Natural neighbour kriging
and its potential for quality mapping and grid design

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Natural Neighbour Kriging
and its potential for quality mapping and grid design

by

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Spatial interpolation is an essential tool in geosciences. Often a limited number of observations, for example elevation or temperature measurements, are conducted and interpolation is used to estimate values at unobserved locations. Kriging is a widely used stochastic interpolation method. Kriging calculates the dissimilarities between data pairs and uses this relationship to determine the interpolation weights in such way that the estimation variance is minimized. Kriging estimates are relatively accurate and yield a smaller prediction error than estimates obtained with other interpolation methods. An additional advantage of kriging, compared to other methods, is that it also gives a quality descriptor, namely the kriging variance. However, kriging requires inversion of matrices and can therefore be a computationally inefficient process when dealing with large datasets. A way to overcome this problem is the use of an interpolation neighbourhood, a selected subset of the input points that are close to the estimation point, rather than using all input points. In this study the use of natural neighbours as interpolation neighbourhood is presented. The natural (or Sibson) neighbours of a certain estimation point are the observations points of which their initial Voronoi tessellation is altered by the introduction of that point. The use of natural neighbours could be a good compromise between the number and spread of input points for kriging. Two case study bathymetry datasets from the North Sea are used to examine the potential of natural neighbour kriging and the suitability of the method for different datasets with distinct signals and configurations. A comparison is made between regular kriging methods and natural neighbour kriging methods. The interpolation results are presented in an insightful way, giving information about the input points and the distribution of the estimation errors, using quadtree decomposition and contour mapping. The kriging variance is used as input parameter for quadtree decomposition to design of an adaptive interpolation grid where cell sizes increase with increasing uncertainty. Natural neighbour kriging is proven to be a useful interpolation method: the computational speed is improved considerably compared to regular kriging methods and the selection of the natural neighbours is local and reflect the configuration of the input data. Moreover, cross validation results have shown that natural neighbour kriging performs well compared to other kriging methods and natural neighbour interpolation.
The past year I have been working on this project to complete my master program in Geoscience and Remote Sensing. Throughout this year I learned a lot about spatial interpolation techniques, especially kriging, and I got to improve my programming skills greatly. I very much enjoyed working on this project and therefore I am thrilled to bits to finally present the summary of my research to you in this report!

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S.C. van der Graaf
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List of abbreviations

**AF**  Anisotropy factor

**AOK**  Anisotropic ordinary kriging

**AOK\textsubscript{NN} / AOK\textsubscript{nn}**  Anisotropic natural neighbour kriging

**AOK\textsubscript{ANN} / AOK\textsubscript{ann}**  Anisotropic natural neighbour kriging using only anisotropic neighbours

**LOO**  Leave one out (cross validation)

**MBES**  Multi beam echo sounder

**MCS**  Multi-channel sparker

**MSE**  Mean squared error

**MSE\textsubscript{10}**  Mean squared error after removal of 10 highest error points

**MSE\textsubscript{20}**  Mean squared error after removal of 20 highest error points

**NEA**  Netherlands Enterprise Agency

**NN**  Natural neighbour interpolation

**OK**  Ordinary kriging

**OK\textsubscript{NN} / OK\textsubscript{nn}**  Natural neighbour kriging

**RD**  Rijksdriehoek

**RNLN**  Royal Netherlands Navy

**SBES**  Single beam echo sounder

**WFS**  Wind farm site
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Introduction

Data acquisition can be a time consuming and expensive process. It is often impossible to gather information throughout the entire research area, and one has to settle for a limited number of observations that are conducted. For example, a restricted number of weather stations needs to account for the temperature overview of an entire region. The temperature must be estimated in between these weather stations in order to cover the entire region.

Estimates of the unknown field values in unsampled locations can be obtained using spatial interpolation techniques. The known data points surrounding an unknown location are weighted to acquire field values at every location. There are various types of interpolation techniques available, all different in what points are considered and how the weights of these estimation points are determined. In general nearby points obtain more weight than distant points, as supported by Tobler’s first law of geography: “Everything is related to everything else, but near things are more related than distant things”. In the sections below two types of interpolation techniques that are relevant for this research, namely kriging and natural neighbour interpolation, are shortly discussed. The next section emphasizes on the problem and project description and the research questions. In the last section an overview of the thesis organization is given.

1.1. Kriging

The theory for kriging, a stochastic interpolation approach, was developed first by the mathematician Georges Matheron in 1951 [Krige (1951)]. The interpolation method was named kriging, after the student that worked out the method during his master research, Danie Krige. The idea of kriging is to calculate the dissimilarity between data points pairs and use this relationship to estimate the interpolation weights. The dissimilarities between the points are used to quantify the spatial dependence of the points in a so-called variogram. This variogram is used to predict the weights at unobserved locations such that it minimizes the estimation variance. Many variations of kriging have been developed until now. These variations mainly differ in the assumptions that are made on the estimated fields. For example, the most straightforward type of kriging, simple kriging, assumes stationarity of the mean over the entire field. The type of kriging that is most suitable for a given dataset depends on the stochastic properties of the field and the availability of the observations. An advantage of kriging is that it also gives a quality description of the result, namely an estimation of the variance [Goovaerts (1997)].

1.2. Natural neighbour interpolation

Natural neighbour interpolation is a weighted average interpolation method developed by Robin Sibson in 1981 [Sibson (1981)]. The method consists of two steps. First, a so-called “Voronoi” tessellation of the observed points is created. These Voronoi cells define all locations that are closest to that point. Second, locally a new Voronoi tessellation is created for each of the estimation point separately. The effect of this new point on the existing tessellation is the measure for the interpolation weights. All observation points of which their Voronoi cell is altered by the introduction of the new estimation point are called the “natural neighbour” of that point. The weight given to each natural neighbour is the area that is ‘stolen’ from its Voronoi cell divided by the total area of the Voronoi cell of the interpolation point [Sibson (1981)], as illustrated in Figure 1.1.
Natural neighbour interpolation is a good method to interpolate large datasets, because only a set of neighbouring points is used for the calculation of the weights. Another advantage of natural neighbour interpolation is that the selection of neighbours is based on the configuration of the dataset, taking into account spatial variations in data density [Dumitru et al. (2013)].

1.3. Problem and project description
The calculation of kriging weights can be a computationally demanding process when dealing with large datasets. The creation of the variogram as well as the inversion of large matrices during kriging can be very time-consuming processes. The common way to overcome this problem is to locally only include a subset of nearby points in the kriging process. This subset of points is often called the interpolation neighbourhood. The main focus of this study is to assess the effectiveness of natural neighbours as interpolation neighbourhood used for kriging. This method will be referred to as 'natural neighbour kriging'. Natural neighbour kriging combines the favourable geometrical aspects of natural neighbours and the stochastic aspects of kriging and therefore is a promising technique. To illustrate the potential of natural neighbour kriging the method and its interpolation results are compared to the results of ordinary kriging and natural neighbour interpolation.

In practice interpolation results are often used without reconsidering the original inputs and its quality. Another important focus of this research is to insightfully visualize the results of natural neighbour kriging, such that it is clear to what extent each input point contributes to the final result and how the estimation errors are distributed. A tool that can be used to display both the geometry of the input and the error distribution of the output is the interpolation grid cell size. In this research the adaptation of the interpolation grid to spatial variations of both the input data and the errors of the results are examined using, among others, quad tree computations and data structures.

1.4. Research questions
The goals of this project are translated to the following main question:

What is the potential of natural neighbour kriging for quality mapping and grid design?

In this project quality mapping means interactive visualisation of the interpolation results, in a way that the associated errors are displayed. Grid design means the determination of the wanted geometry of the interpolation grid based on the input data itself and other relevant parameters, for example the error distribution of the interpolation results.

The following sub questions are derived from this main question:

1. How can the potential of natural neighbour kriging as interpolation technique be assessed?

2. What criteria are relevant for assessing the quality of natural neighbour kriging as an interpolation technique?
3. To what extent does natural neighbour kriging meet these criteria?

4. How does this method compare to other kriging methods based on the previously mentioned criteria?

5. For what type of geostatistical data is natural neighbour kriging interpolation suitable?

6. How can the interpolation result be presented to users in an insightful way, providing information about both the quality of the result and the contribution of the input data points?

7. How can the interpolation grid cell size be adapted to spatial variation in distribution and quality of the input data and interpolation results?

1.5. Thesis overview

The theoretical background information on spatial interpolation is given in the Chapter 2. The methodology of natural neighbour kriging is described in Chapter 3. The first section of Chapter 3 emphasizes on the theory of natural neighbour kriging and the used algorithm. The last section describes the adjustment of natural neighbour kriging for anisotropic datasets. Chapter 4 describes the methods that are used for quality mapping and grid design. Chapter 5 emphasizes on the used datasets and where each dataset is used for. The results for the used datasets will be presented in Chapter 6. The results for quality mapping and grid design are given in Chapter 7. The conclusions and some suggestions for further research are finally presented in the last chapter, Chapter 8.
Spatial interpolation methods

Estimates of unknown field values at unsampled locations can be obtained using spatial interpolation. The known data points surrounding an unknown location are weighted to acquire field values at wanted locations. There are various types of interpolation techniques available, all different in what points are considered and how the weights of these estimation points are determined. In general nearby points obtain more weight than distant points, as supported by Tobler’s first law of geography: “Everything is related to everything else, but near things are more related than distant things” [Tobler (1970)].

In this chapter the interpolation techniques that are relevant for this thesis are explained, kriging, a stochastic interpolation method and two Voronoi-based deterministic interpolation methods. The first section of this chapter emphasizes on how the quality of interpolation results can be assessed in general. The second section emphasizes on the theory of kriging. In the second section two Voronoi-based methods are explained. In the last section the concept of cross-validation is explained.

2.1. Watson criteria

There are a number of criteria proposed in literature studies, most of them by Watson [Watson (1992)], that can be used to describe an interpolation method in general. According to Watson the quality of an interpolation method for geoscientific datasets can be assessed using the following essential properties. A “good” interpolation method should be:

1. **exact**: the data points should be ‘honoured’ by the interpolant, or the interpolant must ‘pass through’ them.
2. **continuous**: the estimated value at each location should be single and unique.
3. **smooth**: the first and second derivative of the function should be obtainable at every location.
4. **local**: the interpolation function should only use neighbouring data points to estimate a value at a given location
5. **adaptable**: the interpolation function should adapt to anisotropic data distributions and should give realistic results.
   Additional considerations are given by Ledoux [Ledoux (2012)], these include the following:
6. **computationally efficient**
7. **automatic**: the method should not rely on user-defined parameters that require a priori knowledge of the datasets.

The quality of the interpolation methods will be discussed based on these abovementioned criteria. Most of these criteria can be either true or false, for example an interpolation method gives exact results or not. This is the case for the first five criteria and therefore these five will be evaluated based on either a (+)- (meaning the criteria is valid) or a (-)-ranking (meaning the criteria is not valid) and these rankings will be given in a
table for each interpolation method. The last two criteria will be discussed separately for each method.

The computational efficiency of an algorithm is a description of the computational resources required for that algorithm. The actual computational efficiency is determined by a complex interplay of computer-based, data-specific and algorithm-specific factors. In this study all computations are performed on the same computer and compared for the same datasets, therefore only algorithm-specific factors will be considered and described using the theoretical computational efficiency. The theoretical computational efficiency is described by the big O notation, also called the Landau symbol, which describes the order of the algorithm and thus how the algorithm responds to changes in input size. The O symbol can be used to describe both the time efficiency as well as the storage efficiency of an algorithm, however in this study only a description of the time complexity is considered. For example, for an algorithm with a theoretical efficiency given by \( O(n) \) time, in which \( n \) is the size of the input values, in the order of \( n \) actions have to be performed to run this algorithm. An example of such an algorithm is finding the smallest number in an unsorted array of length \( n \) [Berg et al. (2008)]. For comparison only the theoretical computational efficiency as given by \( O \) will be considered, for determination and optimization of the actual computational efficiency is beyond the scope of this research.

2.2. Kriging

Kriging is an interpolation technique that obtains optimally accurate predictions in terms of Mean Squared Prediction Error (MSPE). When the kriging assumptions hold, kriging performs better in terms of accuracy as measured by the MSPE than many other methods, for example nearest neighbours and linear interpolation [Cressie (1993)].

Ordinary kriging is the basis kriging technique and it is essentially a weighted average method. This means that the unknown value at a certain location is calculated by weighting the observations at known locations by a list of weight coefficients. The unknown value at a certain location is thus predicted by [Felus (2005)]:

\[
\hat{Z}(s_0) = w_1 \cdot z(s_1) + w_2 \cdot z(s_2) + \cdots + w_n \cdot z(s_n)
\] (2.1)

The distinct difference between other weighted average methods and kriging is that kriging uses a spatial dependence function to calculate the weights coefficients of the observed data points. A spatial dependence function describes the relationship of the observed values as a function of their separation distance. Frequently, variogram models are used as spatial dependence model in kriging. Globally, there are two main steps in kriging, first the variogram estimation and then the actual interpolation step [Felus (2005)].

Optimal kriging estimates can only be achieved when the data satisfies the following conditions [Felus (2005)]:

1. There is no trend or drift in the data. In other words, the expected difference in values between different locations is zero:

\[
E[z(s) - z(s + h)] = 0
\] (2.2)

where \( E \) is the expectation and \( h \) is the separation distance or lag between the points \( s \) and \( s+h \).

2. The variance difference is a function of distance \( h \), and \( h \) only, between two locations \( s \) and \( s+h \):

\[
\text{Var}[z(s) - z(s + h)] = E[z(s) - z(s + h)]^2 = 2 \cdot \gamma
\] (2.3)

where \( \text{Var} \) is the variance and \( \gamma(h) \) is the semi-variogram value at lag \( h \).

When these conditions are met the field is said to be second order stationary. These conditions can either be met initially, or after pre-processing of the dataset.

2.2.1. Variogram estimation

The variogram is a measure for the dissimilarity between data points at different locations. The estimation of the variogram that will be used in the kriging weight estimation consists of two steps. The first step is the calculation of the so-called experimental semi-variogram using all, or a distance-limited set of data points. Then, in order to describe the spatial variability with a continuous function a mathematical function must be fit through this experimental semi-variogram. The experimental semi-variogram is computed as [Felus (2005), Goovaerts (1997)]

\[
\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [z(s_i) - z(s_i + h)]^2
\] (2.4)
where \( N(h) \) is the number of pairs of data locations that are vector \( h \) apart.

The resulting semi-variogram provides a set of discrete variance values for a finite number of lags and distances. In order to obtain a continuous description of the variance with distance a positive definite mathematical function must be fit to the discrete semi-variogram, examples of these function are given in Figure 2.1. These functions are commonly fit in a least-squares sense.

The variogram is the function that is fit to the experimental semi-variogram. There are three characteristic key parameters that describe the spatial relationship given in a variogram: the range, sill and nugget. The distance (value on the x-axis) at which the variogram model flattens out is known as the range. Sample locations with separation distances larger than the range are not spatially correlated. The variance (value on the y-axis) at which the variogram reaches the range is called the sill. The sill depicts the maximum variability between data pairs [Felus (2005)].

Theoretically one would expect the variogram value to be zero at zero separation. The semi-variogram exhibits a nugget or nugget effect if the model intercepts the y-axis at any value larger than zero, e.g. a discontinuity at the origin. The nugget effect can be attributed to measurement errors and in some cases to actual spatial variations at small separation distances. There are various types of admissible mathematical functions of which the following three basic variogram models are most frequently used [Goovaerts (1997)]:

- **Spherical model**
  \[
  g(h) = \text{Sph} \left( \frac{h}{a} \right) = \begin{cases} 
  1.5 \cdot \frac{h}{a} - 0.5 \cdot \frac{h^3}{a^3} & \text{if } h \leq a \\
  1 & \text{otherwise}
  \end{cases} 
  \]  
  (2.5)

- **Exponential model**
  \[
  g(h) = 1 - \exp \left( \frac{-3h}{a} \right) 
  \]  
  (2.6)

- **Gaussian model**
  \[
  g(h) = 1 - \exp \left( \frac{-3h^2}{a^2} \right) 
  \]  
  (2.7)

The spherical model completely levels off at the sill at distance \( a \), the actual range. The exponential and the Gaussian model reach their sill asymptotically, and the practical range, \( a \), is then defined as the distance at which the function reaches 95% of the sill. The spatial dependence between data points is sometimes described by a covariance function \( C \) rather than a variogram function. Also during the actual interpolation step, the relationship given in a variogram is translated to covariance values rather than variances. For bounded variograms, this relationship is expressed as [Goovaerts (1997)]:

\[
\gamma(h) = C(0) - C(h) 
\]  
(2.8)
2. Spatial interpolation methods

2.2.2. Kriging interpolation

The fitted variogram model will be used in kriging to predict the values at the unobserved locations in such way that the results will be unbiased and best. The results are said to be unbiased when the expected values are equal to their true values. The result is called best if the residual variance is minimized [Goovaerts (1997)].

There are three frequently used variants of kriging: simple kriging (SK), ordinary kriging (OK) and universal kriging (UK). These variants are distinguished based on the handling of the fields mean. Simple kriging assumes that the mean is known and constant throughout the whole study area. In practice, the local mean of the field often varies over the study area. Ordinary kriging accounts for local fluctuations of the mean by limiting the stationarity domain of the mean to a local neighbourhood around the estimation location. In ordinary kriging the mean is assumed to be constant in this local neighbourhood, and assumed to be unknown. Universal kriging, also known as trend kriging, also accounts for local variations of the mean. Universal kriging assumes that the mean of the field can be locally modelled by a polynomial trend model rather than a constant value [Goovaerts (1997)]. Ordinary kriging is often seen as the basic kriging technique, for it requires no input information on the mean of the field [Felus (2005)]. The next part of this section will therefore focus on the equations used in ordinary kriging.

