

A disposition of interpolation techniques

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Wetenschappelijke Onderzoekstaken Natuur & Milieu

A disposition of interpolation techniques

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This document was produced in accordance with the Quality Manual of the Statutory Research Tasks Unit for Nature & the Environment (WOT Natuur & Milieu) and has been accepted by Harm Houweling programme coordinator of WOT Natuur & Milieu.

Wot Working Document **190** presents the findings of a research project commissioned by the Netherlands Environmental Assessment Agency (PBL) and funded by the Dutch Ministry of Agriculture, Nature and Food Quality (LNV). This document contributes to the body of knowledge which will be incorporated in more policy-oriented publications such as the Nature Balance and Environmental Balance reports, and Thematic Assessments.

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Wageningen, juni 2010

Abstract

Knotters, M., G.B.M. Heuvelink, T. Hoogland & D.J.J. Walvoort, 2010. *A disposition of interpolation techniques*. Wageningen, Statutory Research Tasks Unit for Nature and the Environment, WOT-werkdocument 190. 90 p. 26 Figs.; 1 Tab.; 170 Refs.

A large collection of interpolation techniques is available for application in environmental research. To help environmental scientists in choosing an appropriate technique a disposition is made, based on 1) applicability in space, time and space-time, 2) quantification of accuracy of interpolated values, 3) incorporation of ancillary information, and 4) incorporation of process knowledge. The described methods include inverse distance weighting, nearest neighbour methods, geostatistical interpolation methods, Kalman filter methods, Bayesian Maximum Entropy methods, etc. The applicability of methods in aggregation (upscaling) and disaggregation (downscaling) is discussed. Software for interpolation is described. The application of interpolation techniques is illustrated in two case studies: temporal interpolation of indicators for ecological water quality, and spatio-temporal interpolation and aggregation of pesticide concentrations in Dutch surface waters. A valuable next step will be to construct a decision tree or decision support system, that guides the environmental scientist to easy-to-use software implementations that are appropriate to solve their interpolation problem. Validation studies are needed to assess the quality of interpolated values, and the quality of information on uncertainty provided by the interpolation method.

Keywords: geostatistics, kriging, time series, space-time interpolation, aggregation, disaggregation, upscaling, downscaling, uncertainty, accuracy

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The Working Documents series is published by the Statutory Research Tasks Unit for Nature & the Environment (WOT Natuur & Milieu), part of Wageningen UR. This document is available from the secretary's office, and can be downloaded from www.wotnatuurenmilieu.wur.nl.

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Preface

We dance around in a ring and suppose,
But the secret sits in the middle and knows.

Robert Frost

This report is written to help environmental researchers at PBL (Netherlands Environmental Assessment Agency) in choosing from the large variety of interpolation techniques. These techniques are used to predict values at unvisited locations or moments in time, using neighboring observations. We are not only uncertain about the *true* value, but we might even be uncertain about the appropriateness of the applied interpolation method. This report pays special attention to interpolation techniques that quantify the first kind of uncertainty. Furthermore, this report aims to help in reducing the second kind of uncertainty.

We are very grateful to all PBL employees who attended the lunch presentation on 19 November 2009. Their questions and remarks helped us a lot to improve the manuscript. We are also grateful to Harm Houweling (WOt) and Peter Janssen (PBL) for their support in all stages of the project, and to George van Voorn (Biometris-WUR) and Piet Verdonschot (Alterra-WUR) for their helpful comments.

Wageningen, March 2010

Martin Knotters, Gerard Heuvelink, Tom Hoogland and Dennis Walvoort

Summary

Introduction

Environmental scientists can choose from a large collection of interpolation techniques. In choosing an appropriate interpolation method several criteria are relevant, such as the applicability in space, time and space-time, the ability to quantify the accuracy of interpolated values, the applicability to numerical and/or categorical variables, the opportunity to incorporate ancillary information, the opportunity to utilize process knowledge, the applicability for aggregation and disaggregation (up- and downscaling), the complexity of application, level of required expertise, and required computation time, the constraints on the size of the dataset and on the conditions of the dataset, and the availability of easy-to-use software implementations. The aim of this report is to structure the volume of interpolation techniques, with respect to these criteria. Because information on uncertainty is indispensable in present-day environmental policy analysis and policy-focused research, we focus on interpolation methods that provide quantitative information on the accuracy of the interpolated values. The main disposition is based on 1) applicability in space, time and space-time, 2) quantification of accuracy of interpolated values, 3) incorporation of ancillary information, and 4) incorporation of process knowledge.

Interpolation in space

Kriging refers to a group of geostatistical interpolation methods in which the value at an unobserved location is predicted by a –usually– linear combination of the values at surrounding locations, using weights according to a model that describes the spatial correlation. The statistical basis of kriging enables to quantify the accuracy of the predicted values by means of the kriging variance. Kriging methods that do not incorporate ancillary information include widely applied methods such as simple kriging, ordinary kriging, universal kriging with spatial coordinates or kriging in the presence of a trend. To interpolate non-Gaussian distributed variables adapted kriging methods can be applied such as indicator kriging, disjunctive kriging, multiGaussian kriging, lognormal kriging and trans-Gaussian kriging. Kriging methods are commonly based on straight line (Euclidian) distance. For interpolation in stream networks kriging methods have been developed on the basis of hydrologic distances, that is, the distance along the stream, in which the flow direction can be taken into account. Other interpolation methods that quantify uncertainty and do not use ancillary information include splines, methods based on Bayesian statistics, regression methods and neural networks.

Kriging methods in which ancillary information can be used include stratified kriging, cokriging, principal component kriging, kriging combined with linear regression (kriging with uncertain data), universal kriging (kriging with an external drift), and regression kriging (kriging with a guess field, residual kriging). Other methods that incorporate ancillary information and that quantify uncertainty are regression methods such as regression trees and artificial neural networks, Bayesian Maximum Entropy (BME) and Markov random fields. Process knowledge can be incorporated by calculating a ‘guess field’ with a physical-mechanistic model, followed by geostatistical interpolation of residuals.

Methods for spatial interpolation that do not quantify uncertainty and that do not incorporate ancillary information include inverse distance weighting, the nearest neighbour algorithm, and triangular irregular networks. Ancillary information can be utilized by stratification, i.e., by dividing an area into subareas. Process knowledge can be utilized by using a physical-mechanistic model to construct a ‘guess field’ of interpolated values.

Interpolation in time

Kriging methods can also be applied for interpolation in time. In modelling the temporal dependence structure, e.g. a variogram, covariance function or correlogram, it is important to be aware of the specific character of processes developing in time. In particular, when secondary variables are used in the model causality should be considered. Time series models such as autoregressive (integrated) moving average (AR(I)MA) models, transfer function-noise (TFN) models and intervention models can be used for data filling, which can be seen as a form of interpolation in time. These models can be used to model regularly observed time series. The state-space approach with Kalman filtering and Kalman smoothing can be applied to interpolate irregularly observed time series. Other methods for interpolation in time that quantify uncertainty are Bayesian time series models and structural time series models.

Interpolation methods that do not quantify uncertainty, such as inverse distance weighting and the nearest neighbour algorithm, can be used for interpolation in time. Physical-mechanistic models can also be applied for interpolation in time.

Interpolation in space and time

Three basic approaches for space-time interpolation with quantified uncertainty can be distinguished: 1) time series models with a spatial extension, 2) geostatistical models with a time extension, and 3) hybrid models. The first category includes the STARMA (space-time ARMA) model, which is an extension to the univariate ARMA model, accounting for correlations between time series observed at neighbouring locations. The second category includes space-time (ST) simple kriging, ST-ordinary kriging and ST-kriging with an external drift. The third category consists of hybrid models combining time series modelling and geostatistical modelling, e.g., geostatistical interpolation of time series model parameters. Ancillary information can be incorporated into ST-kriging methods and regionalized time series models. The Bayesian Maximum Entropy (BME) approach, in which ancillary information is

incorporated, can be extended to the space-time context. The state-space approach can be extended to space-time, incorporating process knowledge. A physically based regionalized time series model can be embedded in an ST-Kalman filter to enable space-time interpolation. Process models (physical-mechanistic models) can be used for space-time interpolation without (direct) quantification of uncertainty.

