axis([Xmin Xmax  Ymin Ymax])
legend('\zeta(h)','Location','NEO');

% Average Zeta Value
AveZeta=sum(zeta)/lag

%Tau Values and plot
xx= sum(abs(br))*2;
rr=sum(abs(bd));
tau=(xx)./(rr)
figure
l=linspace(StartH,EndH,lag);%*****????
z=zeros(lag,1);
plot(l,tau,'r-*',l,z,'k--')
xlabel('Lag h (m)')
ylabel('\tau(h)')
z1=min(tau);
z2=max(tau);
Ymin=z1-(z1*0.1);
Ymax=z2+(z2*0.1);
axis([Xmin Xmax  Ymin Ymax])
legend('\tau(h)','Location','NEO');

%Average Tau
AveTau=sum(tau)/lag

% Kappa Value and plot
jj=(mr).^2;
ori=sum(jj)*2;
ii=zeta./ori;
kappa=1-ii
figure
l=linspace(StartH,EndH,lag);
z=zeros(lag,1);
plot(l,kappa,'b-s',l,z,'k--')
xlabel('Lag h (m)')
ylabel('\kappa(h)')
    z1=min(kappa);        % very high negative values
    z2=max(kappa);
    Ymin=z1+(z1*0.1);
```

```
    Ymax=z2-(z2*0.1);
z1=min(kappa);    % positive
z2=max(kappa);
Ymin=z1-(z1*0.1);
%Ymin=0;
Ymax=z2+(z2*0.1);
axis([Xmin Xmax  Ymin Ymax])
legend('\kappa(h)','Location','NEO');

%Average Kappa
AveKappa=sum(kappa)/lag


%Plot for all spatial decorrelation measures
figure
linspace(StartH,EndH,lag);
z=zeros(lag,1);
plot(l,kappa,'b-s',l,tau,'r-*',l,zeta,'g-v',l,z,'k--')
xlabel('Lag h (m)')
ylabel('Decorrelation')
Ymin=[];
Ymax=[];
   % z1=min(kappa);  % Very negative values
   % z2=max(zeta);
   % Ymin=z1+(z1*0.1);
   % Ymax=z2+(z2*0.1);
Ymin=0;
Ymax=1.05;
axis([Xmin Xmax  Ymin Ymax])
%% Create legend
legend1 = legend('\kappa(h)','\tau(h)','\zeta(h)','Location','NEO');
%%%%%%%%%%%%%Titles
    %h=Title('ACDC using Normal scores and A0_N_S')
    %h=Title('ACDC using Normal scores')
    h=Title('ACDC using Standardised scores and A0_S')
    %h=Title('ACDC using Standardised scores')
    set(h,'FontSize',12,'FontWeight','bold');

%%%%%%%% Eigenvalues of Experimental semivariogram matrices
for i=1:lag
    eig(M(:,:,i))
end

%%%%%%%%%%Average Spatial Decorrelation Measures
AveZeta
AveTau
AveKappa

%%%%%%%%%%Plot the direct semivariograms
m=zeros(0.5*dim*(dim+1),lag);
figure
counter=1;
for counter1=1:dim
    for counter2=1:counter1
        for i=1:lag
            m(counter,i)=M(counter2,counter1,i);
        end
        counter=counter+1;
    end
end

counter=1;
```

```
mr=zeros(0.5*dim*(dim-1),lag); % mr=off diagonal values of exp
semivariogram
md=zeros(dim,lag); % md=diagonal values of exp. semivariograms
for i=1:0.5*dim*(dim+1)
    if i==0.5*counter*(counter+1)
        md(counter,:)=m(i,:);
        counter=counter+1;
    else
        mr(i+1-counter,:)=m(i,:);
    end
end

hold on
l=linspace(StartH,EndH,lag);%****????
z=zeros(lag,1);
plot(l,md,'-*')
plot(l,z,'k--')
xlabel('Lag h (m)')
ylabel('\gamma(h)')
hold off
Ymin=(min(min(md)));
Ymax=(max(max(md)))*1.1;
axis([Xmin Xmax  Ymin Ymax])