The system $d_n = C_0 * w_n$ is called the ordinary kriging equation. The ordinary kriging results will be unbiased and best if the vector $w_n$, the error variance vector, is resolved the following way [Felus (2005)]:

$$w_n = C_0^{-1} * d_n$$ (2.9)

where $C_0$ is called the variance-covariance matrix (or redundancy matrix) and $d_n$ is called the proximity vector:

$$C_n = \begin{pmatrix} C_{1,1} & \cdots & C_{1,2n} & 1 \\ \vdots & \ddots & \vdots & \vdots \\ C_{n,1} & \cdots & C_{n,n} & \vdots \\ 1 & \cdots & 1 & 0 \end{pmatrix}$$ (2.10)

$$d_n = \begin{pmatrix} C_{1,0} \\ \vdots \\ C_{n,0} \\ 1 \end{pmatrix}$$ (2.11)

$$w_n = \begin{pmatrix} w_1 \\ \vdots \\ w_n \\ \lambda \end{pmatrix}$$ (2.12)

The variance-covariance matrix $C_0$ contains the covariance of all pairs of observed data pairs. The proximity vector $d_n$ is the vector of covariances at the prediction location, calculated using the distances between the estimation location and the observed points and the variogram model. The error variance vector $w_n$ consists of the kriging weights for all observed points and the Lagrange multiplier. The ordinary kriging estimate for an unknown locations can be obtained by summing these weights times their values, as stated in (2.1) [Goovaerts (1997)].

An additional result of kriging is the estimation of the interpolation accuracy. The uncertainty of the interpolation results for every prediction location is obtained using the kriging variance formula [Felus (2005)]:

$$MSPE(\hat{z}(s_0)) = d_n^T * C^{-1} * d_n$$ (2.13)

This MSPE, also called the kriging variance, can be used as an additional measure for the comparison of different kriging types.
2.2.3. Method assessment (Ordinary kriging)

An overview of the rankings on the Watson criteria is given in Table 2.1. The results of ordinary kriging satisfy the first five Watson's criteria. The results are not only exact, continuous and smooth, the range value in the variogram makes sure that only local points can obtain weight. Ordinary kriging is also an adaptable method. Moreover, ordinary kriging does not only adapt to anisotropy in input data geometry, it is also possible to adapt the technique for anisotropy in the spatial relation within the data itself. An example of this is the use of anisotropy factors.

The drawback of ordinary kriging is that it is a very computationally inefficient method. Not only does it require the computation of the experimental variogram, which has a time complexity of $O(n^2)$, it also requires inversion calculation of the matrix $C_n$ to compute the weights. The evaluation of a single set of weights at a given location has a computational complexity of $O(n^3)$. For $m$ grid locations the total complexity will increase to $O(mn^3)$, which is very undesirable for large number of input points $n$. The computational complexity can be drastically reduced by using not all input points, but a certain subset [Srinivasan (2004)]. As an illustration, using a interpolation neighbourhood with a fixed number of 10 points instead of 1000 input points will result in a substantial reduction of computation time for inversion of matrix $C_n$ from $O(m \times (1000^3)) = O(m \times (1000,000,000))$ to $O(m \times (10^3)) = O(m \times (1000))$, thus a factor $10^6$!

One can discuss whether ordinary kriging really is a fully automatic method. In principle one can automate the process and let the computer fit the best variogram model in a least-squared sense. However, as the fit of the variogram may be shifted by the presence of fluctuating point that are beyond the range, this may lead to less-accurate representation of the variogram for points that do lie within the range. Therefore it is often better to manually check whether the variogram model proposed by the least-square fit really is the desired model.

An advantage of kriging over deterministic methods such as natural neighbour interpolation is that information on the spatial relation within the field itself is considered in the weight calculation. Deterministic methods only rely on the geometric distribution, not the correlation within the data. Another benefit of in general is of course the quality description of the results, the kriging variance, that comes with the interpolation results.

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Table 2.1: Overview of Watson's criteria for ordinary kriging OK.
2.3. Voronoi-based methods

In this study the concept of natural neighbours is used to define the interpolation neighbourhood for kriging interpolation. The idea of natural neighbours is closely related to the concepts of the Voronoi diagram and the Delaunay triangulation. The Voronoi diagram and the Delaunay triangulation are the two types of spatial tessellations that are relevant for this study. The first part of this section emphasizes on the definitions and relevant properties related to the Voronoi diagram, the Delaunay triangulation and natural neighbours. The second part emphasizes on Voronoi-based interpolation methods.

2.3.1. Definitions and properties

Voronoi diagram

The Voronoi tessellation is the partitioning of a plane into regions that are closest to each of the input points. For ordinary Voronoi diagrams, ‘closest’ is defined in terms of distances in the Euclidean space, e.g. the Euclidean distance between points \( p(x, y) \) and \( q(x, y) \) is given as \( \text{dist}(p, q) = \sqrt{(p_x - q_x)^2 + (p_y - q_y)^2} \). The general and mathematical definition of the ordinary Voronoi diagram in the two-dimensional space are stated the following:

Definition 1 Planar ordinary Voronoi diagram

Given a finite number of distinct points in the Euclidean space, all locations in that space are associated with the closest member(s) of the point set with respect to the Euclidean distance. The result is a tessellation of the plane into a set of regions associated with members of the point set. This tessellation is called the planar ordinary Voronoi diagram (often simply referred to as the Voronoi diagram) generated by the point set, and the regions constituting the Voronoi diagram ordinary Voronoi polygons (or simply Voronoi polygons) [Okabe et al. (1992)].

Definition 2 Planar ordinary Voronoi diagram (mathematical)

Let \( P = p_1, \ldots, p_n \in \mathbb{R}^2 \), where \( 2 < n < \infty \) and \( x_i \neq x_j \) for \( i \neq j \), \( i, j \in I_n \). We call the region given by

\[
V(p_i) = \{ x | \|x - x_i\| \leq \|x - x_j\| \text{ for } j \in I_n \} \quad (2.14)
\]

the planar ordinary Voronoi polygon associated with \( p_i \) (or the Voronoi polygon of \( p_i \)), and the set given by

\[
V = \{ V(p_1), \ldots, V(p_n) \} \quad (2.15)
\]

the planar ordinary Voronoi diagram generated by \( P \) (or the Voronoi diagram of \( P \)). We call \( p_i \) of \( V(p_i) \) the generator point or generator of the \( i \)th Voronoi polygon, and the set \( P = p_1, \ldots, p_n \) the generator set of the Voronoi diagram \( V \) [Okabe et al. (1992)].

These definitions can be extended for a tessellation of Voronoi polygons in the three-dimensional space.

Delaunay triangulation

The Delaunay triangulation is the geometric dual graph of the Voronoi diagram. In a dual graph the vertices and faces of a certain graph are interchanged. In other words, the vertices of the Voronoi diagram are the faces of the Delaunay triangulation and the other way around, as illustrated in Figure 2.2. The straight line embedding of a dual graph is called a geometric dual graph (Figure 2.3). The general and mathematical definition of the Delaunay triangulation are stated as follows:

Definition 3 Delaunay triangulation

Given a Voronoi diagram where generator points are not collinear and their number of three or more but finite, all parts of generator points whose Voronoi polygons share the common Voronoi edge are joined. As a result, a second tessellation is obtained. If this tessellation consists of only triangles, it is called a Delaunay triangulation. If not, it is called a Delaunay pretriangulation or Delaunay diagram. For the Delaunay pretriangulation, non-triangular polygons are partitioned into triangles by non-intersecting line segments joining the vertices. As a results, the Delaunay pretriangulation becomes a triangulation, which is also called a Delaunay triangulation [Okabe et al. (1992)].
Definition 4 Delaunay triangulation (mathematical)

Let \( V(P) \) be a Voronoi diagram generation by a set of \( n \) distinct points \( P = p_1, \ldots, p_n \in \mathbb{R}^2 \), where \( 3 < n < \infty \) that satisfies the non-collinearity assumption; \( Q = q_1, \ldots, q_n \) be the set of Voronoi vertices in \( V \); and \( x_{i1}, \ldots, x_{ik_i} \) be the location vectors of the generator points whose Voronoi polygons share a vertex \( q_i \). We define the set by

\[
T_i = \{ x | x = \sum_{j=1}^{k_i} \lambda_j x_{ij} \} \quad (2.16)
\]

where \( \sum_{j=1}^{k_i} \lambda_j = 1, \lambda_i \geq 0, j \in I_{k_i} \), and let

\[
\varnothing = \{ T_1, \ldots, T_{n_v} \} \quad (2.17)
\]

If \( k_i = 3 \) for all \( i \in I_{n_v} \), we call the set \( \varnothing \) the Delaunay triangulation of \( CH(P) \) spanning \( P \). If there exist at least one \( k_i \geq 4 \), we call the set \( \varnothing \) the Delaunay pretriangulation of \( CH(P) \) spanning \( P \). We partition \( T_i \) having \( k_i \geq 4 \) into \( k_i - 1 \) triangles by non-intersecting line segments joining vertices, and denote the resulting triangles by \( T_{1i}, \ldots, T_{kk_i-2} \). Let

\[
\varnothing = \{ T_{11}, \ldots, T_{1k_1-2}, \ldots, T_{n_v1}, \ldots, T_{n_vk_{n_v}-2} \} \quad (2.18)
\]

We call the set \( \varnothing \) the Delaunay triangulation of \( CH(P) \) spanning \( P \), and the triangles in \( \varnothing \) Delaunay triangles [Okabe et al. (1992)].

There are several ways to create triangulations of a set of points. A triangulation is only called Delaunay when it is angle-optimal, e.g. when the angles of the triangles are maximized. Another important property of a Delaunay triangulation is that the external Delaunay edges in \( \varnothing(P) \) constitute the convex hull \( CH(P) \) of \( P \). The convex hull of a set of points is the smallest convex set such that it contains all points. Another useful property of the Delaunay triangulation is that all circumcircles of Delaunay triangles are empty circles, in other words a Delaunay triangulation satisfies the so-called empty circle criterion, as illustrated in Figure 2.4. The circumcircle of a Delaunay triangle is sometimes called a Delaunay circle [Okabe et al. (1992)].
2.3.2. Natural neighbours
The idea of natural neighbours is closely related to the concept of the Voronoi diagram and the Delaunay triangulation. For an existing set of points in a Delaunay graph, the natural neighbours of point \( p \) are the points sharing a Delaunay edge with \( p \). In other words, all vertices on the Delaunay circles going through point \( p \) are the natural neighbours of \( p \). In terms of Voronoi graphs the natural neighbours are the points whose Voronoi cell is contiguous to the Voronoi cell of point \( \hat{V}_p \). For example, point \( p \) in Figure (5.4) has seven natural neighbours [Ledoux and Gold (2014)].

2.3.3. Interpolation methods
Natural neighbour interpolation
Natural neighbour interpolation, or Sibson interpolation, is a weighted average interpolation method (recall eq. (2.1)). The definition of natural neighbour in existing tessellation is stated in the previous section. When it comes to natural neighbour interpolation the natural neighbours are defined in the same manner, however they relate to the estimation point. The value of each estimation point is solely determined by the values of its natural neighbours. The weight given to each natural neighbour is derived from the change in the Voronoi tessellation caused by the introduction of the estimation point. First an initial Voronoi tessellation is created of the set of known data values. For each estimation point a new Voronoi tessellation is computed, this time for the data points plus that particular estimation point. The initial Voronoi cells of its natural neighbours will be altered in this new tessellation, some of their Voronoi area will be 'stolen'. The amount of area that is stolen is a measure for the weight given to each natural neighbour [Sibson (1981)].

For a two-dimensional case, the weight of each natural neighbour is quantified the following way [Ledoux and Gold (2014)]:

\[
\psi_i = \frac{\text{Area}(\hat{V}_{p_i} \cap \hat{V}_x^+)}{\text{Area}(\hat{V}_x^+)}
\]  

(2.19)

where \( \text{Area}(\hat{V}_{p_i}) \) represents the area of the Voronoi cell of neighbour \( p_i \), and \( \text{Area}(\hat{V}_x^+) \) the area of the Voronoi cell generated around an interpolation point called \( x \) (the plus-sign marks a Voronoi cell in the 'new' tessellation).
The area of two-dimensional Voronoi cells can be computed by decomposing it into triangles and summing their areas. The value of \( w_i \) will always be between 0 and 1. The weight of each natural neighbour \( p_j \) is thus the area of the intersection of the initial and newly generated Voronoi diagrams divided by the area of the Voronoi diagram of the newly introduced point \( x \), as illustrated in Figure (3.5) [Ledoux and Gold (2014)]:

Although the concept of natural neighbour interpolation is quite easy to understand, the implementation is not so straightforward, since it requires both the computation of two Voronoi diagrams (initial and after the introduction of the estimation point) as well as the computation of their respective area [Ledoux and Gold (2014)].

**Laplace interpolation**

Laplace or Non-Sibsonian interpolation is another natural neighbour-based weighted average interpolation method. The first steps of Laplace interpolation are the same as for natural neighbour interpolation: an initial Voronoi tessellation of all known points is computed, then for each interpolation point a new Voronoi tessellation is calculation. The difference is the handling of the weights of each natural neighbour. As for natural neighbour interpolation, the weights are dependent on the area of the newly introduced Voronoi cell. For Laplace interpolation the weights are based on the edge length of the newly introduced Voronoi cell associated with each of the natural neighbours and the distance to each of the natural neighbours, as illustrated in Figure 2.7.

The weight \( w_i \) of each natural neighbour is computed as [Hiyoshi and Sugihara (1999)]:

\[
  w_i = \frac{\alpha_j}{\sum_{j=1}^{n} \alpha_j} \tag{2.20}
\]

where \( \alpha_j \) is computed as:

\[
  \alpha_j = \frac{s_j}{h_j} \tag{2.21}
\]

Here \( s_j \) is the edge length of the Voronoi cell of \( x \) that is associated with natural neighbour \( j \) and \( h_j \) is the distance to the edge of the Voronoi cell of \( x \), as illustrated in Figure 2.7. The computational complexity of Laplace interpolation is thus a function of lengths only, whereas in natural neighbour interpolation the weights are a function of areas in 2-D, or even volumes in 3-D. Therefore Laplace interpolation is computationally more favourable and easier to implement in higher dimensions [Sukumar (2001)].

Of these two Voronoi-based interpolation methods natural neighbour interpolation is used more frequently. Moreover, the results of these two methods are very comparable, and therefore the choice has been made to compare natural neighbour kriging to natural neighbour interpolation only. Comparison with Laplace interpolation is thus considered to be beyond the scope of this study.
2.3.4. Method assessment (Natural neighbour interpolation)

The results of natural neighbour interpolation satisfies all the Watson criteria enumerated earlier this chapter, except that the first derivative obtained by natural neighbour interpolation is undefined at the data points themselves. The results are thus not smooth at the data locations, however, methods have been proposed to overcome this unwanted effect. An overview of the rankings of natural neighbour interpolation on the Watson criteria is given in Table 2.2. [Ledoux (2012)].

A favourable property of the natural neighbour interpolant is that it adapts to anisotropy in data geometry. Even for anisotropic acquisition geometries realistic weight distribution are obtained. Natural neighbour interpolation thus performs well for various geometrical distribution of input data. However, a drawback of the method is that is still is deterministic one. The results may be good in term of geometrical weight distribution, but the actual spatial relation within the data is not captured or considered during interpolation.

Although the implementation of natural neighbour interpolation is not very straightforward, very computationally efficient algorithms have been designed. A example of these is the natural neighbour interpolation algorithm presented by Ledoux and Gold in 2004 [Ledoux and Gold (2014)] which uses the concept of flipping in a triangulation and has a complexity of but $O(n)$ and can thus be considered very computationally efficient.

Natural neighbour interpolation does not rely on user-defined parameters and it is therefore a fully automatic method [Ledoux (2012)].

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Table 2.2: Overview of Watson’s criteria for natural neighbour interpolation. NN.
2.4. Cross-validation

An interpolated map without a description of its quality is generally considered an incomplete result. A general impression of the quality of both ordinary kriging and natural neighbour interpolation is assessed using the Watson criteria in the previous sections. However, to describe how well a certain interpolation method works for a specific dataset, the data-dependent performance, one must use other methods. A common way to validate the performance of an interpolation method for a certain dataset is a technique called cross-validation, or rotation estimation. The idea of cross-validation is to subdivide a dataset into multiple parts, using part of the data as input locations for interpolation and part as validation locations. The input locations are now used to interpolate the values at the validation locations. The ground truth at these locations are known and can thus be compared to the interpolated values here. The differences between the actual values and the interpolated values are used to determine the Mean Squared Error (MSE), which is specified as the squared mean of the differences. The MSE is a good indicator to tell how well an interpolation method will perform in practice. Two commonly used types of cross-validation can be distinguished, leave-one-out and k-fold cross-validation [Geisser (1993)].

2.4.1. Leave-one-out

In leave-one-out cross-validation one of the known location is left out as input and all other locations are used to calculate the value here. This is repeated until all known points have been left out once. The interpolated values and the true values at all locations are then compared and a MSE is calculated based on the differences between these [Geisser (1993)].

2.4.2. K-fold

K-fold is another cross-validation method. For this type of cross-validation the dataset is randomly divided into k equally sized subsets. One of these k subsets is used as validation location and the other k-1 subsets are used as interpolation input to compute the interpolated values here [Geisser (1993)]. The MSE computed varies dependent on the partition of the dataset, since the data is sampled randomly. The spread of the MSE are calculated using the Monte Carlo method. Monte Carlo is a simulation method that repeats a process or calculation with a random sampling as input a number of times, given a spread in outcomes. From the distribution in outcomes the mean MSE and the standard deviation of the MSE are obtained, giving insight in the validity of the method [Robert and Casella (2004)].

Two types of k-fold cross-validation are performed: 2-fold and 10-fold. For 2-fold cross-validation the dataset is divided into two randomly chosen parts. Half of the data points is thus used to interpolate and the other half for validation. The dataset is divided into 10 random subsets for 10-fold cross-validation. Now, 9 of the 10 subsets are used to achieve estimates for the locations of the 10th subset, which is used for validation.
Natural neighbour kriging

The concept of natural neighbour kriging and the designed algorithm are explained in the first section of this chapter. In the second part of the chapter the adjustments for natural neighbour kriging for anisotropic fields are presented.

3.1. Natural neighbour kriging

Natural neighbour kriging is a type of kriging that uses natural neighbours as interpolation neighbourhood for each grid point. Only these natural neighbours are being taken into account for the actual kriging step, considerably reducing the size of variance-covariance matrix $C_{nn}$. A schematic overview of the steps of natural neighbour kriging is given in Figure 3.1. The algorithm steps of natural neighbour kriging are described separately in the next section.