Aggregation and disaggregation

Aggregation, also referred to as *upscaling*, involves transferring information from a smaller (detailed) scale to a larger (coarser) scale. Here, 'scale' refers to the 'support' as it is known in geostatistics, i.e. the size, volume and shape of entities over which is aggregated. If the locations have been selected following a probability-based sampling design, then unbiased estimates of the areal means or totals can be calculated using the inclusion probabilities related to the sampling design. If the observations have been collected at purposively selected locations or sampling rounds, then the observed values need first to be interpolated to a dense grid and next the interpolated values can be aggregated. In the interpolation a model of spatial structure can be applied for weighing the observed values. Uncertainty can be quantified by stochastic simulation of n realisations and next aggregating the results of each realisation. The variance of the n aggregated values (e.g. areal means) reflects the uncertainty about the true aggregated value. In linear kriging, predictions and prediction error variances of space and/or time aggregates can also be obtained with block kriging.

In disaggregation, or *downscaling*, the variation of a variable at a small (detailed) scale is reconstructed, given the value at a larger (coarse) scale. If there is no ancillary information that can be used to explain some of the unknown temporal or spatial variation of the property at the small scale within the larger scale, and there is also not a mechanistic model available describing this (unknown) temporal or spatial variation, then information can be disaggregated using *empirical functions*. If the average value at the larger scale is exactly known *deterministic empirical functions* or *conditional stochastic functions* can be applied in disaggregation. Examples of deterministic empirical functions are splines, linear functions and general additive models. If only the probability function of the average value at the larger scale is known, then *unconditional stochastic functions* can be applied in disaggregation. Mechanistic models and fine scale ancillary information can be used in deterministic and conditional and unconditional stochastic functions for disaggregation.

Brief overview of software

The ArcGIS Geostatistical Analyst provides tools for geostatistical interpolation and analyses. In education, $E\{Z\}$ -kriging can be used to explain the principles of ordinary point kriging, block kriging and the semi-variogram. The statistical package Genstat provides tools for regression analysis, analysis of the spatial correlation structure, geostatistical interpolation and time series modelling. ISATIS is a comprehensive geostatistical software tool developed by Geovariances in France. GSLIB (Geostatistical Software LIBrary) is a collection of geostatistical programs developed at Stanford University over the past 15 years. ILWIS (Integrated Land and Water

Information System) is a stand-alone integrated GIS package developed at the International Institute of Geoinformation Science and Earth Observations (ITC), Enschede, the Netherlands. MATLAB[®] is a high-level technical computing language and interactive environment for algorithm development, data visualization, data analysis, and numeric computation. Several (user-written) toolboxes on geostatistics for MATLAB[®] are available, as well as procedures for time-series analysis and state-space modelling. R is a free software environment for statistical computing and graphics. Many packages are available for spatial statistics. In addition, R also contains packages for time-series analysis and state-space modelling. SAGA (System for Automated Geoscientific Analyses) is an open source GIS developed in Germany (Universität Göttingen, and since 2007 Universität Hamburg). It contains modules for semivariogram analysis, ordinary kriging, universal kriging, and spline interpolation. Surfer (produced by Golden Software) contains interactive tools for variogram analysis and kriging. S+ is a commercial implementation of the S programming language sold by TIBCO Software Inc.. Like its open source counter part R, it has packages for spatial statistics and time-series analysis. Vesper (Variogram Estimation and Spatial Prediction plus ERror, from the Australian Centre for Precision Agriculture) is a program for variogram estimation/modelling and kriging. It is capable of performing kriging with *local* variograms in an automatic way.

Case studies

The application of interpolation techniques was illustrated in two case studies: temporal interpolation of indicators for ecological water quality, and spatio-temporal interpolation and aggregation of pesticide concentrations in Dutch surface waters. The first case study concerns eight irregularly spaced time series of unequal length of ‘multimetric scores’. These scores, ranging from 0 to 1, indicate the ecological water quality in the district water board “Regge en Dinkel”. Inverse distance weighting, ordinary kriging on untransformed data, ordinary kriging after logit-transformation, MultiGaussian kriging and simple kriging with a known varying mean were applied to interpolate in time. In simple kriging with a known varying mean a seasonal trend was fitted and residuals were interpolated. The results of the various methods show large differences, which confirms that choosing an appropriate interpolation method is important.

The second case study concerns space-time interpolation of the concentrations of the pesticide ‘metribuzin’ in Dutch surface waters (ditches). Point measurements were aggregated in time to averages of growing seasons. These averages were interpolated in space and time by regression kriging, among others using water surface type, proportion of area under agriculture and concentrations predicted by a deterministic pesticide distribution model as explanatory variables in a multiple linear regression model. The residuals of this model were interpolated by space-time simple kriging. Spatial aggregation was done with a stochastic simulation procedure, sequential Gaussian simulation. In this way uncertainty about the aggregated values could be quantified and hence the statistical significance of the temporal trend in the aggregated values. Comparison with ‘naive’ upscaling showed meaningful differences.

Concluding remarks

More information about the properties of the interpolation methods is needed to support finding an appropriate interpolation technique for a given problem. In particular, more information is needed about the *performance*, i.e. the *accuracy*, of the interpolation methods. A summary of validation studies and comparative studies will make clear for what situations information on accuracy of interpolation methods is lacking. This can be a starting point for additional validation studies. A valuable next step will be to elaborate the disposition of methods given in this report to a decision tree or decision support system, that guides the environmental scientist to easy-to-use software implementations that are appropriate to solve their interpolation problem. Knowledge of the interpolation problems PBL-workers are facing is crucial in constructing such a tree.

Statistical information on uncertainty or accuracy is used in methods from statistical decision theory, quantitative risk and policy analysis, and uncertainty assessment inspired by post-normal science theory. The *overall* or *global* accuracy of results of any interpolation method can be assessed by an independent validation study, in which observations on the ‘field truth’ are preferably selected by probability sampling. *Local* information on accuracy can only be obtained by applying stochastic interpolation methods. The quality of this local information on accuracy depends on model assumptions which cannot always easily be verified.

To assess the usefulness of information on uncertainty in decision making, the quality of this information should be known. If information on *global* accuracy is obtained by validation with an independent probability sample, the quality of this information can easily be quantified. The quality of information on *local* accuracy, such as the kriging variance, can be assessed by validation or cross-validation. Studies in which the quality of *local* information on uncertainty has been validated are sparse, however. We underline the need of such validation studies, the results of which can be used to support a choice from the interpolation methods that quantify uncertainty as described in this report.

It can be concluded that most interpolation methods can be used in aggregation. Disaggregation is more delicate than aggregation, since assumptions need to be made about the spatial or temporal variation at the smaller scale. A lot of work on disaggregation techniques has been done in the field of climate research, from which other fields of environmental research could benefit.

Samenvatting

Inleiding

Milieuwetenschappers kunnen kiezen uit een grote verzameling interpolatietechnieken. Relevante criteria bij het kiezen zijn de toepasbaarheid in ruimte, tijd en ruimte-tijd, de mogelijkheid om de nauwkeurigheid van de geïnterpoleerde waarden te kwantificeren, de toepasbaarheid op numerieke en/of categorische variabelen, de mogelijkheid om gebruik te maken van hulpinformatie, de mogelijkheid om proceskennis te benutten, de toepasbaarheid voor aggregatie en desaggregatie (op- en neerschaling), de complexiteit, het benodigd kennisniveau, de vereiste rekentijd, en de beschikbaarheid van eenvoudig toepasbare computerprogramma's. Het doel van dit rapport is om interpolatietechnieken te ordenen op basis van deze criteria. Omdat informatie over onzekerheid tegenwoordig onmisbaar is in beleidsanalyses en beleidsgericht onderzoek op het gebied van het milieu, richten wij ons op interpolatiemethoden die kwantitatieve informatie verschaffen over de nauwkeurigheid van de geïnterpoleerde waarden. De hoofdstructuur is gebaseerd op 1) toepasbaarheid in ruimte, tijd en ruimte-tijd, 2) kwantificering van nauwkeurigheid van geïnterpoleerde waarden, 3) gebruik van hulpinformatie en 4) gebruik van proceskennis.

Ruimtelijke interpolatie

Kriging omvat een groep geostatistische interpolatiemethoden waarbij de waarde op een niet-bezochte locatie wordt voorspeld met een (lineaire) combinatie van de waarden op omliggende locaties, met een weging op basis van een model dat de ruimtelijke correlatie beschrijft. De statistische basis van kriging maakt het mogelijk om de nauwkeurigheid van de geïnterpoleerde waarden te kwantificeren met de krigingvariantie. Algemeen toegepaste krigingmethoden waarbij geen hulpinformatie wordt gebruikt zijn *simple kriging*, *ordinary kriging* en *universal kriging* met ruimtelijke coördinaten (of kriging met een trend). Om niet-Gaussisch verdeelde variabelen te interpoleren kunnen methoden worden gebruikt zoals *indicator kriging*, *disjunctive kriging*, *MultiGaussian kriging*, *lognormal kriging* en *trans-Gaussian kriging*. Krigingmethoden maken doorgaans gebruik van Euclidische afstanden. Voor interpolatie in waterlopenstelsels zijn krigingmethoden ontwikkeld die zijn gebaseerd op hydrologische afstanden (de afstand langs de loop), waarbij rekening kan worden gehouden met de stromingsrichting. Andere interpolatiemethoden waarmee onzekerheid kan worden gekwantificeerd, en waarbij geen hulpinformatie wordt gebruikt, zijn onder meer *splines*, methoden gebaseerd op Bayesiaanse statistiek, regressiemethoden en neurale netwerken.