%Legends
legend5 =
legend('Al_2O_3','Fe','SiO_2','TiO_2','LOI','Location','NEO');
 %h=Title('Experimental Direct Semivariograms of Standardised
Variables')
h=Title('Experimental Direct Semivariograms of Normal Score
Variables')
set(h,'FontSize',12,'FontWeight','bold');
```

6.3 Spatial Decorrelation Code Using MAF and PCA Factors

```
%M-File used to obtain  MAF and PCA spatial decorrelation results
clear;
A=xlsread('F:\MAF&PCA_5V.xls','MAF5_S');   % The MAF/PCA factor global
stats

m=size(A,1);

% Inputs
dim=5; % Number of compunds
lag=15; % Number of lags/matrices.
StartH=6.959; % start of H
EndH=209.877;  % last H
Xmin=0;    % min x axis value
Xmax=210;  % max x axis value


p=0;
for i=1:dim
    p=p+i;
end

counter=1;
B=zeros(p*lag,1);
```

```
for i=1:m
    if isnan(A(i,2)) || isnan(A(i,3))

    else
        B(counter)=A(i,3);
        counter=counter+1;
    end
end
display(counter)
display(counter-p*lag)

Fred=zeros(dim,dim,lag);

counter=1;
for c=1:dim
    for r=1:c
        for j=1:lag
            Fred(r,c,j)=B(counter);
            Fred(c,r,j)=Fred(r,c,j);
            counter=counter+1;
        end
    end
end

display(counter-1)


b3=Fred
display(b3) % decorrelated matrices

%Getting the cross validation decorrelated values from the matrices
into
%vectors for plotting

b=zeros(0.5*dim*(dim+1),lag);

counter=1;
for counter1=1:dim
    for counter2=1:counter1
        for i=1:lag
            b(counter,i)=b3(counter2,counter1,i);
        end
        counter=counter+1;
    end
end

figure
counter=1;
br=zeros(0.5*dim*(dim-1),lag);  % br=off diagonal values
bd=zeros(dim,lag);              % bd=diagonal values
for i=1:0.5*dim*(dim+1)
    if i==0.5*counter*(counter+1)
        bd(counter,:)=b(i,:);
        counter=counter+1;
    else
        br(i+1-counter,:)=b(i,:);
    end
end
hold on
l=linspace(StartH,EndH,lag);
z=zeros(lag,1);
```

```
plot(l,br,'*-')
plot(l,z,'k--')
xlabel('Lag h (m)')
ylabel('\gamma(h)')
hold off
%end of boogie
Ymin=-0.15
Ymax=0.15
%Ymin=(min(min(br)))*1.1;
%Ymax=(max(max(br)))*1.1;
axis([Xmin Xmax  Ymin Ymax])% might need to change (,, min value of b
and maximum value of b)

%LEGENDS

legend5 = legend('M1-M2','M1-M3','M2-M3','M1-M4','M2-M4','M3-M4','M1-
M5','M2-M5','M3-M5','M4-M5','Location','NEO');
%legend5 = legend('PC1-PC2','PC1-PC3','PC2-PC3','PC1-PC4','PC2-
PC4','PC3-PC4','PC1-PC5','PC2-PC5','PC3-PC5','PC4-
PC5','Location','NEO');
%h=Title('Cross Semivariograms of MAF Factors using Normal Scores');
h=Title('Cross Semivariograms of MAF Factors using Standardised
Scores')
set(h,'FontSize',12,'FontWeight','bold');
br
% zeta
yy=(br).^2;
zeta=sum(yy)*2
figure
l=linspace(StartH,EndH,lag);%****????
z=zeros(lag,1);
plot(l,zeta,'g-v',l,z,'k--')
xlabel('Lag h (m)')
ylabel('\gamma(h)')
%z1=min(zeta);
z2=max(zeta);
Ymin=0;
%Ymin=z1-(z1*0.1);
Ymax=z2+(z2*0.2);
axis([Xmin Xmax  Ymin Ymax])
legend('\zeta(h)','Location','NEO');