Figure 3.1: Schematic overview of the algorithm steps of natural neighbour kriging for isotropic geospatial datasets.
3.1.1. Algorithm steps
The step-wise procedure of the algorithm used for natural neighbour kriging is described in the section below. The algorithm is written in Matlab.

Trend removal
The spatial relationship of a field can be shadowed by the presence of a trend within the data and therefore it is important to detrend the data first. A common way to do so is to fit a plane to the field in a least-squares sense. The function of the plane, given by $ax + by + cz$, is subtracted from the data to detrend it. After kriging is performed the trend can again be added to the results to obtain the 'original' field, including trend.

Variogram estimation
The dissimilarities between all input point can now be calculated and grouped to obtain an experimental variogram (Equation 2.4). A variogram model is used to fit the experimental variogram.

Imaginary points introduction
The method used to search for the natural neighbours of each grid cell relies on the fact that a Delaunay triangulation exist at each interpolation location. Four imaginary points at the borders of the dataset are introduced in order to interpolate beyond the boundaries of the convex hull on a rectangular grid. The coordinates of these imaginary points are $(x_{min}, y_{min}), (x_{min}, y_{max}), (x_{max}, y_{min}), (x_{max}, y_{max})$. These points are used for the creation of the Delaunay triangulation of the dataset. [Okabe et al. (1992)]

Delaunay triangulation
A Delaunay triangulation of the known points is created using the build-in Matlab function Delaunaytriangulation. The Delaunay triangulation is used to determine the natural neighbours for each grid point.

Natural neighbour search
There are several ways to determine the natural neighbours of a certain point. The algorithm uses the pre-computed Delaunay triangulation of the field to determine the natural neighbours for each interpolation location. The vertices of a Delaunay triangle are the natural neighbours of a certain point if this point lies within the circle spanned by this Delaunay triangle (Figure 3.2) [Cai and Zhu (2005)]. To determine whether a certain point lies within the circle spanned by one of the Delaunay triangles the following formula is used [Berg et al. (2008)]:

$$\det \begin{bmatrix} a_x & a_y & a_x^2 + a_y^2 & 1 \\ b_x & b_y & b_x^2 + b_y^2 & 1 \\ c_x & c_y & c_x^2 + c_y^2 & 1 \\ p_x & p_y & p_x^2 + p_y^2 & 1 \end{bmatrix} > 0 \quad (3.1)$$

In this formula $a(x, y)$, $b(x, y)$ and $c(x, y)$ are the vertices of a Delaunay triangle and $p(x, y)$ is the interpolation point.

The vertices of the Delaunay triangle must be given in clockwise direction. Note that this implementation of natural neighbour identification is not the most computationally efficient one. Optimizing the computational efficiency of the algorithm is beyond the scope of this thesis.

![Figure 3.2: The points that lie within the circles spanned by the Delaunay triangles are the natural neighbours [Cai and Zhu (2005)].](image)
Ordinary kriging
For each grid point the previously mentioned variogram model is used to determine the covariance values for the variance-covariance matrix $C_n$ and for the proximity vector $d_n$ for all natural neighbours of that point. The ordinary kriging system is solved to obtain the weights for each natural neighbour. The values of each natural neighbour are multiplied by the determined weights to obtain an estimate for each grid cell.

Add trend to interpolation results
Finally, to obtain the original field the modelled trend is added to the ordinary kriging estimates for each grid cell. An estimate of the original field including trend is now obtained.
3.2. Anisotropy

Most phenomena in geology exhibit anisotropy. A phenomenon is anisotropic when its spatial variability changes with direction. For example, mineral deposits in river systems often have a larger continuity along the river paths then perpendicular to these.

3.2.1. Types of anisotropy

There are two types of anisotropy, geometric anisotropy and zonal anisotropy. An anisotropy in the data is said to be geometric when the directional semi-variograms have the same shape and sill but different range values. In this case the rose diagram of ranges, which is an representation of the range values in each direction, is given by an ellipse. An anisotropy is said to be zonal if the sill values vary with direction [Goovaerts (1997)]. Examples of angular experimental variograms that describe both a geometric and a zonal anisotropy case are given in Figure 3.3.

![Image of geometric and zonal anisotropy variogram models](Goovaerts (1997)).

Anisotropy modelling in two dimensions requires a function that depends on both distance and direction, or angle. In kriging angular experimental variogram models are used to model anisotropy. For anisotropic signals a more realistic interpolation result is achieved using methods that adjust to anisotropy. An example of such a method is ordinary kriging using anisotropic variogram functions, also called anisotropic ordinary kriging.

3.2.2. Anisotropic ordinary kriging

A way to deal with anisotropy in the data signal is anisotropic ordinary kriging. Anisotropic ordinary kriging is an adjustment of regular ordinary kriging and uses a covariance ellipsoid (Figure 3.4) rather than assuming equal covariances in all directions. To do so the direction of both the minimum and maximum variability and their respective ratios must be determined in an angular (or directional) experimental variogram. The computation of an angular variogram basically comes down to the same computation as for regular experimental variograms, the only difference is that the angle between all pair of points is calculated additionally. The pairs are now not only grouped based on distance, but also based on their respective pairwise angles. This results in a separate experimental variogram for each direction. The angular experimental variogram is used to determine the direction of minimum and maximum variability as well as the so-called anisotropy factor \( \lambda \), which is a description of the ratios of the minimum and maximum direction of the covariance ellipse that is used. The results of anisotropic ordinary kriging will be referred to as AOK [Goovaerts (1997)].

Anisotropic ordinary kriging uses a correction for geometric anisotropy and therefore the directions of the minimum and maximum variability must be perpendicular such that the resulting covariance ellipse is symmetrical. The determination of anisotropy factor \( \lambda \) is not always so straightforward. In case of perfect geometric anisotropy in the signal \( \lambda \) can be determined using the ratio of the minor range to the major range, as \( \lambda = a_\phi / a_\theta \) which is always smaller than 1. Another method is to determine the ratio of the slopes of the angular variogram model in the direction of minimum and maximum variability. Note that this method is only valid when there is a more or less linear relationship in the experimental variogram, for example when a spherical model is used to fit the experimental variogram. These two methods results in basically the same anisotropy factor, but sometimes the latter is more practical, for example when it is unclear where the sill of the experimental variogram is reached [Goovaerts (1997)].
3.2. Anisotropy

Figure 3.4: Example of contour lines of an isotropic covariance and an anisotropic covariance function (covariance ellipsoid) in 3D space [Dorst (2009)].

Please note that the actual covariance ellipsoid based on the angular variogram models rarely results in a perfectly symmetrical ellipsoid, and that the fitted variogram model, just as for regular ordinary kriging, always includes some deviations from the actual experimental models. In the end the goal is to improve the interpolation results and therefore it is important that the used anisotropy factor describes the spatial relationship well in all directions. In some cases there is clearly more weight towards either the minimum or maximum direction, e.g. there are more angular experimental variograms close to the direction of either the minimum or maximum one. Here, using the anisotropy factor purely based on the minimum and maximum direction only will lead to an under- or overestimated covariance in these directions and introduce errors. In this case it is better to be a bit reserved with the used anisotropy factor, so that the resulting covariance ellipse fits most of the angular variograms better.

Once the direction of maximum ($\phi$) and minimum ($\theta$) variability and the anisotropy factor ($\lambda$) are known the used variogram model can be corrected for anisotropy. This is done by rotation and rescaling of the coordinates. First the coordinate axes are rotated clockwise by the angle of the direction of maximum variability $\theta$, also called the azimuth angle, such that the axes correspond to the main axes of the ellipse [Goovaerts (1997)]. The rotated coordinates are now:

$$h_\theta = \begin{bmatrix} h_\phi \\ h_\theta \end{bmatrix} = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} \times \begin{bmatrix} h_x \\ h_y \end{bmatrix}$$

(3.2)

In which $h_\theta$ is the vector containing locations with respect to the axes of maximum $\phi$ and minimum $\theta$ variability. The second step is to rescale the ellipse with respect to the minor range $\alpha_\phi$ into a circle of equal radius. The final coordinates are expressed as:

$$h' = \begin{bmatrix} h'_\phi \\ h'_\theta \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & \lambda \end{bmatrix} \times \begin{bmatrix} h_\phi \\ h_\theta \end{bmatrix}$$

(3.3)

In which $h'$ are the coordinates scaled with anisotropy factor $\lambda$ in the direction of minimum variability $\theta$. Illustration of these two steps can be seen in Figure 3.5 [Goovaerts (1997)].
3. Natural neighbour kriging

3.2.3. Anisotropic natural neighbour kriging

Anisotropic natural neighbour kriging is a method that selects the natural neighbours of each interpolation points and weights these based on anisotropic ordinary kriging. The natural neighbours of a point are thus used as interpolation neighbourhood for anisotropic ordinary kriging. This adjustment of natural neighbour kriging will be referred to as *anisotropic natural neighbour kriging*, abbreviated as *AOK_NN*. The procedure is the same as for normal natural neighbour kriging, only now anisotropic ordinary kriging is used for interpolation rather than regular ordinary kriging. A schematic overview of the procedure is given in Figure 3.6.

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Figure 3.5: Anisotropy correction for the used variogram model. A angular experimental variogram model of the direction of minimum and maximum variability and the corresponding covariance ellipse (upper images). The ellipse composed of the minor and major ranges is corrected by a linear transformation to correspond to a circle of radius $\alpha$, to resemble an isotropic model (bottom images) [Goovaerts (1997)].

**Figure 3.6**: A schematic overview of the steps of anisotropic natural neighbour kriging ($AOK_{NN}$).

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**3.2.3. Anisotropic natural neighbour kriging**

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The procedure is the same as for normal natural neighbour kriging, only now anisotropic ordinary kriging is used for interpolation rather than regular ordinary kriging. A schematic overview of the procedure is given in Figure 3.6.

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Figure 3.6: A schematic overview of the steps of anisotropic natural neighbour kriging ($AOK_{NN}$).
3.2.4. Anisotropy in acquisition geometry

In anisotropic kriging or anisotropic natural neighbour kriging the term anisotropy refers to signal in the data itself. However, if there is a distinct difference between acquisition data density in different directions one can speak about anisotropy in the acquisition geometry. In most of these cases the difference in data density in different directions is adjusted to the anisotropy in the data itself. For example in bathymetric datasets there is often a higher data density in the direction of the highest variation. Naturally one would like to adjust the points taken into account for interpolation to both the anisotropy in the data signal as well as the anisotropy in data geometry.

An often considered pleasant property of the selection of natural neighbours is that it automatically adjusts to the geometry of the input points. In anisotropic kriging the weighting for different points is adapted to anisotropy in the signal. In anisotropic natural neighbour kriging the weighting is still based on the same angular variogram models, however, the selection of the neighbours is dependent on the acquisition geometry only. Three examples of natural neighbour selection for different acquisition geometries are given in Figure 3.7, Figure 3.8 and Figure 3.9. For example, grid points in the middle of rectangular acquisition geometries will have more natural neighbours in the direction of the length of the rectangles than in the direction of the width (Figure 3.9). This property is wanted if the main direction of continuity within the data signal is in correspondence with the direction of the length of the rectangles. This way more points in the direction of continuity are selected, that will obtain relevant weights in kriging. However, the points in the elongated direction will be less relevant if the direction of continuity is perpendicular to this direction. So, an important consideration in the selection of neighbours should be the relationship between the direction of anisotropy in the acquisition geometry with respect to the direction of anisotropy in the signal itself.

**Figure 3.7:** Example of the selection of natural neighbours (orange) for interpolation location (x) for a regular geometry with length/width = 1.

**Figure 3.8:** Example of the selection of natural neighbours (orange) for interpolation location (x) for an acquisition geometry with length/width = 1.5.
The selection of natural neighbours can be adjusted using a different definition of distance to base the neighbours on. A way to do so is to use a distance measure based on the directional continuity within the data signal itself using the range ellipse obtained by angular variogram modelling. More points should be selected in the main direction, the direction of maximum continuity $\theta$, than in the direction of minimal continuity $\phi$ and to do so the data and grid points can be scaled based on their proportion, given by the anisotropy factor $\lambda$. The resulting neighbours are an example of scaled natural neighbours and are referred to as anisotropic natural neighbours.

The data and grid points are rotated by $-\theta$ so the y-axis aligns with the main direction of continuity $\theta$ and then the y-axis is scaled by the anisotropy factor $\lambda$. The new locations are used to determine the anisotropic natural neighbours of each grid point. The anisotropic natural neighbours can be used as interpolation neighbourhood for ordinary kriging, this method will be abbreviated as $AOK_{ANN}$. Please keep in mind that this transformation is only for the selection of the neighbours, the weighting of each neighbour is still based on the actual distances.
3.2.5. Proposed workflow

The following factors play an important role in the determination of the preferred interpolation technique for a particular dataset.

1. Isotropy or anisotropy
2. Type of anisotropy
3. Correctness of the fit variogram model
4. Spatial variability of the signal
5. Data size

Isotropy or anisotropy

There are several ways to determine whether a signal is isotropic or anisotropic. Often one can recognize anisotropic signals by simply looking at the acquired data or known information of the signal. For example, the topography of seafloor sand dunes is formed by the waves having a predominant direction, resulting in recognizable ellipsoidal shapes. These shapes can be recognized in for example bathymetric data and are clearly anisotropic.

Another way to see whether a signal is isotropic or anisotropic is to look at experimental variograms. In some cases anisotropy in the signal is visible as jumps in the regular experimental variogram. Often these jumps show up using smaller bin sizes for the computation of the variogram. These jumps indicate that there are various directional signals that are often being averaged out as the bin size is increased.

Another possibility to see whether a signal is anisotropic is to compute angular experimental variograms. Large differences in sill and range values for different angles indicate that the signal is anisotropic.

Type of anisotropy

The type of anisotropy is determined using the angular experimental variograms. In practice the signal will often exhibit some combination of both geometric and zonal anisotropy. To determine what type of anisotropy is predominant one should look at the variation in range and sill values between the angular experimental variogram of different angles. A distinct difference between the sill values of the two indicates that the signal predominantly exhibits zonal anisotropy. A clear difference in range values on the other hand indicates that there is predominantly geometric anisotropy. Moreover, range and sill differences in the fit isotropic variogram and main direction angular variogram model are also an indication of either geometric (different range values) or zonal anisotropy (different sill values) in the signal [Goovaerts (1997)].

It is safe to use anisotropic ordinary kriging or anisotropic natural neighbour kriging when geometric anisotropy is predominant. It is more difficult to model zonal anisotropy using an anisotropic variogram model, as this is originally a correction for geometric anisotropy. However, reasonable estimates for close range points can be obtained using anisotropic natural neighbour kriging and an anisotropic variogram model that fits well for small range values. This way only nearby points, where the spatial relation is correctly captured in the variogram model, are used.

Correctness of variogram model

In order to obtain optimally accurate predictions with kriging methods the kriging assumptions must hold. In practice this is true if the range and the sill of the experimental variogram are clearly recognizable. The experimental variogram should increase until it flattens out and stabilizes around the sill value. Another consideration should be whether there are large differences between the experimental variogram and the fit variogram model. In some cases the relationship in the data cannot be captured well in a certain variogram model. This can lead to estimation errors, as the kriging weights are determined using the variogram model rather than the experimental variogram. The use of a deterministic interpolation method, such as natural neighbour interpolation, is preferred in cases where either the kriging assumptions do not hold and/or where the experimental variogram deviates much from the variogram model.

Another consideration is the fit of the isotropic model compared to the fit of the anisotropic model. In some
cases the anisotropic variogram model is unable to capture the anisotropy correctly, for example when the signal is only anisotropic in one particular direction. In these cases it is better to use a non-anisotropic interpolation technique, such as natural neighbour interpolation or ordinary kriging, depending on the overall correctness of the isotropic variogram model.

Spatial variability of the signal
A large spatial variability in the signal can lead to deviations from the used variogram model in kriging, as the same model is often used to interpolate the full dataset. Local differences in range, sill, anisotropy factor or direction cannot be captured within one single variogram model, and therefore it can be tricky to interpolate larger areas. In this case better approximations can be obtained locally using natural neighbour interpolation, which is a more locally adaptable technique.

A way to see if the signal is constant over large areas is to subdivide the detrended signal intro multiple parts and to compare the mean and the standard deviation for each of these parts. It is safe to use kriging if the mean and the standard deviation are constant throughout the full area.

Data size
This factor might be a very obvious one, but is certainly not unimportant in the determination of what interpolation technique to use. Ordinary kriging is an increasingly time-demanding process as data size increases. (Anisotropic) natural neighbour kriging or natural neighbour interpolation are less computationally intensive methods and are therefore preferred for large datasets. The consideration is of course also dependent on the availability of computational resources. For example, some super computer can handle much larger datasets than a regular computer or laptop, and also run more computational intensive algorithms.

Workflow questions
The abovementioned factors re translated into six questions that can help determining what interpolation technique is appropriate to use. These questions are:

1. Is the signal isotropic or anisotropic?
2. What is the predominant type of anisotropy?
3. Can the spatial relationship be sufficiently captured by an isotropic or anisotropic variogram model?
4. Are there large spatial variations in the signal?
5. Are the available time and computational resources limiting with respect to the data size?
6. Is the main acquisition direction in correspondence with the main direction of continuity?
The visualisation of the uncertainties of the interpolation results is at least as important as the interpolation results itself. In this section two methods to visualise the quality of the interpolation results are presented: quadtree decomposition and contour mapping. The two fields that are used to describe the quality associated with the interpolation results are the kriging variance and the number of natural neighbours per grid cell. The quadtree decomposition based on these fields is used to design an adaptive grid for interpolation. The adaptive grid adjusts to the quality of the interpolation: the block size of the grid cells increases with increasing uncertainty.