Krigingmethoden waarbij hulpinformatie kan worden gebruikt zijn onder meer *stratified kriging*, *cokriging*, *principal component kriging*, kriging gecombineerd met lineaire regressie (kriging met onzekere gegevens), *universal kriging* (*kriging with an external drift*), en regressiekriging (*kriging with a guess field*, *residual kriging*). Andere methoden waarbij hulpinformatie wordt gebruikt en waarmee onzekerheid kan worden gekwantificeerd zijn regressiemethoden zoals regressiebomen en *artificial neural networks*, *Bayesian Maximum Entropy* (BME) en *Markov random fields*. Proceskennis kan worden benut door een veld te berekenen met een fysisch-mechanistisch model, en vervolgens de residuen te interpoleren met een geostatistische interpolatiemethode.

Methoden voor ruimtelijke interpolatie waarmee geen onzekerheid kan worden gekwantificeerd, en waarbij geen hulpinformatie wordt gebruikt, zijn *inverse distance weighting*, het *nearest-neighbour*-algoritme en *triangular irregular networks*. Hulpinformatie kan worden gebruikt om het gebied in deelgebieden te verdelen (stratificatie). Proceskennis kan worden benut door een geïnterpoleerd veld te construeren met een fysisch-mechanistisch model.

Temporele interpolatie

Krigingmethoden kunnen ook worden gebruikt voor temporele interpolatie. Belangrijk is bij het modelleren van correlatiestructuren rekening te houden met de wijze waarop een proces zich in de tijd ontwikkelt. Als hulpvariabelen worden gebruikt moet rekening worden gehouden met causaliteit. Tijdreeksmodellen, zoals *autoregressive (integrated) moving average*- (AR(I)MA)-modellen, transfer-ruis- (TFN-)modellen en interventiemodellen kunnen worden gebruikt om ontbrekende waarden te schatten, wat kan worden gezien als een vorm van temporele interpolatie. Deze modellen kunnen worden gebruikt om reeksen met regelmatige waarnemingsintervallen te modelleren. De *state-space approach* met *Kalman filtering* en *Kalman smoothing* kan worden gebruikt om reeksen met onregelmatige waarnemingsintervallen te interpoleren. Andere methoden voor temporele interpolatie, waarmee onzekerheid kan worden gekwantificeerd, zijn Bayesiaanse tijdreeksmodellen en structurele tijdreeksmodellen.

Interpolatiemethoden waarmee onzekerheid niet kan worden gekwantificeerd, zoals *inverse distance weighting* en het *nearest-neighbour*-algoritme, kunnen ook worden gebruikt voor temporele interpolatie, evenals fysisch-mechanistische procesmodellen.

Ruimte-tijdinterpolatie

Methoden voor ruimte-tijdinterpolatie waarmee onzekerheid kan worden gekwantificeerd kunnen worden verdeeld in drie categorieën: 1) tijdreeksmodellen met een ruimtelijke component, 2) geostatistische methoden met een temporele component en 3) hybride modellen. De eerste categorie bevat onder meer het STARMA- (*space-time ARMA*-)model, wat een uitwerking is van het univariate ARMA-model, waarbij rekening wordt gehouden met correlaties tussen tijdreeksen die op verschillende locaties zijn waargenomen. De tweede categorie bevat onder meer *space-time (ST) simple kriging*, *ST-ordinary kriging* en *ST-kriging with an external drift*. De derde categorie bestaat uit combinaties van tijdreeks- en geostatistische modellen, bijvoor-

beeld geostatistische interpolatie van tijdreeksmodelparameters. De *Bayesian Maximum Entropy*-benadering, waarbij gebruik wordt gemaakt van hulpinformatie, kan worden uitgebreid naar ruimte-tijdinterpolatie. De *state-space approach* kan eveneens worden uitgebreid naar ruimte-tijd, waarbij gebruik kan worden gemaakt van proceskennis. Een fysisch gebaseerd, geregionaliseerd tijdreeksmodel kan in combinatie met een ST-Kalman filter worden gebruikt voor ruimte-tijdinterpolatie. Procesmodellen (fysisch-mechanistische modellen) kunnen worden gebruikt voor ruimte-tijdinterpolatie zonder (directe) kwantificering van onzekerheid.

Aggregatie en desaggregatie

Bij aggregatie, of opschaling, wordt informatie van een gedetailleerde (fijne) schaal omgezet naar informatie van een grovere schaal. ‘Schaal’ heeft hier betrekking op *support* in geostatistische zin, dat wil zeggen de omvang, het volume en de vorm van eenheden waarover wordt geaggregeerd. Als de locaties zijn geselecteerd volgens een kanssteekproef dan kunnen gemiddelden en totalen zuiver worden geschat door gebruik te maken van de insluitkansen die samenhangen met de betreffende steekproefopzet. Als de waarnemingen zijn verzameld op gericht geselecteerde locaties of tijdstippen, dan moeten de waarnemingen eerst worden geïnterpoleerd naar een fijn grid, en vervolgens kunnen de geïnterpoleerde waarden worden geaggregeerd. Bij de interpolatie kan gebruik worden gemaakt van een model voor de ruimtelijke samenhang om gewichten te berekenen. Onzekerheid kan worden gekwantificeerd door n stochastische simulaties uit te voeren en per realisatie te aggregeren. De variantie van de n geaggregeerde waarden geeft de onzekerheid aan. In geval van lineaire kriging modellen kunnen de predicties en varianties van geaggregeerde waarden ook eenvoudiger met block-kriging worden verkregen.

Bij desaggregatie, of neerschaling, wordt de variatie van een variabele op een gedetailleerde schaal gereconstrueerd, gegeven de waarde op een grovere schaal. Als er geen hulpinformatie of mechanistisch model beschikbaar is dat de onbekende temporele of ruimtelijke variabele kan verklaren, dan kan informatie worden gedisaggregeerd met behulp van empirische functies. Als de gemiddelde waarde op de grovere schaal exact bekend is kunnen deterministische empirische functies en conditionele stochastische functies worden gebruikt. Als er slechts een kansverdelingsfunctie van het gemiddelde op de grovere schaal bekend is, dan kunnen onconditionele stochastische functies worden gebruikt voor desaggregatie. Mechanistische modellen en gedetailleerde hulpinformatie kunnen worden gebruikt in deterministische en conditionele en onconditionele stochastische functies voor desaggregatie.

Kort overzicht van computerprogramma’s

ArcGIS Geostatistical Analyst bevat mogelijkheden voor geostatistische interpolatie en analyses. Voor onderwijsdoeleinden kan $E\{Z\}$ -kriging worden gebruikt om de principes van *ordinary point kriging*, *block kriging* en het semivariogram uit te leggen. Genstat biedt mogelijkheden voor regressieanalyse, analyse van de ruimtelijke correlatiestructuur, geostatistische interpolate en tijdreeksmodellering. ISATIS is een uitgebreid geostatistisch *software*-pakket dat is ontwikkeld door Geovariances in Frankrijk. GSLIB (Geostatistical Software LIBrary) is een verzameling geostatistische programma’s, ontwikkeld aan de Stanford University gedurende de laatste 15

jaar. ILWIS (Integrated Land and Water Information System) is een *stand-alone* geïntegreerd GIS-pakket dat is ontwikkeld door het International Institute of Geoinformation Science and Earth Observations (ITC) in Enschede. MATLAB[®] is een hogere technische programmeertaal en interactieve omgeving voor de ontwikkeling van algoritmes, datavisualisatie, data-analyse en numerieke berekeningen. Er zijn verschillende *toolboxes* voor geostatistiek in MATLAB[®] beschikbaar, evenals procedures voor tijdreeksanalyse en *state-space*-modellering. R is een *free-software*-omgeving voor statistische berekeningen en grafieken. Veel R-*packages* zijn beschikbaar voor ruimtelijke statistiek. Daarnaast bevat R *packages* voor tijdreeksanalyse en *state-space*-modellering. SAGA (System for Automated Geoscientific Analyses) is een *open source* GIS, ontwikkeld aan de Universität Göttingen, en sinds 2007 Universität Hamburg (Duitsland). Het bevat modules voor de analyse van semivariogrammen, *ordinary kriging*, *universal kriging* en interpolatie met *splines*. Surfer (gemaakt door Golden Software) bevat interactieve *tools* voor variogramanalyse en kriging. S+ is een commerciële implementatie van de programmeertaal S (TIBCO Software Inc.). Evenals de *open source* evenknie R, bevat S+ *packages* voor ruimtelijke statistiek en tijdreeksanalyse. Vesper (Variogram Estimation and Spatial Prediction plus Error, van het Australian Centre for Precision Agriculture) is een programma voor het schatten en modelleren van variogrammen en voor *kriging*. Het kan kriging met lokale variogrammen automatisch uitvoeren.