% Average Zeta
AveZeta=sum(zeta)/lag

%tau
xx= sum(abs(br))*2;
rr=sum(abs(bd));
tau=(xx)./(rr)
figure
l=linspace(StartH,EndH,lag);%****????
z=zeros(lag,1);
plot(l,tau,'r-*',l,z,'k--')
xlabel('Lag h (m)')
ylabel('\gamma(h)')
%z1=min(tau);
z2=max(tau);
%Ymin=z1-(z1*0.1);
Ymin=0;
Ymax=z2+(z2*0.1);
axis([Xmin Xmax  Ymin Ymax])
legend('\tau(h)','Location','NEO');
```

```
%Average Tau
AveTau=sum(tau)/lag

%Get the experimental semivariogram
A1=xlsread('F:\ACDC_Standardised.xls','5v'); %Original experimental
semivariogram results
%A1=xlsread('F:\ACDC3V.xls','3v_loi+TiO2');


m=size(A1,1);

% Inputs
dim=5; % Number of compunds
lag=15; % Number of lags/matrices.
StartH=6.959; % start of H
EndH=209.877;  % last H
Xmin=0;    % min x axis value
Xmax=210;  % max x axis value


p=0;
for i=1:dim
    p=p+i;
end

counter=1;
B=zeros(p*lag,1);
for i=1:m
    if isnan(A1(i,2)) || isnan(A1(i,3))

    else
        B(counter)=A1(i,3);
        counter=counter+1;
    end
end
display(counter)
display(counter-p*lag)

Fred1=zeros(dim,dim,lag);

counter=1;
for c=1:dim
    for r=1:c
        for j=1:lag
            Fred1(r,c,j)=B(counter);
            Fred1(c,r,j)=Fred1(r,c,j);
            counter=counter+1;
        end
    end
end

display(counter-1)
M=Fred1

%kappa

% Start of getting the off diagonal values from the origianl
experimental
% semivariograms matrices
```

```
m=zeros(0.5*dim*(dim+1),lag);

counter=1;
for counter1=1:dim
    for counter2=1:counter1
        for i=1:lag
            m(counter,i)=M(counter2,counter1,i);
        end
        counter=counter+1;
    end
end

counter=1;
mr=zeros(0.5*dim*(dim-1),lag); % mr=off diagonal values of exp
semivariogram
md=zeros(dim,lag); % md=diagonal values of exp. semivariograms
for i=1:0.5*dim*(dim+1)
    if i==0.5*counter*(counter+1)
        md(counter,:)=m(i,:);
        counter=counter+1;
    else
        mr(i+1-counter,:)=m(i,:);
    end
end

%end of getting values and start of kappa

jj=(mr).^2;
ori=sum(jj)*2;
ii=zeta./ori;
kappa=1-ii
figure
l=linspace(StartH,EndH,lag);%****????
z=zeros(lag,1);
plot(l,kappa,'b-s',l,z,'k--')
xlabel('Lag h (m)')
ylabel('\gamma(h)')
%z1=min(kappa)
z2=max(kappa);
%Ymin=z1-(z1*0.01)
Ymin=0;
Ymax=z2+(z2*0.1);
axis([Xmin Xmax  Ymin Ymax])
legend('\kappa(h)','Location','NEO');

%Average Kappa
AveKappa=sum(kappa)/lag

%plot all averages
figure
linspace(StartH,EndH,lag);
z=zeros(lag,1);
plot(l,kappa,'b-s',l,tau,'r-*',l,zeta,'g-v',l,z,'k--')
xlabel('Lag h (m)')
ylabel('Decorrelation')
Ymin=[];
Ymax=[];
z1=min(zeta);
Ymin=z1-(z1*0.5);
Ymax=max(kappa)*1.1;
axis([Xmin Xmax  Ymin Ymax])
```

```
%% Create legend
legend1 = legend('\kappa(h)','\tau(h)','\zeta(h)','Location','NEO');
%h=Title('MAF using Normal scores')
h=Title('MAF using Standardised scores')
set(h,'FontSize',12,'FontWeight','bold');
for i=1:15
    eig(M(:,:,i))
end

AveZeta
AveTau
AveKappa
```