4.1. Kriging variance and natural neighbours

The kriging variance is the main quality descriptor of the interpolation results obtained with kriging. The formula (2.13) used to compute the kriging variance is given in Chapter 2. The kriging variance is used to visualise the prediction uncertainties at each location using two methods: quadtree decomposition and contour mapping. Another field that is computed for the natural neighbour methods is the number of natural neighbours per grid cell. In general the number of natural neighbours follows a similar pattern as the kriging variance, the number of neighbours namely increases further away from the input points. The correlation between the kriging variance and the number of natural neighbours is determined by the correlation coefficient $\rho(A, B)$ [Fisher (1958)]:

$$\rho(A, B) = \frac{C(A, B)}{\sigma_A \cdot \sigma_B} \quad (4.1)$$

in which $A$ and $B$ are the matrices containing the values for the kriging variance and the number of natural neighbours, respectively, $C(A, B)$ is the covariance of $A$ and $B$ and $\sigma_A$ and $\sigma_B$ are the standard deviations of the kriging variance and the number of natural neighbours, respectively. The covariance of $A$ and $B$ $C(A, B)$ is computed by [Fisher (1958)]:

$$C(A, B) = \frac{1}{(N - 1)} \sum_{i=1}^{N} (A_i - \mu_A)(B_i - \mu_B) \quad (4.2)$$

in which $N$ is the number of observations in $A$ and $B$, and $\mu_A$ and $\mu_B$ are the mean values of $A$ and $B$, respectively.

The correlation coefficient is a measure of the linear dependence of two fields of observations. Two fields of observations are uncorrelated if the correlation coefficient is zero. There is a positive correlation between two fields of observations when the correlation coefficient is higher than $+0.5$ [Fisher (1958)]. The correlation coefficient of the number of natural neighbours per grid cell and the kriging variances are computed and compared for different kriging methods.
4.2. Quadtree decomposition

Quadtree decomposition is an image analysis technique that subdivides an image into a number of homogeneous blocks. In quadtree decomposition the image is divided into four equal-sized blocks. The quadtree blocks are squares by default, but the regions can also be made rectangular of any other shape. The pixels within each of these blocks are tested to see whether they meet some criteria of homogeneity. The blocks are not subdivided any further if this is the case. If the pixels within one of the blocks do not meet this criterion, the block is subdivided further into four smaller blocks. The pixels within these blocks are tested once again whether they meet the criterion. This process is repeated until all blocks meet the criterion, or until the blocks reach the smallest block size possible (the size of one pixel) or the specified minimum block size [Berg et al. (2008)]. An example of the quadtree decomposition procedure is given in Figure 4.1.

![Quadtree decomposition](image)

Figure 4.1: Example of the procedure steps in quadtree decomposition [Worboys and Duckham (1995)].

The quadtree data structure was first introduced by Finkel and Bentley in 1974. The data structure resulting from quadtree decomposition is a tree data structure, in which each node has four children, or so-called leaves. The tree data structure follows the spatial decomposition of the quadtree, as illustrated in Figure 4.2. A tree data structure has the advantage that it can be stored very compactly, and therefore quadtrees are often used as a way to compress and store images. Other common uses of quadtrees include image representation, pattern recognition and segmentation. A quadtree decomposes the space into adaptable cells that each meet the specified criteria of homogeneity. Larger blocks sizes thus represent areas of little change, whereas small blocks point out highly variable areas. In highly variable areas there is often more need for data, and therefore the adaptable cells resulting from quadtree decomposition are usable tools for data acquisition planning [Finkel and Bentley (1974)].

![Quadtree data structure](image)

Figure 4.2: Example of the quadtree data structure [Worboys and Duckham (1995)].

The criterion that determines whether the image should be subdivided or not do not necessarily have to apply to the values of the image itself. Another possibility is to decompose an image based on an additional information field that applies to that image. For example, an image can be decomposed based on a quality description of that particular image. The specified criterion, or threshold, is tested on the pixels within each blocks of this additional field, but also subdivide the image accordingly.

Quadtree decomposition is used to design an adaptive grid for interpolation. The idea was to design an adaptive grid that adjusts to the quality of the interpolation results: small cell sizes at areas where the uncer-
4.3. Contour mapping

A relatively simple method to visualize the interpolation results and the associated kriging variance is contour mapping. A contour line of a field is a curve along which the field has a constant value [Courant et al. (1996)]. The kriging variance values are plotted as contours on top of the interpolation results. The spacing between the contour lines shows the distribution of the kriging variance, the colouring of the contours displays the kriging variance value.

The two methods (quadtree decomposition and contour mapping) are tested on the results of layer A of subset 1 of the Borssele windmill farm dataset. The two main input matrices are the results for natural neighbour kriging on a small interpolation grid of 128 x 128 in size and for anisotropic natural neighbour kriging on a larger interpolation grid of 512 x 512. These two matrices have been chosen to on the one hand illustrate the effect of different interpolation grid sizes and on the other hand illustrate the differences between an isotropic and an anisotropic method as input.
This chapter emphasizes on the used datasets. Throughout this study three datasets are used: a small test dataset after Davis, and two case study datasets, data from the Borssele windmill farm and single beam echo sounder data to monitor Tidal sand waves. The three datasets are used for different purposes:

- The performance of natural neighbour kriging is both qualitatively as quantitatively compared to natural neighbour interpolation and ordinary kriging using a test dataset after Davis.

- The quantitative performance of the isotropic methods (natural neighbour interpolation, ordinary kriging and natural neighbour kriging) and the anisotropic methods (anisotropic ordinary kriging and anisotropic natural neighbour kriging) are compared using cross validation techniques for the case study dataset of the Borssele windmill farm from Fugro.

- The cross validation results for the Fugro dataset are used to create a workflow schematic that can be used to determine the appropriate interpolation method depending on the type of signal.

- The workflow is tested on another case study dataset: a single beam echo sounder dataset that it often used to monitor Tidal sand waves.

- The results of the Borssele windmill farm are used as input parameters for interpolation quality visualisation. Two types of quality visualisation methods are introduced: quadtree decomposition and contour mapping.
5.1. Davis' testdata

The Davis' height dataset created by Davis in 1973 is commonly used as test data set for interpolation. The dataset consist of 52 height values in a local coordinate system and is given in Figure 5.1. For this study the units used in the dataset are modified to the metric system. The dataset is used to compare three isotropic interpolation methods: natural neighbour interpolation, ordinary kriging and natural neighbour kriging.

The interpolation results of these three methods are compared and the mean prediction errors are estimated using two types of cross validation: leave-one-out cross validation and subset cross validation. Two types of subset cross validation are used, 2-fold, where the dataset is divided into two random parts, and 10-fold, where the dataset is divided into 10 random parts. The division of the points is randomly done a thousand times and each time the mean squared prediction error is computed. This is done for the full dataset and for the interior of the dataset only, keeping the convex hull fixed as input, as illustrated in Figure 5.2. Moreover, the methods are compared in a more qualitative sense based on their score on the Watson criteria. Also, the weighting and amount of natural neighbours is considered, and different variogram models are used for natural neighbour kriging to obtain a general understanding of the method.
5.2. Borssele windmill farm

The next case study is data from the Borssele Windmill Farm. The Borssele Windmill Farm zone is approximately 344 km$^2$ in size and is located 22.2 km from shore. The area is sub-divided into five different sites. In total an offshore wind capacity of approximately 1400 MW is planned in this zone. The location of the planned windmill farm and surrounding areas, as well as the location of the sites are given in Figure 5.3.

![Figure 5.3: Location of the Borssele Windmill Farm boundary (left) and location of different subzones (right).](image)

5.2.1. Data description

The data that is used for interpolation is collected by a multi-channel seismic sparker system (MCS). The seismic sparker systems are acoustic underwater systems that emit low frequency pulses of around 1 kHz, depending on the wanted depth range [Lurton (2010)]. The different frequency ranges of different acoustic systems are given in Figure 5.4. The pulses are receives by an array of receivers called hydrophones. The seismic sparker is used for deeper penetration into the seabed to inspect the underlying geology. The seismic waves penetrate up to 100 of meters and are used to create a cross-section of the ground along the sailed survey lines. In the seismic cross-section distinguishable surfaces will show up when there is a change in the so-called acoustic impedance, which is the product of the seismic wave velocity and the rock density. These surfaces often represent different geological layers, but can also represent structural features, for example geological faults [Sheriff and Geldart (1995)].

![Figure 5.4: Frequency ranges of main underwater acoustic systems and associated usable ranges [Lurton (2010)].](image)

The windmill park has been divided into different sections. The seismic sparker data is available for two of
5. Experiments

These sections: Wind Farm Section I (WFS I) and Wind Farm Section II (WFS II). The depths of the top of different geological units and subunits have been interpreted within these regions along the sailed survey lines. The main acquisition direction is southwest to northeast, which resembles the direction of maximum variability for most layers. Also perpendicular, northwest-southeast tracks have been acquired. Figure 5.5 shows the survey lines of the seismic sparker.

Figure 5.5: The survey lines acquired by the seismic sparker (blue) and the outline of WFS I and WFS II (black).

5.2.2. Geological units

Several geological units could be recognized on the seismic-cross sections. Five main seismic units have been identified based on their seismic facies and stratigraphical boundaries, named unit A, B, C, D, E and F. The geological units are of Quaternary (less than 1.8 million years) and Tertiary (65 to 1.8 million years) age and are of different geological origins [Skinner et al. (2004)]. The uppermost unit, unit A, consists of horizontally stratified marine and coastal deposits originating from the Quaternary. The next unit, unit B, is an unconformity surface of erosional origin between deposits from the Quaternary and the Tertiary. The underlying units from Tertiary age are dipping layers, consist of river and shallow marine deposits and locally contain sand deposits with patches of gravel or clay [Agency (2016)].

<table>
<thead>
<tr>
<th>Name</th>
<th>Number of points</th>
<th>Average depth (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base A</td>
<td>651,410</td>
<td>-35</td>
</tr>
<tr>
<td>Base B</td>
<td>639,231</td>
<td>-41</td>
</tr>
<tr>
<td>Base C1</td>
<td>162,371</td>
<td>-50</td>
</tr>
<tr>
<td>Base C2</td>
<td>198,788</td>
<td>-54</td>
</tr>
<tr>
<td>Base D</td>
<td>291,495</td>
<td>-63</td>
</tr>
<tr>
<td>Base E1</td>
<td>391,107</td>
<td>-69</td>
</tr>
<tr>
<td>Base E5b</td>
<td>374,632</td>
<td>-84</td>
</tr>
<tr>
<td>Base F1b</td>
<td>646,796</td>
<td>-114</td>
</tr>
<tr>
<td>Base F2</td>
<td>462,528</td>
<td>-113</td>
</tr>
</tbody>
</table>

Table 5.1: Overview of Borssele windmill farm data.

The purpose of the multi-channel sparker data is to create an isopach map of the different geological units that shows the thickness and depth of each unit at each location. These maps are used to assist the design.
of offshore structures and foundations for the windmill farm. Moreover, the data is used to identify locations of structural complexities and other potential geohazards, such as accumulations of shallow gas, that should be avoided. The results and interpretations of the data were also used to develop a plan for the geotechnical survey, which included location determination for, among others, boreholes and cone penetration tests. The data size of the geological unit is quite large (Table 3.1). Per unit a more or less continuous interpretation is given along the survey lines, consisting of approximately 160,000 points to 650,000 points depending on the extent of the interpretation [Agency (2016)].

Different interpolation methods are compared for two selected subsets of the data, one located within WFS I and another one located in WFS II. The locations of the two subsets are shown in Figure 5.6. The geological units that are continuously interpreted and thus used within the first subset are unit A, unit B, subunits C1 and C2, unit D, subunit E1 and subunit F1b. In the second subset continuous descriptions of unit A, B, subunit E5a and E5b and subunits F1b and F2 are available and used.

Figure 5.6: Example of seismic cross-section obtained by the seismic sparker and interpretations of different geological units. The overlapping borehole and cone penetration test results are plotted on top of the section as red lines [Agency (2016)].
5.2.3. Selected subsets
Two subsets have been selected, one in Wind Farm Section I and another one in Wind Farm Section II. The locations of the selected subsets is given in Figure 5.7. There are different interpreted geological units available for each of these two subsets. The amount of points per unit is reduced to 1% because there are only limited computational resources available. The remaining amount of points still constitute a reasonable representation of each unit such that it reflects both the acquisition geometry and the signal of the data in a sufficient way for the goal of the analysis, which is the comparison of the different interpolation methods. The amount of point within subset 1 and 2 are given in Table 5.2.

![Subset WFS I](image1) ![Subset WFS II](image2)

Figure 5.7: Locations of subset 1 (left) and subset 2 (right).

<table>
<thead>
<tr>
<th>Subset 1</th>
<th>Number of points</th>
<th>Xmin (m)</th>
<th>Xmax (m)</th>
<th>Ymin (m)</th>
<th>Ymax (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Subset 1</td>
<td>271</td>
<td>503,500</td>
<td>506,500</td>
<td>5,733,000</td>
<td>5,736,000</td>
</tr>
<tr>
<td>Subset 2</td>
<td>292</td>
<td>502,400</td>
<td>505,400</td>
<td>5,716,200</td>
<td>5,719,200</td>
</tr>
</tbody>
</table>

Table 5.2: Overview of WFS I subset 1 and WFS II subset 2.

The regions used for interpolation and error computation are given in Figure 5.8.

![Subset WFS I base A (m)](image3) ![Subset WFS II base A (m)](image4)

Figure 5.8: Regions used for cross validation for WFS I and WFS II. The used points are represented by the large circles, the other points represented by smaller dots are given as additional input for the calculations.
5.3. Tidal sand waves

The next case study dataset consists of two types of echo sounder datasets that are used for tidal sand wave monitoring. The sea floor is covered by different rhythmic features. One of the most relevant of these are the tidal sand waves. Tidal sand waves are characterized by wavelengths of hundreds of meters and amplitudes of up to several meters [Dorst, 2009]. The bathymetric measurements are acquired by the Royal Netherlands Navy (RNLN) with two types of vessels, a single-beam and a multi-beam echo sounder (SBES and MBES). The main purpose of these acquisitions is to create and update nautical charts that enable safe navigation at sea. The tidal sand waves are highly dynamics and therefore need to be closely monitored at some locations. The echo sounder data is used in several studies to estimate the sand wave dynamics. These studies play an important role in resurveying planning.

5.3.1. Data description

Single- and multi beam systems are also acoustic underwater systems. The distinct difference between these two systems and the seismic sparker data from Fugro is the frequency range. The single beam and multi beam echo sounder systems have a frequency range from approximately 10 to 100 kHz (see Figure 5.4), whereas the seismic sparker system from Fugro uses sound with a much lower frequency. Moreover, the single- and multi-beam echo sounders use one single receiver, whereas the seismic sparker system uses multiple receivers in an array [Lurton (2010)].

The single- and multi beam echo sounders both emit a single ping at the time and receive its response. A single beam echo sounder emits and receives one ping at the time. The depth of the seafloor is computed using the travel time and the velocity of this one ping. The dataset acquired by a single beam echo sounder consists of separate sea floor depth points along the sailed lines of the survey vessel. A multi beam echo sounder also emits one single ping. However, the receiver splits the returning signal into incoming beams of different angles. The angle from the ship to the seafloor is used to compute the seafloor depth at different locations. The dataset of a multi beam echo sounder has a much higher point density than the single beam echo sounder, as one single ping results in multiple seafloor depths at different locations.

The data has been acquired west of the coast of the Netherlands. The coordinates of both datasets are in Rijksdriehoek (RD). The single beam echo sounder dataset acquired in June 2003 is used to validate the workflow proposed in the previous section. The single beam dataset consists of 349,642 points, the different survey lines have a spacing of 125 meters. Figure 5.9 shows the seafloor depths obtained by the single beam echo sounder. The focus will be on two selected subsets that are indicated in black. Figure 5.10 shows the two subsets and the subdivision of each subset that is used for subset cross-validation. The number of points and the extent of the two selected subsets are given in Table 3.3. The areas indicated in red show the subsets that have been used for subset cross validation.

![Tidal sand wave dataset (depth seafloor (m))](image)

Figure 5.9: Tidal sand wave SBES dataset acquired in June 2003 and the two test locations (black squares).
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Table 5.3: Overview of Zandgolf data subset 1 and subset 2.

<table>
<thead>
<tr>
<th></th>
<th>Number of points</th>
<th>Xmin (m)</th>
<th>Xmax (m)</th>
<th>Ymin (m)</th>
<th>Ymax (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Subset 1</td>
<td>1632</td>
<td>556,600</td>
<td>557,400</td>
<td>5,816,500</td>
<td>5,817,300</td>
</tr>
<tr>
<td>Subset 2</td>
<td>1563</td>
<td>576,600</td>
<td>577,400</td>
<td>5,817,500</td>
<td>5,818,300</td>
</tr>
</tbody>
</table>

5.3.2. Measurement error variance
The measurement error variance of the single beam and multi beam echo sounder surveys are used to model a nugget effect, the offset of the variogram at zero distance, for kriging. Adding a nugget effect to the variogram model leads to smoother estimates, as the results are not forced to fit the data points exactly. The measurement variances are computed by Dorst (2009) and are a function of depth. The resulting measurement error variances are the sum of the variances of different error sources from the devices and external factors, for example water level reduction. A complete description of the error sources for the different vessels used by RNLN please consult Dorst (2009). The measurement error variance \( \sigma_{p,s}^{(e)2} \) of single-beam depth measurements is [Dorst (2009)]:

\[
\sigma_{p,s}^{(e)2} = 1.4 \times 10^{-6} \cdot d_{p,s}^2 + 0.014 \tag{5.1}
\]

in which \( d_{p,s}^2 \) is the depth of the seafloor.

Figure 5.10: Subdivision of subset 1 and 2 for subset cross validation.

The used nugget effect is the measurement error variance computed for the average seafloor depth for each subset. The single beam echo sounder dataset is used to validate the workflow that follows from the analysis of the results of the Borssele Windmill Farm. The workflow resulting from the Fugro dataset is applied to the dataset. The outcome of the workflow is compared to cross validation results for the two subsets of the dataset.
6

Results for interpolation methods

In this chapter the results of this study are presented. In section 4.1 natural neighbour interpolation, ordinary kriging and natural neighbour kriging are compared for the Davis test dataset. Section 4.2 focusses on the results for the Borssele windmill farm case study dataset. In section 4.3 the results for the Tidal sand waves case study dataset are presented.