Case studies

In twee *case studies* is de toepassing van interpolatietechnieken geïllustreerd: temporele interpolatie van indicatoren voor de ecologische waterkwaliteit, en ruimte-tijdinterpolatie en aggregatie van concentraties van bestrijdingsmiddelen in Nederlandse oppervlaktewateren. De eerste *case study* betreft acht tijdreeksen, met onregelmatige waarnemingsintervallen en ongelijke lengtes, van ‘multimetrische scores’. Deze scores, met waarden tussen 0 en 1, geven de ecologische waterkwaliteit aan in het waterschap ‘Regge en Dinkel’. Temporele interpolatie is uitgevoerd met *inverse distance weighting*, *ordinary kriging* van niet-getransformeerde gegevens, *ordinary kriging* na logit-transformatie, *MultiGaussian kriging* en *simple kriging* met een bekend variërend gemiddelde. Bij *simple kriging* met een bekend variërend gemiddelde is een seizoenstrend gefit en zijn de residuen daarvan geïnterpoleerd. De resultaten van de interpolatietechnieken verschillen onderling sterk, wat bevestigt dat het zin heeft om te zoeken naar een geschikte interpolatiemethode.

De tweede *case study* betreft ruimte-tijdinterpolatie van concentraties van het gewasbeschermingsmiddel ‘metribuzin’ in Nederlandse oppervlaktewateren (sloten). Puntwaarnemingen zijn in de tijd geaggregeerd tot gemiddelden voor groeiseizoenen. Deze gemiddelden zijn ruimtelijk en temporeel geïnterpoleerd met regressie-kriging. Hierbij is een meervoudig lineair regressiemodel gebruikt met als verklarende variabelen onder andere het type oppervlaktewater, de oppervlaktefractie landbouwgrond, en concentraties die zijn voorspeld met een deterministisch model voor de verspreiding van bestrijdingsmiddelen. De residuen van dit regressiemodel zijn geïnterpoleerd met *ST simple kriging*. Voor ruimtelijke aggregatie is stochastische simulatie toegepast (sequentiële Gaussische simulatie). Zodoende kon de onzekerheid over de geaggregeerde waarden worden gekwantificeerd, en de significantie van temporele trends in de geaggregeerde waarden. De aldus verkregen temporele trend in de landelijke gemiddelde concentratie bleek beduidend te verschillen van de trend verkregen met ‘naïeve’ opschaling.

Concluderende opmerkingen

Om het vinden van een geschikte interpolatiemethode te kunnen ondersteunen, is er meer informatie nodig over de eigenschappen van deze methoden. In het bijzonder is er meer informatie nodig over de nauwkeurigheid van interpolatiemethoden. Een overzicht van validatiestudies en vergelijkende studies moet duidelijk maken voor welke situaties informatie over de nauwkeurigheid ontbreekt. Dit kan het vertrekpunt zijn voor aanvullende validatiestudies. Een zinnige volgende stap is om het overzicht dat dit rapport geeft uit te werken tot een beslisboom of beslissingsondersteunend systeem, dat milieuwetenschappers de weg wijst naar eenvoudig toepasbare *software* voor het oplossen van hun interpolatieproblemen. Bij het construeren van een dergelijke beslisboom is het belangrijk inzicht te hebben in de interpolatieproblemen waarmee medewerkers van PBL te maken hebben.

Statistische informatie over onzekerheid of nauwkeurigheid wordt gebruikt bij toepassing van methoden uit de statistische beslissingstheorie, bij kwantitatieve risico- en beleidsanalyse en bij onzekerheidsanalyses vanuit de theorie van *post-normal science*. Voor elke interpolatiemethode kan de *overall* of globale nauwkeurigheid worden gekwantificeerd met een onafhankelijk validatie-onderzoek, waarbij de veldwaarnemingen bij voorkeur zijn verzameld middels een kanssteekproef. *Lokale* informatie over de nauwkeurigheid kan alleen worden verkregen door stochastische interpolatiemethoden toe te passen. De kwaliteit van deze lokale informatie over nauwkeurigheid hangt af van modelveronderstellingen die niet altijd eenvoudig kunnen worden geverifieerd.

Om te kunnen beoordelen of informatie over onzekerheid bruikbaar is in beslisprocessen, moet de kwaliteit van deze informatie bekend zijn. Als informatie over de *globale* nauwkeurigheid is gebaseerd op een validatie met een onafhankelijke kanssteekproef, dan kan de kwaliteit van deze informatie eenvoudig worden gekwantificeerd. De kwaliteit van *lokale* informatie over nauwkeurigheid kan worden gekwantificeerd door middel van validatie of *cross-validatie*. Validatiestudies naar de kwaliteit van *lokale* informatie over nauwkeurigheid zijn echter schaars. Wij benadrukken de noodzaak van dergelijke studies, waarvan de resultaten kunnen worden benut bij het ondersteunen van een keuze uit de interpolatiemethoden die in dit rapport worden beschreven.

De meeste interpolatiemethoden kunnen worden gebruikt bij het aggregeren van informatie. Desaggregatie is moeilijker dan aggregatie, omdat er veronderstellingen moeten worden gemaakt over de ruimtelijke of temporele variatie op de meer gedetailleerde schaal. In het klimaatonderzoek is veel ervaring met desaggregatie opgedaan, waarvan andere gebieden van milieuonderzoek zouden kunnen profiteren.

Chapter 1

Introduction

1.1 Background and problem definition

Environmental scientists can choose from a large collection of interpolation techniques developed during the past decades. The methods vary from general algorithms to specific methods tailored to specific applications, from simple to complex algorithms, from strictly data-based methods to methods incorporating process knowledge, from deterministic to stochastic methods, etc. Interpolation methods have been reviewed and compared in several studies. Recently, Li and Heap (2008) reviewed spatial interpolation methods for environmental scientists in Australia. Denby et al. (2005) reviewed interpolation and assimilation methods for European scale air quality assessment and mapping. Hengl (2007) summarized a variety of methods for geostatistical interpolation of environmental variables in a practical guide, and described available hands-on software. The performance of methods for spatial interpolation have been compared by, e.g., Dubois et al. (2003) and Dubois (2005). The INTAMAP project (www.intamap.org) provides methods and open source software for real time, web-based automatic interpolation.

Choosing an appropriate interpolation method from this large variety of techniques might be cumbersome. Several criteria are relevant in making a choice:

- applicability in space, time and space-time;
- quantification of accuracy of interpolated values;
- applicability to numerical and/or categorical variables;
- incorporation of ancillary information;
- incorporation of process knowledge;
- applicability for aggregation and disaggregation (up- and downscaling);
- complexity of application, level of required expertise, and required computation time;
- constraints on the size of the dataset and on the conditions of the dataset;
- availability of easy-to-use software implementations.

1.2 Aim

The aim of this report is to structure the volume of interpolation techniques, with respect to the criteria mentioned above. The underlying statistical models, the interpolation algorithm as well as available software will be described. The suitability for the Netherlands Environmental Assessment Agency (PBL) will be discussed. Because information on uncertainty is indispensable in present-day environmental policy analysis and policy-focused research (Morgan and Henrion, 1990; Van der Sluijs et al., 2003) we focus on interpolation methods that provide quantitative information on the accuracy of the interpolated values. We emphasize that the *overall* accuracy of interpolations (e.g., a map) can be assessed by an independent validation study, whatever the applied interpolation method is. *Local* information on accuracy can only be obtained by applying stochastic interpolation methods, however. The quality of this local information on accuracy depends on model assumptions which cannot always easily be verified.

The main disposition is based on 1) applicability in space, time and space-time, 2) quantification of accuracy of interpolated values, 3) incorporation of ancillary information, and 4) incorporation of process knowledge. In the description of the categories of methods the applicability to numerical and/or categorical variables, the applicability for aggregation and disaggregation, complexity of application, required computation time, constraints on the size and conditions of the dataset and availability of software implementations will be discussed.