6.1. Davis’ testdata
In the following section the results of natural neighbour kriging, abbreviated as OK\textsubscript{nn}, for the Davis dataset are given and compared to the results of ordinary kriging OK and natural neighbour interpolation NN. The height dataset is quite small, and therefore there was no computational need to use any other type of interpolation neighbourhood for the ordinary kriging method. First the interpolation results for all three methods and their differences are qualitatively discussed. Then the results of these three interpolation methods are compared quantitatively, first based on the Watson criteria and then in a more quantitative manner, using three types of cross-validation techniques: leave-one-out, 2-fold and 10-fold cross-validation. The two kriging techniques, natural neighbour kriging and ordinary kriging are compared in terms of kriging variance. Also the weights of each natural neighbour in ordinary kriging are computed and summed to describe the suitability of natural neighbour as selected interpolation neighbourhood.

6.1.1. Height differences
In Figure 6.1 the interpolated heights using ordinary kriging, natural neighbour kriging and natural neighbour interpolation are given. At first sight the results look quite similar. The clearest deviation between the kriging methods and natural neighbour interpolation can be distinguished in the down-right area: here, the effect of the highest point in the area seems to be more local for natural neighbour interpolation.
Figure 6.1: Interpolated heights for ordinary kriging (OK), natural neighbour kriging (OK_{nn}) and natural neighbour interpolation (NN).

Figure 6.2 illustrates the absolute differences between the interpolated heights. These differences are but given to shortly demonstrate the (dis)similarities between the three methods. One can clearly recognize the influence of the natural neighbours points as input for natural neighbour kriging and natural neighbour interpolation, as these two methods give similar results. Also, one is still able to see the similarities between natural neighbour kriging and ordinary kriging, as these to also have low differences in interpolation results. Of course, these differences are highest for the two least-similar techniques: ordinary kriging and natural neighbour interpolation.
6.1. Davis' test data

Figure 6.2: Absolute height differences between ordinary kriging (\(OK\)), natural neighbour kriging (\(OK_{nn}\)) and natural neighbour interpolation (\(NN\)).

6.1.2. Watson's criteria

Watson's criteria are used to compare the natural neighbour kriging method in general. To obtain a better understanding of the behaviour of the results of natural neighbour interpolation the used range and sill values of the used variogram model were modelled. Variations in sill values did not have a distinct effect on the resulting interpolation, as they results in a scaling of the covariance matrix \(C_{nn}\) only. Range variations did have a effect on the results, as they will change the non-diagonal values in the covariance matrix \(C_{n}\).

Variogram variations

The results of the variogram variations illustrates that the method does not always give smooth results. Figure 6.3 shows the effect of varying range values on a small area of the test data set. The interpolation for range values of 0.1 m, 1 m, 10 m and 100 m are shown.

The figure shows that there are jumps in the interpolated heights for small range values. These jumps or artefacts have a close relation to the cumulative weights in ordinary kriging, shown in Figure 6.4. For a range of 0.1 meters the weights given to the natural neighbours in ordinary kriging is very low for all locations, except close to the input points. The interpolation result for this range value is very blocky and clearly shows where there is a jump in the set of used natural neighbours. For a range of 1 meter the jumps only seem to occur when the cumulative weight percentage in ordinary kriging is much smaller than 100 %, for example in the upper right corner of the image. The interpolation result for range values of 10 meters and 100 meters seems smooth and the artefacts have disappeared. The cumulative weight percentage in ordinary kriging for both
6. Results for interpolation methods

<table>
<thead>
<tr>
<th>Criteria</th>
<th>OK</th>
<th>OK$_{NN}$</th>
<th>NN</th>
</tr>
</thead>
<tbody>
<tr>
<td>exact</td>
<td>(+)</td>
<td>(+)</td>
<td>(+)</td>
</tr>
<tr>
<td>continuous</td>
<td>(+)</td>
<td>(+)</td>
<td>(+)</td>
</tr>
<tr>
<td>smooth</td>
<td>(+)</td>
<td>(+ -)*</td>
<td>(+ -)**</td>
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<tr>
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<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>local</td>
<td>(+)</td>
<td>(+)</td>
<td>(+)</td>
</tr>
<tr>
<td>adaptable</td>
<td>(+)</td>
<td>(+)</td>
<td>(+)</td>
</tr>
<tr>
<td>computationally efficient</td>
<td>(-)</td>
<td>(+ -)*</td>
<td>(+)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>automatic</td>
<td>(+ -)*</td>
<td>(+ -)*</td>
<td>(+)</td>
</tr>
</tbody>
</table>

* smooth when the field is not under sampled
** first derivative undefined at data points, but methods available to solve this

Table 6.1: Overview of Watson’s criteria for ordinary kriging OK, natural neighbour kriging OK$_{NN}$ and natural neighbour interpolation NN.

these range values is larger than 100 % at any location (see Figure 6.4).

The artefacts appear due to the way kriging handles interpolation at locations that are further away from the known points than the range. At these locations there is no spatial relation to the known points anymore, and therefore kriging estimates the heights here by a weighted-average of known points. In natural neighbour kriging only the natural neighbours are used, and therefore the heights at these locations are limited to an average of the natural neighbours only, rather than a larger set of points or even all points. The artefacts seem to occur only when the known points have no spatial relation anymore, e.g. are further away from each other than the range. The results of natural neighbour interpolation will be smooth if this is not the case. To avoid these artefacts the to be interpolated field must thus not be under sampled.

**Computational efficiency**

Natural neighbour kriging has an additional step compared to ordinary kriging, namely the identification of the natural neighbours for each grid cell. This makes natural neighbour kriging computationally less favourable for very small datasets. However, for increasingly large datasets natural neighbour kriging becomes more and more computationally efficient, since it reduces the size of variance-covariance matrix $C_{nn}$ considerably. Recall that the weights calculation in kriging has a time complexity of $O(mn^3)$, $n$ being the number of input points and $m$ being the number of grid points. The number of grid points remains the same, but the number of input points reduces to only a few natural neighbours per grid cell. This will result in a significant improvement of the computational efficiency, making natural neighbour kriging more favourable for larger datasets.
**Comparison with ordinary kriging and natural neighbour interpolation**

An overview of the rankings on Watson's criteria for all three methods is given in Table 4.1. These rankings can be summarized the following manner:

All three methods are exact, continuous, local and adaptable. Ordinary kriging is a smooth method. Natural neighbour kriging is smooth on the condition that the field is not under sampled and natural neighbour interpolation the first derivative is undefined at data points. Natural neighbour interpolation is most computationally efficient of these three methods. The larger the dataset, the more favourable natural neighbour kriging becomes in terms of computational efficiency compared to ordinary kriging. Natural neighbour interpolation is an automatic method, both kriging methods can be fully automatic, but checking the variogram model manually is often preferred.

These criteria are qualitative descriptors of how well a certain interpolation method works in general, but do not say anything about the quantitative performance of the method. Cross-validation techniques are used to quantify the MSE for each method in the next sections.
6. Results for interpolation methods

6.1.3. Cross-validation

Leave-one-out

The results of leave-one-out cross-validation for natural neighbour kriging, ordinary kriging and natural neighbour interpolation are given in Figure 6.5, Figure 6.6 and Figure 6.7. The MSE obtained using by cross-validating all points is 762 m$^2$ for natural neighbour interpolation, 645 m$^2$ for ordinary kriging and is 582 m$^2$ for natural neighbour kriging. Here, the height values estimated using natural neighbour kriging resemble the true height the most.

The drawback of using all data points for cross-validation is that some edge- and extrapolation-effects are included in the determined MSE. One way to overcome this is to only validate the results within the interior of the dataset, keeping the points on the edges of the dataset fixed. Therefore another cross-validation calculation is done using only the interior points. The points on the convex hull of the dataset are used as fixed, known points and the remaining points are used for validation, as illustrated in Figure 5.2. The resulting MSE are 349 m$^2$ for natural neighbour interpolation, 392 m$^2$ for ordinary kriging and 344 m$^2$ for natural neighbour kriging. In this particular case the MSE is again lowest for natural neighbour interpolation. After improving the variogram model used for both kriging methods another validation calculation is performed on the interior points of the dataset. The experimental variogram is now computed using the interior points only, leading to a better fit within this region. Now, a spherical model with a range of 3.3 meter and a sill of 1470 is used. By doing so the MSE improves to 269 m$^2$ for ordinary kriging and to 340 m$^2$ for natural neighbour kriging. Now the MSE is lowest for ordinary kriging.
6.1. Davis’ testdata

Figure 6.5: Cross-validation results for ordinary kriging (OK), natural neighbour kriging (OK_{nn}) and natural neighbour interpolation (NN) using all points, along with the associated standard deviations for the kriging methods. For both kriging methods the spherical variogram model with a range of 3.3 meter and a sill of 1470 is used.

K-fold
Initially two types of k-fold cross-validation, 10-fold and 2-fold, are used and modelled using 1000 Monte Carlo simulation runs. The results are given in Figure 6.8 and Figure 6.9. The upper image in Figure 6.8 shows a histogram of the Monte-Carlo runs for 10-fold cross validation using all data points. The mean MSE for natural neighbour interpolation is 798 m², for ordinary kriging 636 m² and for natural neighbour kriging 614 m². The standard deviation of the MSE for these methods is 125 m² for natural neighbour interpolation, 64 m² for ordinary kriging and 61 m² for natural neighbour kriging. Natural neighbour kriging has the lowest mean MSE as well as the lowest standard deviation.
Figure 6.6: Cross-validation results for ordinary kriging (OK), natural neighbour kriging ($OK_{nn}$) and natural neighbour interpolation (NN) along with the associated standard deviations for the kriging methods. The cross-validation is performed on the points within the interior of the dataset, the point on the convex hull are fixed. For both kriging methods the spherical variogram model with a range of 3.3 meter and a sill of 1470 is used.

The lower image in Figure 6.8 shows the histogram for the Monte Carlo simulation of 2-fold cross-validation using all data points. The mean MSE for natural neighbour interpolation is 1045 m$^2$, for ordinary kriging 781 m$^2$ and for natural neighbour kriging 813 m$^2$. The standard deviation of the MSE for these methods is now 427 m$^2$ for natural neighbour interpolation, 133 m$^2$ for ordinary kriging and 163 m$^2$ for natural neighbour kriging. Both the mean MSE and the standard deviation are now lowest for ordinary kriging instead of natural neighbour kriging.

Again the procedure is repeated so it included only the interior points, keeping the points on the convex hull fixed. The results are given in Figure 6.9. Two different variogram models are used. For the upper image a spherical model with range 3.3 meters and sill 1470 is used. The mean MSE for natural neighbour interpolation is 443 m$^2$, for ordinary kriging 470 m$^2$ and for natural neighbour kriging 433 m$^2$. The standard deviation is now 76 m$^2$ for natural neighbour interpolation, 100 m$^2$ for ordinary kriging and 78 m$^2$ for natural neighbour kriging. The mean MSE and the standard deviation for all three methods has drastically improved. For the bottom image a spherical model with range 2.2 meters and sill 850 is used. The mean MSE of ordinary kriging is now 377 m$^2$ and the standard deviation 68 m$^2$. For natural neighbour interpolation the mean MSE is 443 m$^2$ and the standard deviation 79 m$^2$, and for natural neighbour kriging the mean MSE is 429 m$^2$ and the standard deviation 77 m$^2$. The results of ordinary kriging are now improved greatly, whereas the results of natural neighbour kriging are only slightly improved.
Figure 6.7: Cross-validation results for ordinary kriging (OK), natural neighbour kriging (OKnn) and natural neighbour interpolation (NN) along with the associated standard deviations for the kriging methods. The cross-validation is performed on the points within the interior of the dataset, the point on the convex hull are fixed. For both kriging methods a spherical variogram model with a range of 2.2 meter and a sill of 850 is used, which has a better fit for the interior points.
6. Results for interpolation methods

6.1.4. Kriging variance
The kriging variance is computed for both ordinary kriging and natural neighbour kriging. Figure 6.10 shows the results for ordinary kriging and natural neighbour kriging and the absolute differences between the two. The computed kriging variance is equal for both methods close to the known locations. In between the known locations, the kriging variance of the results for natural neighbour kriging is somewhat higher than for ordinary kriging. The mean and the maximum difference are computed within the convex hull area. The mean variance difference is 10.9 m$^2$. 

Figure 6.8: 2-fold and 10-fold cross-validation results for ordinary kriging (OK), natural neighbour kriging (OK$_{nn}$) and natural neighbour interpolation (NN) using all points.
6.1.5. Ordinary kriging weights

Only the natural neighbours of each grid cell obtain weights in natural neighbour kriging, their total weight sums to 1. To see whether the selection of natural neighbours only is sufficient, one can look at the weights given to these natural neighbours in ordinary kriging. The cumulative weights of the natural neighbours in percentages in ordinary kriging are shown in Figure 6.11. High cumulative weight percentages would illustrate that the natural neighbours in ordinary kriging comprise a significant amount of the kriging weight. Low percentages, however, would mean that to some extent relevant points in ordinary kriging are disregarded by the selection of natural neighbours. Note that the cumulative weights in ordinary kriging can reach values over a 100 % because of the existence of negative kriging weights. Negative weights for example arise when points nearby the estimation location screen points located behind them.
Throughout the whole area the cumulative weights are over 100%, with a mean of 110% in the convex hull area. The maximum cumulative weight value is 126%. At these locations there seems to be a significant amount of screening in ordinary kriging. The high cumulative weights show that the natural neighbours indeed constitute the relevant points in ordinary kriging for this particular dataset.
6.1.6. Computational speed

Figure 6.12 gives an overview of the function calls for ordinary kriging and natural neighbour kriging of the Davis dataset for an interpolation grid of 100 x 100 points. The left image shows the Matlab profiler time for ordinary kriging. The total time it took to compute the ordinary kriging interpolation was 270 seconds (indicated in red). The right image shows the Matlab profiler for natural neighbour kriging. The time the total computation took was only 49 seconds (indicated in red). Of these 49 seconds 15 seconds were needed to determine the natural neighbours of each interpolation point. The kriging step itself took only 27 seconds. The computational speed of natural neighbour kriging is thus improved considerably compared to ordinary kriging.

Figure 6.12: Matlab profiler for ordinary kriging operation (left) and natural neighbour kriging operation (right) for an interpolation grid of 100 x 100 points for the Davis dataset.
6.1.7. Conclusions
The comparison of natural neighbour kriging (OK$_{nn}$), ordinary kriging (OK) and natural neighbour interpolation (NN) based on Watson's criteria has led to the following main conclusions:

- Ordinary kriging scores best on the first five Watson criteria.
- Natural neighbour interpolation is computationally most efficient.
- Natural neighbour kriging becomes more computationally favourable to ordinary kriging for increasingly large datasets.

The comparison of natural neighbour kriging, ordinary kriging and natural neighbour interpolation using the Davis dataset has led to the following conclusions:

- The kriging variances of natural neighbour kriging are larger than those of ordinary kriging.
- The cumulative weight of the natural neighbours in ordinary kriging illustrates that the selection of natural neighbours constitute the relevant points in ordinary kriging.
- The weight computation speeds up considerably using natural neighbours for ordinary kriging.
6.2. Borssele windmill farm

In the following section the results for the two subsets of the Borssele Windmill data are presented. For both subsets the variogram models and the prediction errors for \( \text{NN}, \text{OK}, \text{OK}_{\text{NN}}, \text{AOK}, \text{AOK}_{\text{NN}} \) obtained using leave-one-out and subset cross validation are presented.

6.2.1. Analysis steps

The methods mentioned in the previous chapters, natural neighbour interpolation (\( \text{NN} \)), ordinary kriging (\( \text{OK} \)) and natural neighbour kriging (\( \text{OK}_{\text{NN}} \)) and three methods that include adjustments to anisotropy are compared. For each layer both an isotropic experimental variogram and anisotropic angular experimental variograms are computed. All the variogram models used are spherical.

For leave-one-out cross validation the whole subset is used and the mean squared errors are computed for each point. The mean squared error is a value that is sensitive to outliers and therefore, to show the distribution of the errors more clearly, a graph is created that shows the development of the mean squared error by removing the largest errors one-by-one. The x-axis represents the amount of points removed and the y-axis the mean squared error calculated over the remaining points. An example of such a graph is given in Figure 6.13. Moreover, a graph is created where the mean squared errors is divided in the two prominent directions, south-west and north-east, to see the distribution of the errors in these two directions. These mean squared error graphs are computed for each geological unit within the two subsets (see Appendix C).

![Mean Squared Error Graphs](image_url)

Figure 6.13: Development of the MSE (m²) for natural neighbour interpolation for unit A in subset WFS I. The left image represents the mean squared errors for leave-one-out cross-validation: the total error is in black, the red line represents the errors in the south-west to north-east lines and the blue line represents the errors in the north-west to south-east directions. The right image represents the mean squared errors obtained using subset cross validation. The red line are the errors in the main, south-west to north-east direction, and the blue line in the north-west to south-east direction.

For subset cross validation the region is divided into two separate parts: data obtained in the main, south-west to north-east, acquisition direction and the data in the less densely sampled cross-line acquisition direction, oriented from north-west to south-east. Two mean squared error development graphs for each of these directions are computed and plotted for each layer.

An overview of the resulting mean squared errors for each interpolation technique for each geological unit is plotted in a table where the values are coloured from green (lowest error) to red (highest error). The goal of this analysis is to get insight about what interpolation techniques should be used for a particular field and why. The results are used to propose a workflow that will allow the user to choose an appropriate interpolation technique based on the type of signal.
Three experimental variograms have been computed for each of the units within the subsets: an isotropic, regular variogram and two angular variograms. The isotropic experimental variogram has been used to determine the variogram model values for ordinary kriging and natural neighbour kriging. The angular experimental variogram is used to obtain the anisotropic variogram model for anisotropic ordinary kriging and anisotropic natural neighbour kriging. The first angular variogram uses a smaller angle bin value of 15 degrees and has been used to search for the directions of minimum and maximum variability. The second angular variogram uses a larger angle bin of 30 degrees which results in less lines and a clearer image and therefore it is used to check whether the determined range, sill and anisotropy factor values are correct.