We emphasize that this study is a review of interpolation methods rather than a textbook that describes underlying theory in detail. Readers interested in background information of methods are provided with references to relevant literature.

1.3 How to read this report?

Methods for interpolation in space, time and space-time are described in Chapters 2, 3 and 4, respectively. Methods that quantify uncertainty are described in the first section of these chapters, methods that do not quantify uncertainty in the second. Within these sections we describe methods that do not use ancillary information, methods using ancillary information, and methods incorporating process knowledge, respectively. Chapter 5 presents a table that summarizes the interpolation methods described in the previous three chapters.

Chapter 6 discusses the applicability of interpolation methods for aggregation and disaggregation (also referred to as up- and downscaling). Chapter 7 gives a brief overview of available software for interpolation. Chapter 8 demonstrates the application of interpolation methods in two case studies. The first case study concerns temporal interpolation of multimetric scores for ecological surface water quality. Inverse distance weighting (IDW) and four kriging methods are applied. The second case study concerns the spatio-temporal interpolation and aggregation of pesticide concentrations in Dutch surface waters. The report ends with a general discussion and conclusions in Chapter 9, including a discussion on information on accuracy and its quality.

Chapter 2

Interpolation in space

2.1 Methods that quantify uncertainty

2.1.1 Methods without use of ancillary information

Methods based on kriging

Kriging refers to a group of geostatistical interpolation methods in which the value at an unobserved location is predicted by a linear combination of the values at surrounding locations, using weights according to a model that describes the spatial correlation. The statistical basis of kriging enables to quantify the accuracy of the predicted values by means of the kriging variance. The kriging variance is a measure of the accuracy of the interpolated values, or, in other words, a measure of the uncertainty about the true values. For an introduction to kriging we refer to Isaaks and Srivastava (1989), and for theoretical backgrounds to Cressie (1993) and Goovaerts (1997). Kriging methods are widely applied for the interpolation of spatially distributed environmental variables. The map of kriging variances characterizes the local accuracy of the spatial predictions. It should be noted that the kriging variance is based on various assumptions (e.g. the stationarity assumption) and does not take the uncertainty about the model of spatial structure or variogram into account. A model-free assessment of the global uncertainty about the interpolation error can only be obtained by an independent validation study based on a probability sample (e.g., Brus et al. (2010)).

Simple kriging (SK) is based on a stationary random function model

$$Z(\mathbf{s}) = m + R(\mathbf{s}), \quad (2.1)$$

with \mathbf{s} being a vector of spatial coordinates, m the stationary mean or systematic component, and $R(\mathbf{s})$ the stochastic component with zero mean, constant variance, and with spatial covariance $C(\mathbf{h})$, the vector \mathbf{h} representing the lag distance between two locations. The random function Z is assumed to have generated the unknown reality z , which is observed at a limited set of point locations and which needs to be interpolated. See Figure 2.1 for a notional example in 1D of a realization of the random function model in Eq. 2.1. The covariance $C(\mathbf{h})$ is defined as

$$C(\mathbf{h}) = E \{Z(\mathbf{s} + \mathbf{h})Z(\mathbf{s})\} - [E \{Z(\mathbf{s})\}]^2, \quad (2.2)$$

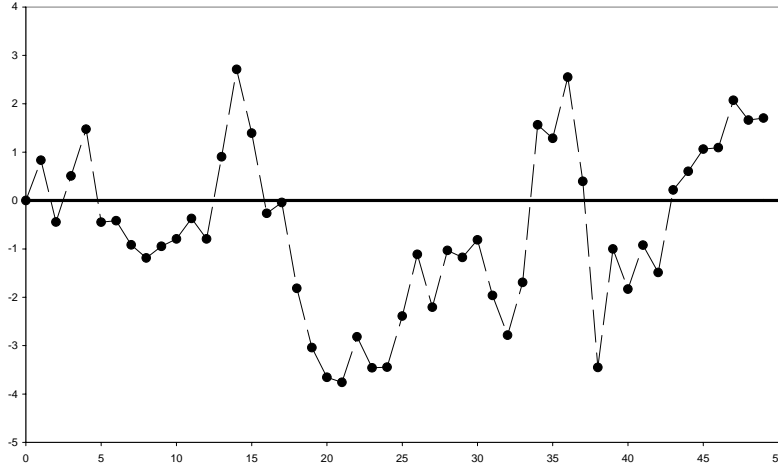


Figure 2.1: Notional example in 1D of the random function model in Eq. 2.1. Solid line: m . Dashed line: $z(\mathbf{s})$.

where E is the expectation. Alternatively to the covariance, the variogram γ is defined as half the variance of the increment $\{Z(\mathbf{s} + \mathbf{h}) - Z(\mathbf{s})\}$. For a stationary random function the variogram is

$$\begin{aligned} 2\gamma(\mathbf{h}) &= \text{Var} \{Z(\mathbf{s} + \mathbf{h}) - Z(\mathbf{s})\} \\ \gamma(\mathbf{h}) &= C(0) - C(\mathbf{h}), \forall \mathbf{s}. \end{aligned} \quad (2.3)$$

The value of z at an unsampled location \mathbf{s}_0 is estimated on the basis of the values $Z(\mathbf{s}_i)$ at locations $\mathbf{s}_1, \dots, \mathbf{s}_n$ by

$$\hat{Z}_{\text{SK}}(\mathbf{s}_0) = \sum_{i=1}^n \lambda_i(\mathbf{s}_0) Z(\mathbf{s}_i) + \left[1 - \sum_{i=1}^n \lambda_i(\mathbf{s}_0) \right] m, \quad (2.4)$$

in which $\lambda_i(\mathbf{s}_0)$ are the kriging weights. These are determined by minimizing the kriging variance or variance of spatial predictions, leading to the following conditions:

$$\sum_{j=1}^n \lambda_j(\mathbf{s}_0) C(\mathbf{s}_j - \mathbf{s}_i) = C(\mathbf{s}_0 - \mathbf{s}_i), \forall i = 1 \dots n. \quad (2.5)$$

The corresponding minimized kriging variance is:

$$\sigma_{\text{SK}}^2(\mathbf{s}_0) = C(0) - \sum_{i=1}^n \lambda_i(\mathbf{s}_0) C(\mathbf{s}_0 - \mathbf{s}_i). \quad (2.6)$$

Simple kriging has been described in many textbooks on geostatistics, e.g., Journel and Huijbregts (1978), Goovaerts (1997) and Diggle and Ribeiro (2007). Li and Heap (2008) discussed simple kriging their review of interpolation methods. Pebesma (2004) described the implementation of simple kriging in the software package `gstat` (see Chapter 7). Brus and Heuvelink (2007) described the application of the simple kriging algorithm in stochastic simulation.

In *ordinary kriging* (OK) the sum of the weights $\sum_{i=1}^n \lambda_i(\mathbf{s}_0)$ is constrained to be equal to 1. As a result the last term in Eq. (2.4) equals zero, which means that no

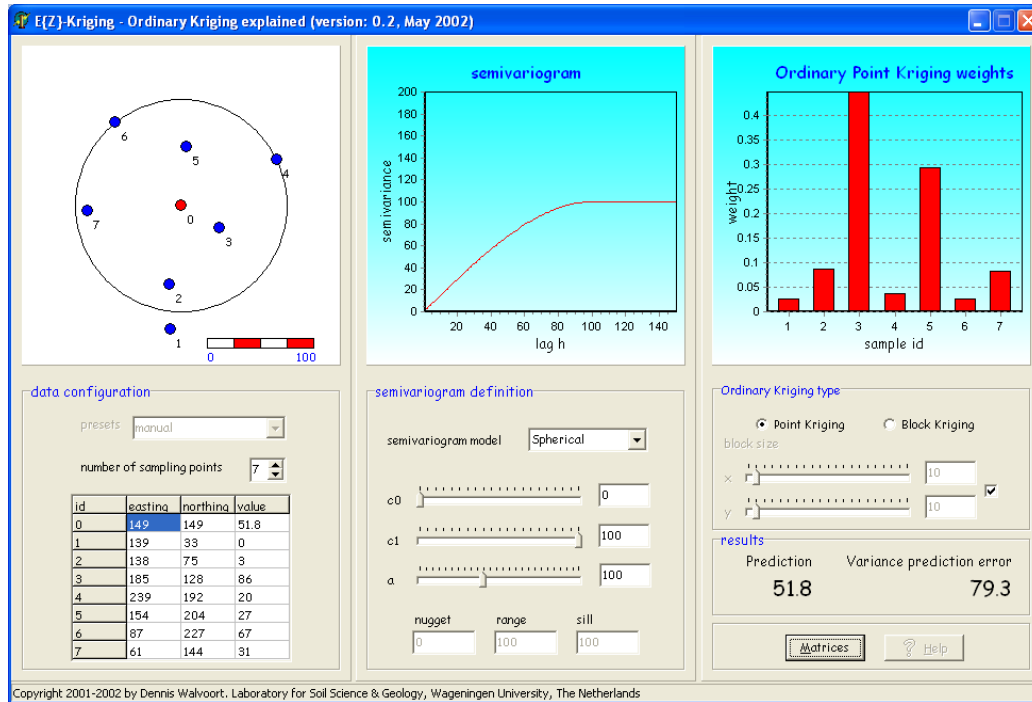


Figure 2.2: Illustration of kriging weights for ordinary kriging. Based on the educational program E{Z}-kriging, see Chapter 7.

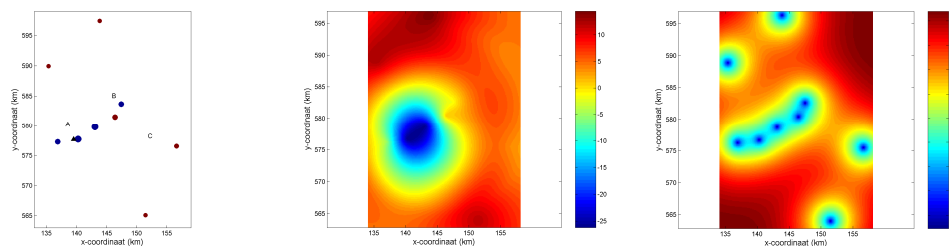


Figure 2.3: Ordinary kriging of the drop in the level of the bottom of the ‘Wadden Sea’ (period 1994-2004). Left: observations. Center: interpolated values. Right: kriging standard deviation. See also Figure 2.5.

prior knowledge on the stationary mean m is needed. Figure 2.2 gives an example of the kriging weights in OK, which is based on the educational software program E{Z}-kriging, see Chapter 7. OK has been described in many textbooks, e.g. Journel and Huijbregts (1978), Isaaks and Srivastava (1989) and Webster and Oliver (2007). Its performance in spatial predictions has been assessed in many studies, e.g. Knotters et al. (1995), Zimmerman et al. (1999), Schloeder et al. (2001), Erxleben et al. (2002), Atkinson and Lloyd (2003), Jones et al. (2003), Pebesma (2004), Denby et al. (2005), Savelieva (2005), He et al. (2005), Brus and Heuvelink (2007), Diggle and Ribeiro (2007), Hengl (2007), Schuurmans et al. (2007), Li and Heap (2008), Luo et al. (2008), Bargaoui and Chebbi (2009) and Kleijnen (2009). Mishra et al. (2009) applied ordinary kriging to parameters of soil profile depth distribution functions, and next estimated soil organic matter contents from the interpolated parameters. Figure 2.3 gives an example of interpolation by ordinary kriging.

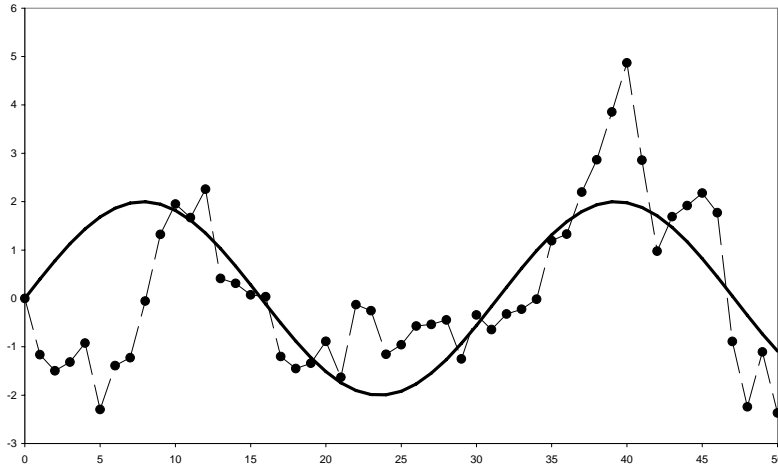


Figure 2.4: Notional example of the random function model in Eq. 2.7. Solid line: $m(\mathbf{s})$. Dashed line: $z(\mathbf{s})$.

Universal kriging with spatial coordinates (Matheron, 1969) is also referred to as *kriging in the presence of trend* or ‘drift’ (Webster and Oliver, 2007) and *kriging with a trend model* (Goovaerts, 1997, KT). The stationary mean μ in Eq. (2.1) is replaced by a smoothly varying, deterministic trend component, the level of which depends on the spatial coordinates \mathbf{s} :

$$Z(\mathbf{s}) = m(\mathbf{s}) + R(\mathbf{s}). \quad (2.7)$$

Figure 2.4 gives a notional example in 1D of this random function model. The trend component can be defined as $m(\mathbf{s}) = E\{Z(\mathbf{s})\}$ and is modelled as a (local) function from the coordinates vector, whose unknown parameters are fitted from the data:

$$m(\mathbf{s}) = \sum_{k=0}^K a_k(\mathbf{s}) f_k(\mathbf{s}). \quad (2.8)$$

Here, the functions f_k are so-called base functions and must be known. A trend in two-dimensional space can be modelled, for example, by a linear model,

$$m(\mathbf{s}) = m(x, y) = a_0 + a_1x + a_2y, \quad (2.9)$$

($K = 2$), or a quadratic model:

$$m(\mathbf{s}) = m(x, y) = a_0 + a_1x + a_2y + a_3x^2 + a_4y^2 + a_5xy, \quad (2.10)$$

($K = 5$).

The residual component $R(\mathbf{s})$ is modelled as a stationary random function with zero mean and covariance $C_R(\mathbf{h})$. The value of z at an unsampled location \mathbf{s}_0 is estimated by

$$\hat{Z}_{\text{KT}}(\mathbf{s}_0) = \sum_{i=1}^n \lambda_i(\mathbf{s}_0) Z(\mathbf{s}_i), \quad (2.11)$$

and the KT system is:

$$\begin{cases} \sum_{j=1}^n \lambda_j(\mathbf{s}_0) C_R(\mathbf{s}_i - \mathbf{s}_j) + \sum_{k=0}^K \mu_k(\mathbf{s}_0) f_k(\mathbf{s}_i) = C_R(\mathbf{s}_i - \mathbf{s}_0), i = 1, \dots, n \\ \sum_{j=1}^n \lambda_j(\mathbf{s}_0) = 1 \\ \sum_{j=1}^n \lambda_j(\mathbf{s}_0) f_k(\mathbf{s}_j) = f_k(\mathbf{s}_0), k = 0, \dots, K, \end{cases} \quad (2.12)$$

where the $\mu_k(\mathbf{s}_0)$ are Lagrange multipliers (Goovaerts, 1997, p. 140, Eq. (5.26)). *Kriging with a trend model* has, amongst others, been described by Goovaerts (1997) and Webster and Oliver (2007). Its performance has been assessed by, for example, Caruso and Quarta (1998), Zimmerman et al. (1999), Pebesma (2004), Denby et al. (2005), He et al. (2005), Diggle and Ribeiro (2007) and Luo et al. (2008).

In the kriging methods described above the target variable z is related to a point with spatial coordinates \mathbf{s} . *Block kriging* is applied if the target quantity is the average value over a block of specific dimensions, for example the average Cd concentration over a 1-hectare field if remedial measures are applied to 1-hectare areas (Goovaerts, 1997). It should be mentioned that the block can have any size or shape. For a description of the block kriging estimator we refer to Isaaks and Srivastava (1989) and Goovaerts (1997). Typically, block kriging does not affect the interpolated values much, but it does decrease the kriging standard deviation, particularly in cases with large short-distance spatial variation (Webster and Oliver, 2007). The performance of block kriging has been assessed, for example, by Bio et al. (1999), Van Horssen et al. (2002), Hengl (2007) and Li and Heap (2008).