The estimated variogram models are now used to perform two types of cross-validation to predict the errors associated with the different interpolation techniques. The short-range correctness of the interpolation techniques is tested with leave-one-out cross validation and the correctness on a longer range is tested by subset cross-validation.
6.2.2. Subset Wind Farm Section I

Wind Farm Section I is the northernmost of the two sub regions. The geological units that have been interpreted within this subset are unit A, unit B, subunits C1 and C2, unit D, subunit E1 and subunit F1b. Although subunit F1b was available, it could not be used for kriging interpolation, as there seemed to be a misinterpretation in one of the cross-line cross sections, blowing up the experimental variogram values. Therefore subunit F1b is left out of consideration for comparison.

Variogram modelling

The variogram models given in Figure 6.14 have been used to interpolate the data. In this table also the main direction of continuity $\theta$ and the used anisotropy factor $\lambda$ are given for each geological unit.

<table>
<thead>
<tr>
<th>WFS I</th>
<th>isotropic model</th>
<th>anisotropic model</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>range</td>
<td>sill</td>
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<tr>
<td>A</td>
<td>2000</td>
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<tr>
<td>B</td>
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</tr>
<tr>
<td>C1</td>
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<td>1.50</td>
</tr>
<tr>
<td>C2</td>
<td>2300</td>
<td>2.20</td>
</tr>
<tr>
<td>D</td>
<td>3500</td>
<td>3.80</td>
</tr>
<tr>
<td>E1</td>
<td>3500</td>
<td>2.60</td>
</tr>
</tbody>
</table>

Figure 6.14: Table containing variogram model values for the layers within subset WFS I.
Isotropic variograms

The isotropic variogram model values are based on the experimental variograms computed for each layer within subset WFS I. The experimental variograms are plotted in 6.15. Please note that the x- and y-values on which the variograms are plotted are different for each unit. The different experimental variograms have different range and sill values. The experimental variogram for unit B clearly has a much lower range value, which is expected since this layer is an unconformity rather than an actual geological layer.

Figure 6.15: Experimental variograms for subset 1 of each geological unit.
Anisotropic variograms
The anisotropic variogram model values are based on the angular experimental variograms computed for each layer within subset WFS I. The angular experimental variograms, computed with steps of 30 degrees, are plotted in 6.20. The angular experimental variograms of unit A have different sill values and therefore the signal in unit A seems to be predominantly zonal anisotropic. The angular experimental variograms of unit B are similar and unit B thus seems not to be anisotropic. The angular experimental variograms for C1 and C2 show both features of geometric and zonal anisotropy, but both layers seem to be mainly geometric anisotropic, as most variograms have similar sill values. The same holds for unit D and unit E1. Although the sill of the experimental variogram in the direction of $\frac{1}{6}\pi$ is much lower than those of the other variograms, the other variograms do have a similar sill values, indicating geometric anisotropy.

Figure 6.16: Angular experimental variograms with $\theta_{\text{step}} = 30$ degrees and $n_{\text{bins}} = 20$ for subset 1 of each geological unit.
Cross-validation

The development of the mean squared errors computed using cross-validation are given in Figure 6.17 for unit A, B and C1 and in Figure 6.18 for unit C2, D and E1. A full description of the results is given in Appendix C. The majority of the layers are anisotropic (A, C1, C2, D, E1) and the anisotropic methods resulted in smaller errors, except for unit D. For most of the anisotropic layers \( AOK_{AX} \) performed best in general, followed by \( AOK_{ANN} \). Unit B is isotropic, and the isotropic interpolation methods thus resulted in smaller errors.

Figure 6.17: Table containing cross-validation MSE (m²) values for different interpolation techniques for unit A, B and C1 in WFS I.

Figure 6.18: Table containing cross-validation MSE (m²) values for different interpolation techniques for unit C2, D and E1 in WFS I.
6.2.3. Subset Wind Farm Section II
Wind Farm Section I is the northernmost of the two sub regions. The geological units that have been interpreted within this subset are unit A, unit B, subunits E5a and E5b and subunits F1b and F2.

Variogram modelling
The variogram models given in Figure 6.19 have been used to krige the data. The main direction of continuity $\theta$ and the used anisotropy factor $\lambda$ are also given in this table.

<table>
<thead>
<tr>
<th>WFS II</th>
<th>Isotropic model</th>
<th>anisotropic model</th>
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<td>A</td>
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<tr>
<td>B</td>
<td>400</td>
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</tr>
<tr>
<td>E5a</td>
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</tr>
<tr>
<td>E5b</td>
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</tr>
<tr>
<td>F1b</td>
<td>1600</td>
<td>4.50</td>
</tr>
<tr>
<td>F2</td>
<td>1600</td>
<td>6.50</td>
</tr>
</tbody>
</table>

Figure 6.19: Table containing variogram model values for the layers within subset WFS II.

Isotropic variograms
The isotropic variogram model values are based on the experimental variograms computed for each layer within subset WFS I. The experimental variograms are plotted in 6.20. The experimental variograms all have different range and sill values. The slopes of the experimental variograms mainly look more or less linear, supporting a spherical variogram model which also has a linear slope. For this subset the sill values of the isotropic experimental variograms increase with depth for all layers.

Figure 6.20: Experimental variograms for subset 2 of each geological unit.
**Anisotropic variograms**

The anisotropic variogram model values are based on the angular experimental variograms computed for each layer within subset WFS II. The angular experimental variograms, computed with steps of 30 degrees, are plotted in 6.21. The majority of the angular experimental variograms for unit A reach approximately the same sill value, resembling predominantly geometric anisotropy in the signal. The angular experimental variograms for unit B, just like for subset 1, are close together and unit B thus seems not to show a clear anisotropy in the signal. The angular experimental variograms both for unit E5a and unit E5b show a variation of sill values, and the signal thus seems to be predominantly zonal anisotropic. The angular experimental variograms for both unit F1b and F2 clearly show both features of geometric as well as zonal anisotropy, geometric anisotropy being seemingly predominant.

Figure 6.21: Angular experimental variograms with $\theta_{\text{step}} = 30$ degrees and $\text{n}_{\text{bins}} = 20$ for subset 2 of each geological unit.
Cross-validation

The development of the mean squared errors computed using cross-validation are given in Figure 6.22 for unit A, B and E5a and in Figure 6.23 for unit E5b, F1b and F2. A full description of the results is given in Appendix C. The majority of the layers (A5a, E5b, F1b and F2) are anisotropic and here the anisotropic methods gave smaller errors. For all these layers anisotropic natural neighbour kriging (both AOKNN and AOKAN) performed better than anisotropic ordinary kriging. The differences between AOKNN and AOKAN are small and comparable for all the anisotropic layers, only for layer A AOKAN gave smaller errors than AOKNN for all cross validation methods. Layer B is an isotropic unit and the isotropic methods thus gave smaller errors in general.

Figure 6.22: Table containing cross-validation MSE (m²) values for different interpolation techniques for unit A, B and E5a in WFS II.

![Figure 6.22](image)

Figure 6.23: Table containing cross-validation MSE (m²) values for different interpolation techniques for unit E5b, F1b and F2 in WFS II.

![Figure 6.23](image)
6.2.4. Anisotropic natural neighbours

Figure 6.24 shows the number of natural neighbours per grid cell and the number of anisotropic natural neighbours per grid cell for $\theta = 1/6 \pi, \lambda = 0.5$ and for $\theta = 4/6 \pi, \lambda = 0.5$. Figure 6.24 shows that the number of anisotropic neighbours that are selected increases when the acquisition geometry and the direction of main continuity of the signal align. The number of anisotropic natural neighbours decreases if the acquisition geometry and the direction of main continuity of the signal are perpendicular.

Figure 6.24: Number of natural neighbours (left), number of anisotropic neighbours determined using $\theta = 1/6 \pi, \lambda = 0.5$ (middle) and anisotropic neighbours determined using $\theta = 4/6 \pi, \lambda = 0.5$ (right).
6.2.5. Full subset interpolation
The comparison of the different interpolation methods is done using a subset of only 1% of the data points. It is also possible to use the full dataset as input for natural neighbour kriging. To illustrate the effect of varying data sizes, and to compare their resulting computational speed for this type of geometry in particular, three interpolations are computed: one using all the available points in subset 1 (27,100 points), one using 10% of the points (2,710 points) and one using only 1% of the points (271 points).

The three interpolations are computed for subset 1 of unit A using anisotropic natural neighbour kriging. The experimental variogram computation using 10% of the points and using all data points resulted in a very similar variogram model, so the same anisotropic variogram model for unit A is used as the one stated in Figure 6.13.

Figure 6.25: Anisotropic natural neighbour kriging result of geological layer A subset 1 using 1% of the points (up left), 10% of the points (up right), and all points (bottom figure).
The anisotropic natural neighbour kriging results using 1% of the points, 10% of the points and all points are given in Figure 6.25. At first sight the results seem very similar. The absolute differences between the interpolation results using all points, compared to the interpolation results using 10% and 1% of the points is given in Figure 6.26. The left image in Figure 6.26 illustrates that the differences between the results using all points and using only 1% of the points are quite large at some places, but in general the absolute difference is no more than 0.1 meters. The right image in Figure 6.26, on the other hand, shows that the difference between the results using all points and 10% of the points is much smaller, the absolute difference between the two is below 0.01 meters everywhere. Moreover, the absolute difference in kriging variance is computed and given in Figure 6.27. Figure 6.27 shows that the absolute difference in kriging variance comparing using 100% and 1% of the points is quite large, whereas the absolute difference in kriging variance comparing using 100% and 10% of the points is also much smaller.

Figure 6.26: Absolute difference in anisotropic natural neighbour kriging result of geological layer A subset 1 in meters using all points compared to using 1% of the points (left) and 10% of the points (right).

Figure 6.27: Absolute difference in kriging variance (m$^2$) of geological layer A subset 1 using all points compared to using 1% of the points (left) and 10% of the points (right).
6.2. Borssele windmill farm

**Amount of natural neighbours**
The selection of natural neighbours is based on the acquisition geometry. For regular, evenly spread acquisition geometries (for example the geometry of the Davis dataset) the amount of natural neighbours is small at all interpolation locations, leading to a huge computational advantage compared to regular kriging methods. This huge advantage remains for increasingly large data sizes of these type of acquisition geometries, as the amount of selected natural neighbours remains small at all locations.

The spread of points of the acquisition geometry of the Borssele windmill farm dataset, on the other hand, is not evenly distributed. The amounts of natural neighbours that are selected as interpolation neighbourhood does increase with increasing data size, and the computational advantage compared to regular kriging methods is therefore reduced to some extent. Moreover, the amount of natural neighbours varies a lot per location. For example, close to the input points fewer natural neighbours are selected than in the middle of an acquisition rectangle. Interpolation locations that use a lot of natural neighbour as interpolation neighbourhood govern the computational speed of the interpolation, as the covariance matrix will be relatively large at these locations.

**Computational speed**
The amounts of natural neighbours that is selected for each case is reflected by the computational speed of the interpolation. Figure 6.28 shows the Matlab profiler for the interpolation using all points within subset 1. The profiler shows that the interpolation took about 5 hours. This is quite long, however, please do note the following points. First of all, the most time-consuming step was not the kriging step (krig) itself, but the computations of the distances between points (edist). This illustrates that, compared to regular kriging where the kriging step itself prevails, the computational speed is still higher than for regular kriging methods. Second of all, the computation could be speed up considerably using parallel computations for each acquisition rectangle, as the selection of natural neighbours will never pass the borders of these rectangles.

![Figure 6.28: Matlab profiler for anisotropic natural neighbour kriging of subset 1 using all the points.](image-url)
Table 6.29: Matlab profiler for anisotropic natural neighbour kriging of subset 1 using 10% of the points.

<table>
<thead>
<tr>
<th>Function Name</th>
<th>Calls</th>
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<th>Self Time</th>
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<td>13.581 s</td>
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<td>6.811 s</td>
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<tr>
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</tr>
<tr>
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</tr>
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<td>0.127 s</td>
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</tr>
</tbody>
</table>
6.2.6. Conclusions
The comparison of isotropic interpolation methods $NN$, $OK$ and $OK_{NN}$ and anisotropic methods $AOK$, $AOK_{NN}$ and $AOK_{ANN}$ for two subsets of the Borssele windmill farm dataset has led to the following conclusions:

- Almost all layers are anisotropic and for these layers the anisotropic interpolation methods resulted in smaller prediction errors. Unit B is an exception and is isotropic.
- For most layers $AOK_{NN}$ and $AOK_{ANN}$ gave smaller errors than $AOK$.
- More anisotropic natural neighbours are selected per grid cell when the main acquisition direction is in the same direction as the main continuity of the signal.
- Interpolation of the full dataset using natural neighbour kriging is possible. The computation is quicker than regular.
- There is a possibility to speed up natural neighbour kriging using parallel computations, or by reducing the number of input points.
- The natural neighbour kriging results using all points compared to 10% of the points are almost identical, however, natural neighbour kriging using 10% of the points is significantly faster.
6.2.7. Workflow schematic
Based on the results for the Fugro dataset the following workflow is proposed. The workflow schematic given in Figure 6.30.

Figure 6.30: Schematic workflow for the determination of the appropriate interpolation technique.
For each geological unit the workflow is followed. The methods proposed by the workflow are given in Table 4.2. The proposed methods are compared to the results of the cross validation given in Appendix C. The last column checks whether the proposed method was within the top two of the methods with the lowest predication errors. The overall score of the workflow is 8 out of 12, which comes down to 67%.

<table>
<thead>
<tr>
<th>Unit</th>
<th>Subset</th>
<th>Proposed method</th>
<th>yes / no</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>WFS I</td>
<td>$AOK_{ANN}$</td>
<td>yes</td>
</tr>
<tr>
<td>B</td>
<td>WFS I</td>
<td>$OK_{NN}$</td>
<td>yes</td>
</tr>
<tr>
<td>C1</td>
<td>WFS I</td>
<td>$AOK_{ANN}$</td>
<td>yes</td>
</tr>
<tr>
<td>C2</td>
<td>WFS I</td>
<td>$AOK_{ANN}$</td>
<td>no</td>
</tr>
<tr>
<td>D</td>
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<tr>
<td>B</td>
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<td>$OK_{NN}$</td>
<td>yes</td>
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<tr>
<td>F2</td>
<td>WFS II</td>
<td>$AOK_{NN}$</td>
<td>yes</td>
</tr>
</tbody>
</table>

Table 6.2: Overview of the proposed method by the workflow for each layer and whether the cross validation result indicated that this method was one of the two best methods (yes) or not (no).
6.3. Tidal sand waves

In the following section the results for two subsets of the single beam echo sounder data are presented. For both subsets the variogram models and the prediction errors for $NN$, $OK_{NN}$, $AOK_{NN}$ and $AOK_{ANN}$ obtained using leave-one-out and subset cross validation are presented.

6.3.1. Subset 1

The isotropic variogram model that is used for subset 1 has a range of 130 meters and a sill of $1.4 \, m^2$. The angular variogram model has a range of 600 meters, a sill of $1.5 \, m^2$, $\theta = 2/3 \pi$ and $\lambda = 0.2$. Subset 1 has a mean depth of -26.5 meters, resulting in a nugget effect of $0.01498 \, m^2$.

Figure 6.32 shows the experimental variogram and the angular experimental variogram computed for subset 1. The angular experimental variograms show that the direction of main continuity $\theta$ is the direction of $2/3 \pi$. The angular experimental variogram shows that the variance decreases in most directions for distances of around 500 meters. The angular experimental variograms approximately reach the same sill value, indicating that the signal is geometric anisotropic.

![Experimental variogram subset 1 Zandgolf, $n_{\text{bins}} = 20$](image1.png)

![Directional experimental variograms for subset 1 Zandgolf ($\theta_{\text{step}} = 30^\circ$, $n_{\text{bins}} = 20$)](image2.png)

Figure 6.31: Experimental variogram with $n_{\text{bins}} = 20$ for subset 1 of the Zandgolf dataset (left) and the angular experimental variograms with $\theta_{\text{step}} = 30$ degrees and $n_{\text{bins}} = 20$ (right).

Figure 6.33 shows the mean squared error development graphs for all four methods for subset 1. The graphs on the left represent the mean squared error computed using leave-one-out cross validation and the graph on the right represents the mean squared prediction errors computed using subset cross validation. The mean squared errors computed using leave-one-out cross validation are small for all methods. The mean squared prediction errors computed with subset cross validation show that $OK_{NN}$ gave the highest errors, followed by $NN$. The anisotropic methods $AOK_{NN}$ and $AOK_{ANN}$ gave much better results. The interpolation method that gave the lowest errors was $AOK_{ANN}$. 
6.3.2. Subset 2

The isotropic variogram model that is used for subset 2 has a range of 220 meters and a sill of 0.38 m². The angular variogram model has a range of 800 meters, a sill of 0.5 m², $\theta = 2/3\pi$ and $\lambda = 0.35$. Subset 2 has a mean depth of -23.1 meters, resulting in a nugget effect of 0.01475 m².

Figure 6.32 shows the experimental variogram and the angular experimental variogram computed for subset 2. The range of the isotropic variogram is similar subset 1, the sill however is much smaller. The same is seen in the angular experimental variograms. The range values are similar, and the direction of main continuity is the same, however, the sill value is smaller.

![Figure 6.32: Experimental variogram with $n_{\text{bins}} = 20$ for subset 2 of the Zandgolf dataset (left) and the angular experimental variograms with $\theta_{\text{step}} = 30$ degrees and $n_{\text{bins}} = 20$ (right).](image)

Figure 6.34 shows the mean squared error development graphs for all four methods for subset 2. The graphs on the left represent the mean squared error computed using leave-one-out cross validation and the graph on the right represents the mean squared prediction errors computed using subset cross validation. The mean squared errors computed using leave-one-out cross validation is similar for all methods, but somewhat higher for the anisotropic methods. The mean squared errors computed with subset cross validation are lowest for $AOK_{NN}$, followed by $AOK_{ANN}$. The cross validation results for natural neighbour interpolation gave the highest errors.
6.3.3. Workflow questions
The answers to the question in the proposed workflow for the full tidal sand wave dataset are:

*Is the signal isotropic or anisotropic?*

The signal is anisotropic. The anisotropy is clearly visible in the data itself (see Figure 3.19), and it is also recognizable in the experimental angular variograms.