In the kriging methods described above the value of the target variable is predicted at unvisited locations, or average values for areas of interest are estimated, and the accuracy is quantified by the kriging variance. In *indicator kriging* the kriging algorithm is applied to indicator data:

$$I(\mathbf{s}; z) = \begin{cases} 1 & \text{if } Z(\mathbf{s}) \leq z \\ 0 & \text{otherwise.} \end{cases} \quad (2.13)$$

Indicator kriging provides estimates of the conditional cumulative distribution function (ccdf) of $Z(\mathbf{s})$:

$$F(\mathbf{s}; z_k | (n)) = P\{Z(\mathbf{s}) \leq z_k | (n)\}, \quad (2.14)$$

in which z_k , $k = 1, \dots, K$ indicates a set of threshold values discretizing the range of variation of z , and (n) indicates the set of n neighbouring data values $Z(\mathbf{s}_i) = z(\mathbf{s}_i)$, $i = 1, \dots, n$. The performance of indicator kriging has been evaluated by, for example, Atkinson and Lloyd (2003). Note that in indicator kriging the ccdf is not described by its parameters, but that probabilities that threshold values z_k are exceeded are estimated at unvisited locations. For details on indicator kriging we refer to Isaaks and Srivastava (1989), Goovaerts (1997) and Webster and Oliver (2007). Indicator kriging may be applied 1) if the target variable has a non-Gaussian distribution, 2) for interpolation of categorical variables. Recent examples of the application of indicator kriging in spatial risk assessment are given by Goovaerts (2008), who applied indicator kriging in the geostatistical analysis of health and exposure data, and by Stelzenmüller et al. (2010), who predicted species occurrence probabilities of fishes for the UK continental shelf.

Several kriging methods other than indicator kriging have been developed to interpolate non-Gaussian distributed variables. Like indicator kriging, *disjunctive kriging* (Deutsch and Journel, 1998; Journel and Huijbregts, 1978; Webster and Oliver, 2007) can be applied to derive ccdf models characterizing the uncertainty about $z(\mathbf{s})$ at an unvisited location. In indicator kriging the direct and cross indicator covariances are inferred from the data. In disjunctive kriging, a parametric model of the bivariate distribution with rather restrictive assumptions is used, which is characterized by a transform of the original data and the covariance of those transforms. Deutsch and Journel (1998) advised to apply a Multi-Gaussian approach or median indicator

kriging instead of disjunctive kriging. *Multi-Gaussian kriging* with transformation of the target variable (Goovaerts, 1997; Deutsch and Journel, 1998) is particularly useful when the distribution of the z -data deviates from the normal distribution, as is the case with many environmental variables. Multi-Gaussian kriging starts with a transformation of the original z -data into y -values with a standard normal histogram (the so called *normal score transform*). Next, the y -values can be interpolated to any unvisited location by simple kriging, ordinary kriging or kriging with a trend model. Inference of the normal cdf $G(\mathbf{s}; y | (n))$ can be obtained by estimating its two parameters, mean and variance, at any unvisited location. It should be noted that 1) the Multi-Gaussian assumption is hard to validate, and 2) the normal score transform is not unbiased.

In *lognormal kriging* (Journel and Huijbregts, 1978) the target variable z is transformed to the logarithmic scale before the values are interpolated using the kriging system. After backtransformation to the original scale, the interpolated values are *median* unbiased estimates. The exponentiation in the backtransformation might make lognormal kriging sensitive to errors in the interpolation process, since these errors are exponentiated. For that reason several geostatisticians prefer Multi-Gaussian kriging and indicator kriging above lognormal kriging (Deutsch and Journel, 1998), although it must be noted that the normal score and indicator transforms suffer from the same problems. *Trans-Gaussian kriging* (Cressie, 1993; Diggle and Ribeiro, 2007) is a more general form of lognormal kriging and refers to kriging using transformations to the Gaussian distribution such as Box-Cox-transformations:

$$z^* = \begin{cases} (z^\lambda - 1)/\lambda & \text{if } \lambda \neq 0, \\ \log(z) & \text{if } \lambda = 0. \end{cases} \quad (2.15)$$

In *factorial kriging* (Goovaerts, 1997; Deutsch and Journel, 1998; Webster and Oliver, 2007) a random function (RF) model with two or more *independent* stochastic components or factors is considered:

$$Z(\mathbf{s}) = Z_0(\mathbf{s}) + Z_1(\mathbf{s}) + \dots + Z_L(\mathbf{s}), \quad (2.16)$$

(note the difference with the RF model in Eq. (2.7)). The Z -covariance is the sum of the $L + 1$ component covariances. Factorial kriging becomes interesting if one wants to separate the factors (e.g., physical processes or human activity) causing the spatial distribution of a variable. If these factors are related to different scales and operate different from one another, then for each factor separately a variogram can be considered.

Geostatisticians composed many variations on the kriging themes described above. Often these methods are tailored to specific study areas and research aims. A complete overview would be beyond the scope of this study. Kriging methods accounting for ancillary information will be discussed in Subsection 2.1.2. A number of remaining kriging methods that do not incorporate ancillary information will be discussed briefly here. As in indicator kriging in *Geostatistical classification and class kriging* (Allard, 2003) the range of variation of the z -variable is discretized by cutoffs, dividing the range of z into classes. The cutoffs are optimized by minimizing the sum of products of within-class variance and number of elements within the class over all classes. In *Poisson kriging* (Goovaerts and Gebreab, 2008) the variable of interest is a rate, for instance the mortality rate (number of recorded mortality cases divided by the size of the population at risk). *Bayesian kriging* has been applied by Biggeri et al. (2006) to predict the risk of parasite infection. *Robust kriging* (Fournier and

Furrer, 2005) has been developed to be less sensitive to erroneous measurements in interpolation. *Variation decomposition + kriging with a relative variogram and non-stationary residual variance* (Raty and Gilbert, 2003) shows some similarities with factorial kriging since variation is considered at various scales. *Detrending combined with kriging* (Genton and Furrer, 2003) is based on the RF-model given in Eq. (2.7). The deterministic trend is described by a nonparametric surface, and after subtracting this surface from the data, the residuals are kriged. Finally, the kriged values are added to the deterministic trend surface. A similar approach is *neural network residual kriging*, described in Demyanov et al. (2003), in which the deterministic trend component is modelled by an artificial neural network. *Modified residual kriging* (Erxleben et al., 2002) is also based on the RF-model given in Eq. (2.7). As contrasted to *kriging with a trend model* the parameters of the trend model are not estimated simultaneously with the calculation of the kriging weights, but separately. First, a parametric model describing the deterministic trend surface is fitted. Next, this surface is subtracted from the z -values and the residuals are kriged. Finally, the kriged values are added to the deterministic trend surface. Walvoort and De Gruijter (2001) developed *compositional kriging*, which aims to satisfy the constant sum and nonnegativity constraints of compositional data, expressed as fractions or percentages. Diggle and Ribeiro (2007) defined generalized linear models for geostatistical data that provide a sound statistical basis for non-Gaussian spatially dependent variables.

All kriging methods described above are based on Euclidian distance (straight line distance). The Euclidian distance might not be appropriate to interpolate chemical or biological variables that are dispersed within surface water systems such as stream networks. Knotters et al. (2009) give an overview of kriging methods tailored to interpolation within stream networks. Ver Hoef et al. (2006) and Peterson et al. (2007) developed kriging methods based on the *symmetric hydrologic distance* (SHD). The SHD is the distance between two points in a stream network, measured along the stream segments connecting these two points. Peterson and Urquhart (2006) and Peterson et al. (2006) developed a kriging method based on *weighted asymmetric hydrologic distance* (WAHD), which is unidirectional because movement between sites is restricted to either the upstream or downstream direction. Spatial weights represent the relative influence of one site on another. Sites that are not connected have zero spatial weight. The segment proportional influence (PI) of an incoming stream segment is calculated by dividing its watershed area by the total upstream watershed area at the confluence or survey site. The PI of one site on another is the product of the segment proportional influences found in the path between the flow-connected sites. Spatial weights are calculated by taking the square root of the PI's. Lyon et al. (2008) developed a kriging method that incorporates landscape characteristics in an adjusted distance metric. This approach has similarities with WAHD. The symmetric hydrologic distance between two points is weighted for the similarity in characteristics of areas that contribute to the stream in which the points are situated. Skøien et al. (2006) and Skøien and Blöschl (2007) presented *topological kriging* (Top-kriging) for interpolation in stream networks based on 'regularisation' of the variogram from between-point to between-catchment level. Chokmani and Ouarda (2004) and Guillemette et al. (2009) followed an approach in which a 'physiographical space' is constructed using the results of principal component analysis (PCA) and canonical correlation analysis (CCA). In this physiographical space the target variable is interpolated by kriging.

Splines

Spline functions are polynomials which are fitted in a flexible way through observations of z . The performance of splines, thin plate splines, thin plate smoothing splines with tensions or Laplacian smoothing splines has been evaluated in many studies (Voltz and Webster, 1990; Hutchinson, 1995; Guenni et al., 1996; Brus et al., 1996; Schloeder et al., 2001; Saveliev et al., 2005; Hengl, 2007; Li and Heap, 2008; Hofstra et al., 2008; Luo et al., 2008). Methods of radial basis functions (RBF) based on splines have been discussed by Thielen (2003) and Denby et al. (2005). Hofierka (2005) evaluated the Regularized Spline with Tension. If accuracy is quantified locally interpolation based on splines tends to kriging. For a discussion on the similarity between thin plate smoothing splines and kriging we refer to Dubrule (1984) and Hutchinson and Gessler (1994).