*What is the predominant type of anisotropy?*

The predominant type of anisotropy is geometric. The angular experimental variograms all level off at approximately the same sill value.

*Can the spatial relationship be sufficiently captured by an anisotropic variogram model?*

Yes. The variogram model can capture the main relationship of both the normal and the angular experimental models, although there are some features that are excluded from the used variogram models (for example the small amplitude wave-like features).

*Are there large spatial variations in the signal?*

No. Although the sill values for the experimental variograms of subset 1 and 2 are different, the range values, the direction of main continuity $\theta$ and the anisotropy factor $\lambda$ are similar. The standard deviation of the depth values of both subsets are of the same order ($\sigma_s^1 = 1.1$ and $\sigma_s^2 = 0.6$).

*Are the available time and computational resources limiting with respect to the data size?*

Yes. Only the more computationally efficient methods are considered.

*Is the main acquisition direction in correspondence with the main direction of continuity?*

No. The main acquisition direction is in the north-south direction (approximately 10 degrees). The main direction of continuity is 120 degrees.

According to the workflow $AOK_{NN}$ should be used to interpolate the dataset. The cross validation results have shown that both anisotropic methods $AOK_{NN}$ and $AOK_{ANN}$ resulted in the smallest errors, for subset 1 $AOK_{ANN}$ gave the lowest errors and for subset 2 $AOK_{ANN}$. The differences were small though, so the workflow resulted in a reasonable proposal.
6.3.4. Conclusions
The comparison of isotropic interpolation methods $NN$ and $OK_{NN}$ and anisotropic methods $AOK_{NN}$ and $AOK_{ANN}$ for two subsets of the Tidal sand wave dataset has led to the following conclusions:

- The angular variogram models show that the signal is geometric anisotropic.
- The cross validation results for the anisotropic methods resulted in the smallest prediction errors, the isotropic methods gave much higher errors.
- The method that resulted in the smallest error was $AOK_{ANN}$ for subset 1 and $AOK_{NN}$ for subset 2.
- The workflow suggested $AOK_{NN}$ as the appropriate interpolation technique.
6.4. Discussion
The results of this project could be improved several ways. The main suggestions for improvement are stated below.

**Variogram modelling**
Although the used variogram models were fit to the data with great care, they could be improved in different ways. Most experimental variograms exhibited some kind of wave-like features beyond the range and sill values. These features often made automatic variogram fitting impossible, as they would move the variogram model to also fit these features best in a least-square sense. Therefore many variogram models were partially chosen manually.

The type of variogram model (e.g. spherical, exponential, Gaussian) could be altered to fit the data better. Although the Gaussian model gave the best fit to most of the experimental variograms for both datasets, its use lead to oversmoothing of the data and therefore resulted in erroneous results. For example, the use of a Gaussian relationship created unwanted wave-like features in between neighbouring data points. Some of these effects were still present after introduction of a nugget effect and therefore other types of variogram models were used. Another possible improvement is the anisotropic variogram models that are used for the anisotropic kriging methods. As mentioned before, the anisotropic variogram model that fits the direction of maximum and minimum variability best does not necessarily fit best in all directions. Moreover, the directions of maximum and minimum continuity are selected based on angular experimental variograms with a minimal angle bin of 15 degrees. This means that each angular experimental variogram includes all points that lie within a range of -7.5 degrees and +7.5 degrees from each other. The direction of the minimum and maximum continuity could be improved by for example directional gradient computations.

**Nugget effect**
The kriging interpolations of the geological layers of the Borssele windmill dataset could be smoothened by introduction of a nugget effect. The choice is made not to use a nugget effect, as the main error source in seismic depths results from the time-to-depth conversion using a velocity model. Errors in this time-to-depth conversion step lead to translations of the depth of the geological units as a whole, rather than deviations within the geological units itself. The measurement errors in the layers itself are negligible compared to the errors that may result from time-to-depth conversion. Adding a small nugget effect, however, could have improved the results slightly.

**Cross validation**
The cross validation results could be improved by enlarging the interpolation grid size or the amount of input points, to see the effects on the actual data size better. Unfortunately the computers used for this study did not have enough computational power to deal with larger grid or data sizes. Moreover, more subsets could be used for cross validation to provide a better description of the data signals as a whole.

**Workflow**
The proposed workflow could be improved, for example by adding more steps or more methods. A drawback of the current workflow, however, is that already a lot of knowledge of the to be interpolated dataset is required. One could wonder whether the improvement of the interpolation result is worth this extra amount of time. This, of course, depends on the needed quality of the interpolation results. Therefore another consideration should always be where the interpolation results will be used for, and thus whether optimizing the results is really necessary.
Figure 6.33: Cross validation results for subset 1. The graphs on the left show the mean squared error development graphs for leave-one-out cross validation, the graphs on the right show the mean squared error development graphs for subset cross validation.
Figure 6.34: Cross validation results for subset 2. The graphs on the left show the mean squared error development graphs for leave-one-out cross validation, the graphs on the right show the mean squared error development graphs for subset cross validation.
Results for quality mapping and grid design

In this section several ways to visualise the interpolation results along with an estimation of the associated prediction errors are presented. The results of natural neighbour kriging and anisotropic natural neighbour kriging for the base of geological layer A of subset 1 of the Borssele windmill farm data have been used to generate the results.

A way to design an adaptable grid for interpolation is the use of quadtree decomposition. To create a quadtree decomposition any separate data layer can be used. Preferably the grid size increases as the quality of the interpolation decreases. To achieve this an adaptive grid based on quadtree decomposition of the kriging variance is presented in the next section. First, a small size interpolation grid of natural neighbour kriging is presented of 128 x 128 points. Then, the result of anisotropic natural neighbour kriging on a larger interpolation grid, 512 x 512, is decomposed based on its kriging variance values. The interpolation results of subset 1 of the Borssele windmill farm for the base of geological layer A are used to test the method.

7.1. Kriging variance and natural neighbours

The kriging variance is computed for each interpolation grid cell. The kriging variance gives an estimation of the prediction errors for each interpolated location. The kriging variance increases further away from input points, the rate at which it increases depends on the used variogram model.

The distribution of the number of natural neighbours for each interpolation grid cell resembles the pattern the kriging variance follows. The correlation between the two fields is defined by the correlation coefficient. The resulting correlation coefficients $\rho$ of the number of natural neighbours and the kriging variance for different interpolation methods is given in Table 7.1. The correlation coefficients are computed for the small sized grid of 128 x 128 points results for subset 1 of the base of geological layer A. The kriging variance associated with the interpolation results of different methods is compared to the number of natural neighbours for each location. The computed correlation coefficients for all methods are approximately 0.9, which indicates a rather strong relationship between the two fields. The results show that the number of natural neighbours increase as the kriging variance increases for this particular acquisition geometry.

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<tr>
<td>OK$_{NN}$</td>
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<tr>
<td>AOK</td>
<td>0.87</td>
</tr>
<tr>
<td>AOK$_{NN}$</td>
<td>0.87</td>
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</table>

Table 7.1: Correlation coefficient $\rho$ for number of natural neighbours and kriging variance of different methods.
7. Results for quality mapping and grid design

7.1.1. Natural neighbour kriging
The interpolation results of natural neighbour kriging for base A of subset 1 on a grid of 128 x 128 points in size and the associated kriging variance are shown in Figure 7.1. The resulting kriging variance close to the input points is small and increase gradually further away from the points. The resulting pattern is very regular.

![Figure 7.1](image1.png)

**Figure 7.1**: Natural neighbour kriging interpolation (left) and kriging variance values in m$^2$ (right).

The same interpolation result and the number of natural neighbours per grid cell are given in Figure 7.2. The general pattern is regular as well, although small distance variations in the acquisition geometry lead to irregularities. The pattern within each of the acquisition rectangles is somewhat different.

![Figure 7.2](image2.png)

**Figure 7.2**: Natural neighbour kriging interpolation (left) and amount of natural neighbours (right).
7.1.2. Anisotropic natural neighbour kriging

The interpolation results of anisotropic natural neighbour kriging for base A of subset 1 on a larger grid of 512 x 512 points in size and the associated kriging variance are shown in Figure 7.3. The kriging variance associated with anisotropic natural neighbour kriging increases more rapidly in northwest-southeast direction than in northeast-southwest direction. The resulting kriging variances are higher than those of natural neighbour kriging.

![Figure 7.3: Anisotropic natural neighbour kriging interpolation (left) and kriging variance values in m² (right).](image1)

The same interpolation result and the number of natural neighbours per grid cell are given in Figure 7.4.

![Figure 7.4: Anisotropic natural neighbour kriging interpolation (left) and amount of natural neighbours (right).](image2)
7.2. Quadtree decomposition

The adaptive grid resulting from quadtree decomposition is used to illustrate variations in interpolation prediction errors. Three different field are used as input values for quadtree decomposition. An overview of the used input data fields, the used threshold values and the resulting quadtree block size distributions are given in Table 7.2. For the small interpolation grid of natural neighbour kriging (128 x 128) the square root of the kriging variance values and the number of natural neighbours are used as input for quadtree decomposition. For the larger interpolation grid of anisotropic natural neighbour kriging (512 x 512) the square root of the kriging variance is used as input. The block size distributions of the resulting quadtree decompositions show that the larger input grid resulted in a broader range of quadtree block sizes.

<table>
<thead>
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<th>Field</th>
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<th>Threshold</th>
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<th>4 x 4</th>
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</thead>
<tbody>
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<td>4356</td>
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<td>208</td>
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<tr>
<td>Number of natural neighbours</td>
<td></td>
<td>128 x 128</td>
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<td>1136</td>
<td>1920</td>
<td>449</td>
</tr>
<tr>
<td>Square root kriging variance</td>
<td>AOK\textsubscript{NN}</td>
<td>512 x 512</td>
<td>0.045</td>
<td>38576</td>
<td>31744</td>
<td>4129</td>
</tr>
</tbody>
</table>

Table 7.2: Quadtree input field, threshold and resulting block size distribution.

The variogram model that is used to determine the kriging variance values for geological layer A is a spherical model. The relationship given in a spherical variogram model is linear, until the model flattens and reaches the sill and range values. The kriging variance associated with kriging results computed with a spherical variogram model cannot be directly used as quadtree input. The quadtree blocks are namely based on changes in the input field. The flattening of the spherical variogram model towards the sill and range values results in larger changes in kriging variance around these values and in quadtree decomposition. This will lead to smaller block sizes. To overcome this problem the square root of the kriging variance is given as input for quadtree decomposition. The square root of the kriging variance computed with a spherical variogram model increases more rapidly close to the input data points and levels off at larger distances. The histograms of the kriging variance (left) and the square root of the kriging variance (right) are given in Figure 7.5 for natural neighbour kriging and in Figure 7.6 for anisotropic natural neighbour kriging. The histograms of the kriging variance show a more or less horizontal trend, whereas the histograms of the square root kriging variance values are shifted towards the right and show a gradually increase in histogram count as the value increases. Note that these Figures show the scaled histogram values, where all values are scaled to be between 0 and 1.

![Histogram of scaled kriging variance (OK\textsubscript{NN})](image1)

![Histogram of scaled square root of kriging variance (OK\textsubscript{NN})](image2)

Figure 7.5: Histogram of scaled kriging variance (left) and scaled square root of kriging variance (right) of OK\textsubscript{NN}. 
7.2. Quadtree decomposition

Kriging variances associated with exponential variogram models can be directly used as input for quadtree decomposition for the computation of error dependent block sizes, as the relationship in an exponential variogram model already increases first rapidly and then gradually flattens off.

Figure 7.6: Histogram of scaled kriging variance (left) and scaled square root of kriging variance (right) of $AOK_{NN}$. 
7.2.1. Natural neighbour kriging

Figure 7.7 shows the quadtree decomposition based on the square root of the kriging variance of natural neighbour kriging on a grid of 128 x 128 in size. The quadtree decomposition is plotted on top of the interpolation results. The used quadtree threshold is 0.10 m$^2$. The smallest block sizes are around the input points. The block size gradually increases towards the middle of the acquisition rectangles.

Figure 7.7: Quadtree decomposition based on square root of kriging variance $OK_{NN}$ on top of natural neighbour kriging results.
The mean kriging variance values per quadtree block are plotted in Figure 7.8. The resulting pattern is very regular and the blocks of different sizes more or less represent the same mean kriging variance values. For example, the largest blocks of 4 x 4 in size are almost all coloured green and represent mean kriging variance values of around 0.5 m$^2$.

Figure 7.8: Mean kriging variance per quadtree block $\hat{K}_{N,N}$. 
The kriging variance and the number of natural neighbours is closely related, and therefore the number of natural neighbours for each location is tested as quadtree input. An advantage of using the number of natural neighbours as quadtree input is that it could be used to define an interpolation grid prior to the interpolation calculation itself, as only the locations of the acquisition points need to be known to compute it. The quadtree decomposition based on the number of natural neighbours is given in Figure 7.9. The resulting quadtree grid in Figure 7.9 is less regular than the quadtree grid created with the kriging variance as input.

Figure 7.9: Quadtree decomposition based on number of natural neighbours on top of natural neighbour kriging results.
Figure 7.10 shows the mean number of natural neighbours per grid cell. In general the cell size still increases with increasing distance from the input points, however this relationship is less pronounced compared to using the kriging variance as input.

Figure 7.10: Mean number of natural neighbours per quadtree block.
7.2.2. Anisotropic natural neighbour kriging

Figure 7.11 shows a zoomed-in part of the quadtree decomposition based on the square root of the kriging variance plotted on top of the interpolation results of anisotropic natural neighbour kriging. The quadtree threshold that is used is 0.045 m². The points that are used as input to compute the interpolated depths are plotted on top of the image as white dots. The blocks in Figure 7.11 are small close to the input points and increase in size further away from them. The effect of the anisotropic variogram model that is used can be clearly recognized in the quadtree partitioning, as the size of the blocks increase more rapidly in the northwest-southeast direction compared to the northeast-southwest direction.

Figure 7.11: Quadtree decomposition based on square root of kriging variance $AOK_{NN}$ on top of anisotropic natural neighbour kriging results.
The mean kriging variance of each of the blocks is plotted in Figure 7.12. The quadtree block size increases with increasing kriging variance, although not all blocks of the same size have the same mean kriging variance value. The blocks are smallest close to the input points and their size increases further away from these. The pattern is clearer recognizable compared to the quadtree decomposition of natural neighbour kriging, which had a much smaller grid (128 x 128). Please note that the rapid increase of kriging variance in the down-left corner is due to the fact that the edge of subset 1 is reached here.

Figure 7.12: Mean kriging variance per quadtree block $AOK_{NN}$. 
7.3. Contour mapping
Another way to visualise both the interpolation result and the associated quality is contour mapping. The kriging variance is converted to contour lines and plotted on top of the interpolation results. The kriging variance contour lines are curves where the kriging variance value is constant. The colour of the contour lines represents the value along each curve. The kriging variance contours give an overview of the estimated prediction error for each location.

7.3.1. Natural neighbour kriging
The kriging variance contours of natural neighbour kriging are plotted on top of a grey-scale interpolation using natural neighbour kriging in Figure 7.13. The kriging variance contours computed have a spacing of 0.1 m², each curve thus represents steps of 0.1 m² in kriging variance. The white dots represent the locations of the input points. The colorbar underneath the image represents the interpolated depth values in meters and the colorbar on the left side of the image represents the kriging variance values of the contours. The resulting image once again shows the regular pattern in kriging variance.

![Figure 7.13: Interpolation of depth values (m) with OK\textsubscript{NN} and kriging variance contours.](image)
7.3.2. Anisotropic natural neighbour kriging

Figure 7.14 shows contour values of the kriging variance mapped on top of the interpolated depth obtained using anisotropic natural neighbour kriging. The kriging variance contours also represent a spacing of 0.1 m². The resulting pattern is again very regular. The anisotropy in the signal is clearly represented by the contour spacing: the kriging variance clearly increases more rapidly in the northwest-southeast direction.

Contrary to the kriging variance quadtrees, where there is quite a large difference between the results of the two grids of different sizes, the contour map of the small grid (128 x 128) and the large grid (512 x 512) are alike. An advantage of this type of quality visualisation is thus not depend as much on the size of the input grid.
7.4. Conclusions
In the previous section several ways to present the quality of the interpolation results are discussed. The main conclusions of the previous section include:

- There is a strong correlation between the kriging variance and the number of natural neighbours per grid cell for this acquisition geometry.
- Quadtree decomposition is a good method to visualise prediction errors per location, and is also suitable as a tool for adaptive grid design.
- Contour mapping is another relatively simple way to visualise prediction errors for each location.

The quadtree decomposition of the small grid (128 x 128) for natural neighbour kriging and the larger grid (512 x 512) for anisotropic natural neighbour kriging for subset 1 of geological base A of the Borssele windmill dataset has led to the following main conclusions:

- Quadtree decomposition is successfully used to design an adaptive grid where block sizes increase as the prediction errors increase.
- The kriging variance is a suitable input parameter for the creation of adaptable grid using quadtree decomposition.
- Increasing the number of interpolation grid points leads to more blocks and a larger variety of block sizes, and results in a clearer relationship between block size and prediction errors.
- The number of natural neighbours per grid cell is also used as input for the creation of an adaptable grid using quadtree decomposition. However, the resulting adaptable grid is less constant than the interpolation grid created with the kriging variance values as input, as the number of natural neighbours is more sensitive to irregularities in the acquisition geometry.

7.5. Discussion
The quadtree decomposition could be improved using larger grids or more input points. Both the kriging variance and the number of natural neighbours per grid cell would then reflect a more realistic representation of the full dataset. However, the general principle is still proven to work.
Conclusions and further research

8.1. Conclusions

The answers to the sub questions are summarized the following way:

*How can the potential of natural neighbour kriging as interpolation technique be assessed? What criteria are relevant for assessing the quality of natural neighbour kriging as an interpolation technique? To what extent does natural neighbour kriging meet these criteria?*

The potential of natural neighbour kriging as an interpolation technique can be assessed in a qualitative way using the Watson criteria and in a quantitative way using cross validation techniques.

Qualitatively, natural neighbour kriging scores well on the Watson criteria. The interpolation results obtained using natural neighbour kriging are *exact, continuous, local* and *adaptable*. The results are *smooth* if the field is not under sampled. Moreover, only a limited number of points are used as interpolation neighbourhood for kriging, making the technique relatively *computationally efficient* and the technique can be made *automatic* using automatic variogram fitting functions.

Quantitatively, the cross validation results have shown that natural neighbour kriging provides a better weighting of the natural neighbours than natural neighbour interpolation. The quantitative performance of natural neighbour kriging, however, is highly dependent on the used input data field and therefore needs to be compared to other techniques per case.

*How does this method compare to other kriging methods based on the previously mentioned criteria?*

The comparison of natural neighbour kriging and ordinary kriging, both for isotropic and anisotropic cases, lead to the following main conclusions:

Natural neighbour kriging is computationally more efficient than ordinary kriging. The computational efficiency of the kriging computation improves significantly for increasingly large dataset using the natural neighbours as interpolation neighbourhood. Moreover, the selection of natural neighbours are local and adaptable, automatically reflecting the acquisition geometry of the input dataset. Whether the selection of natural neighbours reflects the relevant points in interpolation sufficiently is dependent on the type of data signal and needs to be examined for each signal.

*For what type of geostatistical data is natural neighbour kriging interpolation suitable?*

Natural neighbour kriging is suitable for isotropic data fields. The two adjustments of natural neighbour kriging for anisotropic data, anisotropic natural neighbour kriging and anisotropic natural neighbour kriging that uses anisotropic natural neighbours, are suitable for anisotropic data fields. The anisotropic variants of natural neighbour kriging are suitable for both geometric and zonal anisotropic fields, as the results are very local.
Natural neighbour kriging is less suitable for fields that have large covariance at large separate distances, for example fields with returning wave-like events, as these large distance points might not be included in the natural neighbour selection.

How can the interpolation result be presented to users in an insightful way, providing information about both the quality of the result and the contribution of the input data points?

The main quality descriptor of natural neighbour kriging is the kriging variance. The contribution of the input data points is reflected by the number of natural neighbours per grid cell. There is a positive correlation between the kriging variance and the number of natural neighbours per grid cell. Quadtree decomposition and contour mapping based on these two fields are useful tools for visualisation of the interpolation results along with the estimated prediction errors.

How can the interpolation grid cell size be adapted to spatial variation in distribution and quality of the input data and the interpolation result?

An adaptive interpolation grid is designed using quadtree decomposition. Two input fields are used, the kriging variance and the number of natural neighbours per grid cell. The adaptive grid based on the kriging variance is very regular and reflects the quality of the interpolation results well. The adaptive grid based on the number of natural neighbours per grid cell more sensitive to irregularities in data acquisition and therefore less regular, but also globally reflects the quality of the interpolation results.

Finally, the answers to the sub questions are summarized to conclude on the main research question:

What is the potential of natural neighbour kriging for quality mapping and grid design?

Natural neighbours kriging is a promising interpolation technique that is successfully used to interpolate several types of data signals. The quality parameters associated with natural neighbour kriging, the kriging variance and the number of natural neighbours per grid cell, provide a description of the quality of the interpolation results and are successfully used for grid design. Overall, natural neighbour kriging is concluded to have great potential as an interpolation method itself, as well as for its use in quality mapping and grid design.
8.2. Suggestions for further research

8.2.1. Computational challenges
The selection of natural neighbours for the interpolation neighbourhood for kriging will never cross the borders of each acquisition rectangle. Therefore there is a possibility to divide up the kriging computation into separate computations for different acquisition rectangles. The kriging results could be calculated parallel for each acquisition rectangle, speeding up the computation even more.

Another consideration is the possibility to update the natural neighbour kriging results locally. The natural neighbours of each interpolation grid cell are saved in a data structure and can be looked up in case of local updates. The natural neighbour data structure can be used to search for all grid points that used the now updated values as neighbourhood for kriging. The kriging estimation only needs to be updated for these grid points, instead of redoing the computation for the full area. An example of this updating procedure is given in Appendix A.

8.2.2. Quadtree decomposition
The number of natural neighbours of each interpolation grid cell as input for quadtree decomposition resulted in a quite irregular pattern for the Borssele windmill farm dataset. The use of the number of natural neighbours per grid cell, however, has two wanted properties: the field can be used to compute an adaptive grid prior to the interpolation step itself and it is correlated with the kriging variance. To obtain a more regular quadtree pattern a synthetic dataset that follows the general pattern of the actual acquisition geometry could be used. The synthetic dataset would not have the small irregularities that you see in actual data, and would therefore result in an adaptive grid that is more regular. An adaptive grid based on the number of natural neighbours could also be used to estimate the prediction error distribution for natural neighbour interpolation.

Other input field that can be used for the creation of an adaptive grid using quadtree decomposition could also be investigated. For example, a simple distance related measure to the closest points. An adaptive grid that is created prior to the interpolation step can also be used to define the limits for the interpolation step itself. For example, the quadtree blocks could potentially be used as blocks for block kriging, another kriging methods that computes just one estimation per block.

8.2.3. Proposed workflow
This study only focuses on ordinary kriging, but of course there are also other types of kriging that can also be compared. It would be interesting to include simple and universal kriging in the comparison and to add these methods to the proposed workflow. Another interesting topic would be to quantify the questions that are stated in the workflow. For example, when exactly is there too much spatial variability in the signal.

8.2.4. Data size input
The seismic interpretation of the geological layers for the Borssele windmill dataset is more or less continuous, resulting in a very large dataset. An interesting questions would be whether it is really necessary to use the full dataset or whether using only a percentage of the dataset is enough to obtain a good interpolation. Reducing the data size seems appealing, as it leads to considerably faster computations. The interpolation results using all points and using 10% of the points gave very similar results, both in terms of the interpolation itself and also in terms of kriging variance. It would be interesting to study what percentage of the Borssele windmill farm dataset should be used to obtain an optimal balance between quality of the results and computational time.
Local updating using saved natural neighbours per grid point

The natural neighbours of each interpolation point are saved to be used in natural neighbour kriging. In this project the natural neighbour of each interpolation point were saved in a matrix in Matlab, each row representing the natural neighbours of one interpolation point. This natural neighbour matrix is useful for local updating of the natural neighbour kriging results.

A simple example is illustrated using the Davis test dataset. First the natural neighbour kriging interpolation is computed for the original dataset. The natural neighbour kriging interpolation, as well as the natural neighbours of each interpolation point are saved. Then the value of one of the points is updated. The natural neighbour matrix is used to search for interpolation grid points that use the updated point, using the index of this point, and these grid points are saved. Let’s call all grid points that use updated value the influence area of that updated point. A new kriging interpolation is then computed only for the grid points within the influence area. The stepwise procedure is as follows:

1. Compute the natural neighbour kriging interpolation.
2. One or multiple values are updated.
3. Find the influence area of the updated points using the natural neighbour matrix (or any other data structure).
4. Update the natural neighbour kriging interpolation locally.
Figure A.1 shows the procedure for the Davis dataset. The height of the indicated points is changed from 820 meters to 920 meters. The first image shows the initial natural neighbour kriging interpolation. The second image shows the influence area of the updated points, the area indicated in yellow. The interpolation is only updated within this area. Finally, the locally updated natural neighbour kriging interpolation is shown in the lower image.

Figure A.1: Illustration of the updating procedure for the Davis dataset.
Experimental variogram computation using natural neighbours

The experimental variogram is normally computed using all data pairs. However, it is also possible to compute the experimental variogram with a more local approach, namely using only the natural neighbours of each input point. The experimental variogram using only the natural neighbours is computed for two different cases, for the Davis test dataset and subset 1 of base A of the Borssele Windmill dataset. The results are plotted in Figure B.1 and Figure B.2. The left images show the normal experimental variogram of each of the two cases. The right images show the experimental variograms using only the natural neighbour of the input points.

Figure B.1: Experimental variogram using all points (left) and using only natural neighbours (right) for the Davis test dataset.

Figure B.1 shows these two experimental variograms for the Davis test dataset. The black dots represent all the computed variogram values, and the red dots represent the final experimental variogram binned per 0.25 meters. The two experimental variograms are similar for lag distances up to approximately 1.5 meters. The differences are large for larger lag distances, this is of course due to the fact that most natural neighbours are located close to the input points. There are only a small number of variogram values computed for larger distances, as there are only a few points that have natural neighbours located far away from them.
Figure B.2 shows both variograms for subset 1 of base A. Once again the black dots represent all computed variogram values, whereas the red dots represent the final experimental variogram binned per 100 meters. The two experimental variograms are similar for small lag distances of up to approximately 500 meters. For larger lag distances there is a once again a large difference between the two.

Although the normal experimental variogram and the experimental variogram using only natural neighbours are very similar for small lag distances for both cases, they are very different for larger lag distances, due to the lack of natural neighbours here. The problem is that it becomes very difficult to determine the range and sill values in the experimental variogram that only uses the natural neighbours, as the variogram values at larger lag distances are determined by a few points only. On the one hand, only the natural neighbours of each point are used for natural neighbour kriging, and these points are represented in the first part of the experimental variogram computed with only the natural neighbours. This means that the experimental variogram values for most relevant points is captured well in the variogram computed with natural neighbours. On the other hand, the range and sill values must be determined in order to convert the variogram values to covariances. For both cases there are few to no points around the range values as determined using the normal experimental variogram. Moreover, in the experimental variogram using only the natural neighbours there are no clear range or sill recognizable. Determining erroneous range and sill values could lead to incorrect conversion from the variogram to the covariance function, potentially messing up the relative importance of the used points for interpolation. For example, the experimental variogram computed using only natural neighbours (right image) in Figure B.2 suggests that the range value is around 1000 meters, whereas the experimental variogram (left image) illustrates that the actual range is much larger and in fact undeterminable.

The use of only natural neighbours pairs is thus not sufficient for the computation of the experimental variogram, as range and sill values are tricky to determine, making correct conversion to a covariance function difficult.
Borssele windmill farm: interpolation method comparison

C.1. Subset Wind Farm Section I

C.1.1. Unit A
The method with the smallest errors is $AOK_{ANN}$, followed by $AOK_{NN}$. The worst performing method is ordinary kriging. In general the anisotropic methods perform better than the isotropic methods. However, natural neighbour interpolation gave relatively smaller errors than the other two isotropic methods. The top three performing methods are:

1. $AOK_{ANN}$
2. $AOK_{NN}$
3. $AOK$

Predominantly zonal anisotropy, main acquisition direction parallel to main direction continuity signal.

C.1.2. Unit B
The method with the smallest errors are ordinary kriging, natural neighbour interpolation and natural neighbour kriging. The worst performing method with the highest mean squared errors is $AOK_{ANN}$, followed by anisotropic ordinary kriging. The top three performing methods are:

1. $OK$
2. $OK_{NN}$
3. $NN$

Isotropic unit.

C.1.3. Unit C1
The best performing method is $AOK_{NN}$, with relatively small mean squared errors for both leave-one-out and subset cross validation. The worst performing method is ordinary kriging. Natural neighbour interpolation gives the smallest mean squared errors for close-range points (leave-one-out cross validation), but performs worse looking at longer distances (subset cross validation). The top three performing methods are:

1. $AOK_{NN}$
2. $AOK_{ANN}$
3. $OK_{NN}$

Predominantly geometric anisotropy, main acquisition direction more or less parallel to main direction continuity signal.
C.1.4. Unit C2
The anisotropic methods perform better than the isotropic methods, $AOK_{NN}$ having the lowest errors in general. Natural neighbour interpolation and ordinary kriging gave the highest errors. The top three performing methods are:

1. $AOK_{NN}$
2. $OK_{NN}$
3. $AOK_{ANN}$

Predominantly geometric anisotropy, main acquisition direction more or less parallel to main direction continuity signal.

C.1.5. Unit D
The isotropic methods perform better than the anisotropic methods. Natural neighbour interpolation and natural neighbour kriging perform best. The anisotropic methods perform worse, $AOK_{ANN}$ gave the highest mean squared errors in general. The top three performing methods are:

1. $NN$
2. $OK_{NN}$
3. $OK$

Predominantly geometric anisotropy, main acquisition direction more or less parallel to main direction continuity signal.

C.1.6. Unit E1
The anisotropic methods perform best, $AOK_{NN}$ giving the lowest mean squared errors in general. The second best performing method is anisotropic ordinary kriging. $AOK_{ANN}$ performs well for longer range estimation (subset), however, gave the highest mean squared errors for leave-one-out cross validation. The top three performing methods are:

1. $AOK_{NN}$
2. $AOK$
3. $AOK_{ANN}$

Predominantly geometric anisotropy, main acquisition direction more or less parallel to main direction continuity signal.
C.2. Subset Wind Farm Section II

C.2.1. Unit A
In general the anisotropic methods perform better than the isotropic ones. $AOK_{ANN}$ gave the smallest errors in general, followed by $AOK_{NN}$. Ordinary kriging gave the highest errors of all methods. The top three performing methods are:

1. $AOK_{ANN}$
2. $AOK_{NN}$
3. $NN$

Predominantly geometric anisotropy, main acquisition direction more or less parallel to main direction continuity signal.

C.2.2. Unit B
The best performing method with the lowest errors was natural neighbour kriging, followed by anisotropic natural neighbour kriging. Ordinary kriging and anisotropic ordinary kriging gave the highest errors. The top three performing methods are:

1. $OK_{NN}$
2. $AOK_{NN}$
3. $NN$

Isotropic unit.

C.2.3. Unit E5a
Although the isotropic methods gave smaller errors for leave-one-out cross validation, the anisotropic methods clearly perform better for longer range estimation. The best performing method is $AOK_{NN}$, followed by $AOK_{ANN}$. The top three performing methods are:

1. $AOK_{NN}$
2. $AOK_{ANN}$
3. $AOK$

Predominantly zonal anisotropy, main acquisition direction perpendicular to the direction of main continuity of the signal.

C.2.4. Unit E5b
All methods, except for ordinary kriging, gave reasonable and comparable results. The best performing methods were natural neighbour interpolation and natural neighbour kriging. The top three performing methods are:

1. $NN$
2. $OK_{NN}$
3. $AOK_{NN}$

Predominantly zonal anisotropy, main acquisition direction perpendicular to the direction of main continuity of the signal.
C.2.5. Unit F1b
The best performing methods were those that use natural neighbours as interpolation neighbourhood, $AOK_{ANN}$ performing best followed by $AOK_{NN}$. The worst performing method was anisotropic ordinary kriging. The top three performing methods are:

1. $AOK_{ANN}$
2. $AOK_{NN}$
3. $OK_{NN}$

Predominantly geometric anisotropy, main acquisition direction perpendicular to the direction of main continuity of the signal.

C.2.6. Unit F2
In general the anistropic methods performed better than the isotropic ones, $AOK_{NN}$ giving the smallest errors. Although anisotropic ordinary kriging gave higher errors for short range estimation (leave-one-out), it gave reasonable results for long range estimation (subset cross validation). The worst performing methods were natural neighbour interpolation and ordinary kriging. The top three performing methods are:

1. $AOK_{NN}$
2. $AOK_{ANN}$
3. $OK_{NN}$

Predominantly geometric anisotropy, main acquisition direction perpendicular to the direction of main continuity of the signal.
Figure C.1: Angular experimental variograms with $\theta_{\text{step}} = 15$ degrees and $n_{\text{bins}} = 10$ for subset 1 of each geological unit.
Figure C.2: Angular experimental variograms with $\theta_{\text{step}} = 15$ degrees and $n_{\text{bins}} = 10$ for subset 2 of each geological unit.
C.4. Mean squared error development graphs

Figure C.3: Mean squared error development after removal of # highest error points for leave-one-out cross-validation of unit A in WFS I.

Figure C.4: Mean squared error development after removal of # highest error points for subset cross-validation of unit A in WFS I.
Figure C.5: Mean squared error development after removal of $\#$ highest error points for leave-one-out cross-validation of unit B in WFS I.

Figure C.6: Mean squared error development after removal of $\#$ highest error points for subset cross-validation of unit B in WFS I.
Figure C.7: Mean squared error development after removal of # highest error points for leave-one-out cross-validation of unit C1 in WFS I.

Figure C.8: Mean squared error development after removal of # highest error points for subset cross-validation of unit C1 in WFS I.
Figure C.9: Mean squared error development after removal of # highest error points for leave-one-out cross-validation of unit C2 in WFS I.

Figure C.10: Mean squared error development after removal of # highest error points for subset cross-validation of unit C2 in WFS I.
Figure C.11: Mean squared error development after removal of $\#$ highest error points for leave-one-out cross-validation of unit D in WFS I.

Figure C.12: Mean squared error development after removal of $\#$ highest error points for subset cross-validation of unit D in WFS I.
Figure C.13: Mean squared error development after removal of # highest error points for leave-one-out cross-validation of unit E1 in WFS I.

Figure C.14: Mean squared error development after removal of # highest error points for subset cross-validation of unit E1 in WFS I.
Figure C.15: Mean squared error development after removal of $\#$ highest error points for leave-one-out cross-validation of unit A in WFS II.

Figure C.16: Mean squared error development after removal of $\#$ highest error points for subset cross-validation of unit A in WFS II.
Figure C.17: Mean squared error development after removal of # highest error points for leave-one-out cross-validation of unit B in WFS II.

Figure C.18: Mean squared error development after removal of # highest error points for subset cross-validation of unit B in WFS II.
C.4. Mean squared error development graphs

Figure C.19: Mean squared error development after removal of \# highest error points for leave-one-out cross-validation of unit E5a in WFS II.

Figure C.20: Mean squared error development after removal of \# highest error points for subset cross-validation of unit E5a in WFS II.
Figure C.21: Mean squared error development after removal of # highest error points for leave-one-out cross-validation of unit E5b in WFS II.

Figure C.22: Mean squared error development after removal of # highest error points for subset cross-validation of unit E5b in WFS II.
Figure C.23: Mean squared error development after removal of \# highest error points for leave-one-out cross-validation of unit F1b in WFS II.

Figure C.24: Mean squared error development after removal of \# highest error points for subset cross-validation of unit F1b in WFS II.
Figure C.25: Mean squared error development after removal of # highest error points for leave-one-out cross-validation of unit F2 in WFS II.

Figure C.26: Mean squared error development after removal of # highest error points for subset cross-validation of unit F2 in WFS II.