Methods based on Bayesian statistics

The *maximum entropy estimator* has been described by, e.g., Lee (2003). For applications with ancillary information we refer to Section 2.1.2, under “Other methods”. The maximum entropy method is also used to model the spatial distribution of species for which *occurrence-only* (or presence-only) data are available (Phillips et al., 2006, Maxent). Other methods to interpolate occurrence-only data are the Genetic Algorithm for Rule-Set Prediction (Stockwell and Peters, 1999, GARP), Ecological Niche Factor Analysis (Hirzel et al., 2002, ENFA).

Bayesian automating fitting functions are described by, e.g., Palaseanu-Lovejoy (2005), and *hierarchical Bayesian models* by Biggeri et al. (2006). Van de Kastele et al. (2005) applied geostatistical interpolation based on Bayesian inference to interpolate the annual number of ozone exceedance days in the Netherlands.

Regression methods

Regression on spatial coordinates or *trend surface analysis* can be used in spatial interpolation (He et al., 2005; Hengl, 2007; Li and Heap, 2008; Luo et al., 2008). It should be noted that the residuals are assumed to be spatially independent in trend surface analysis. In many situations this assumption will be too strong, and *universal kriging with spatial coordinates* is preferred.

Methods based on neural networks

Methods based on neural networks are data-driven and do in general not incorporate physical knowledge. Studies in which neural networks methods are evaluated are Pisoni et al. (2008) (Artificial Neural Networks), Rigol-Sanchez (2005), Timonin and Savelieva (2005), Dutta et al. (2005) and He et al. (2005) (Back-Propagation Artificial Neural Networks and Radial Basis Functions Neural Networks).

Other methods

Besides the methods described above, many other, less general, methods for spatial interpolation exist to which we briefly refer here. Denby et al. (2005) and Uboldi et al. (2008) evaluated *Optimal Interpolation* (Gandin, 1963) in mapping meteorological variables (see also Subsection 4.1.3). Ingram et al. (2005) evaluated the use of *Sparse Gaussian Processes* in spatial interpolation. Haskard et al. (2007) described Anisotropic Matérn Correlation and Spatial Prediction Using REML for interpolation of soil salinity data. Hofstra et al. (2008) evaluate the performance of *Conditional Interpolation* (CI) which has specifically been developed for gridding precipitation. Sadahiro (1999) compared four methods for *areal interpolation*, in which data are transferred from one zonal system to another (in contrast to point interpolation): areal weighting method, point-in-polygon method, kernel method and ‘intelligent methods’ that use supplementary data such as satellite images or landuse data in areal interpolation to improve estimation accuracy. Teegavarapu (2009) combined Association rule mining (ARM) and ordinary kriging to estimate missing precipitation records.

2.1.2 Methods using ancillary information

Stratified kriging

Ancillary information is often present in the form of so called choropleth maps, for example a soil map or a land use map. If it is likely that the mean of the target variable, its variance or both differ between the map units (strata), then a stratified kriging approach might improve the accuracy of spatial predictions. Examples are given by Hernandez-Stefanoni and Ponce-Hernandez (2006) and Brus and Heuvelink (2007). The following aspects need attention in stratified kriging:

1. Are variograms estimated for each stratum separately or is one variogram estimated for the whole study area?
2. How are discontinuous or gradual transitions at the stratum delineations dealt with?

Ad 1: Accurate variogram modelling requires at least 100-150 observations (Webster and Oliver, 1992), and short as well as long distances between the data locations. If these requirements are not fulfilled at stratum level, then only a variogram for the whole study area can be estimated.

Ad 2: Boucneau et al. (1998) described modifications of ordinary kriging to model discontinuous or gradual transitions at the delineations of strata.

Cokriging methods

In *cokriging* (Isaaks and Srivastava, 1989; Goovaerts, 1997; Deutsch and Journel, 1998) the RF-model of Eqs. (2.1) and (2.7) are extended with more than one variable:

$$Z_i(\mathbf{s}) = m_i(\mathbf{s}) + R_i(\mathbf{s}), \quad (2.17)$$

with $i, i = 1 \dots N_v$ indicating the i th variable. z_1 is referred to as the primary variable, $z_i, i = 2 \dots N_v$ as the secondary variables. In *simple cokriging* each local mean $m_i(\mathbf{s})$ is considered to be known and constant in the entire study area. In *ordinary cokriging* the means $m_i(\mathbf{s})$ are assumed to be constant but unknown within local neighborhoods. Ordinary cokriging has two drawbacks, following from the constraint that the weights for the secondary data have to sum to zero. The first is that some of the weights may be negative, thus increasing the risk of getting unacceptable estimates, e.g. negative metal contents. The second is that most of the weights tend to be small, thus reducing the influence of the secondary data. As a remedy *standardized ordinary cokriging* was introduced (Isaaks and Srivastava, 1989; Goovaerts, 1997), in which knowledge of the stationary means of both the primary and secondary variables is used. These means can be estimated from the sample means. In the standardized ordinary cokriging system the sum of the weights for primary and secondary data is constrained to 1. The sample means are used to rescale the secondary variables in advance so that their means equal that of the primary variable. However, Papritz (2008) showed that using sample means to apply standardized ordinary cokriging is in fact inferior to ordinary cokriging. In *cokriging with trend models* the means $m_i(\mathbf{s})$ are modelled as linear combinations of known functions $f_{ki}(\mathbf{s})$, analogous to Eqs. (2.8) to (2.12) (also called *universal cokriging* (Pebesma, 2004)). An alternative is *modified residual cokriging* (Erxleben et al., 2002), in which the parameters of the trend model for the primary variable are not estimated simultaneously with the calculation of the kriging weights, but separately. First, a parametric model describing the deterministic trend surface is fitted. Next, this surface is subtracted from the z -values and the residuals are interpolated by cokriging, using secondary variable(s). Finally, the co-kriged residuals are added to the deterministic trend surface.

A practical disadvantage of cokriging is the possible instability of the cokriging system. More specifically, the matrix containing the covariances and cross-covariances between the variables is sensitive to instability, in particular when the secondary variables are much more densely sampled than the primary variable. A solution to this problem is to use only the secondary datum closest to the location \mathbf{s}_0 to be interpolated to, referred to as *collocated cokriging* (Goovaerts, 1997; Deutsch and Journel, 1998). Cokriging can also be performed within strata, analogous to stratified kriging (Hernandez-Stefanoni and Ponce-Hernandez, 2006; Li and Heap, 2008). In several studies the performance of cokriging has been evaluated and compared with methods in which kriging and regression are combined (Ahmed and de Marsily, 1987; Knotters et al., 1995; Brus and Heuvelink, 2007; Coulibaly and Becker, 2007; Hengl, 2007; Luo et al., 2008).

Principal component kriging

Principal component kriging (Goovaerts, 1997) aims to reduce the *cokriging* of N_v variables to the *kriging* of N_v principal components. This means that N_v variograms of principal components are estimated, that each of the N_v principal components is estimated separately at each location \mathbf{s} , and that finally the estimate of z_i at \mathbf{s} is reconstituted as a linear combination of the principal component estimates at that location plus the mean m_i . In contrast to cokriging, in principal component kriging only those data locations where all N_v variables z_i are observed can be considered.

Combinations of regression and kriging

Kriging combined with linear regression (Delhomme, 1978), also referred to as *kriging with uncertain data*, is based on the RF-model for a primary variable in Eq. (2.1). Two types of data on the primary variable are considered: errorless observations and imprecise data obtained by linear regression with secondary variables. It is assumed that the regression errors are 1) nonsystematic (i.e., random), 2) spatially uncorrelated between themselves, and 3) uncorrelated with the variable. Next the inaccuracy of the regression predictions can be accounted for by simply subtracting the variance of prediction errors from the diagonal elements of the kriging (covariance) matrix. Although cokriging has a better theoretical foundation, kriging combined with linear regression showed a relatively good performance in comparative studies by Ahmed and de Marsily (1987) and Knotters et al. (1995). As compared to cokriging, kriging combined with linear regression needs much less computational effort. As compared to various methods to be described below, in kriging combined with linear regression, data on the secondary variables do not need to be available at the prediction points. Data on both the primary and the secondary variables need to be available at a sufficiently large number of locations to fit the regression model.

Universal kriging, kriging with an external drift or kriging with a trend model (Ahmed and de Marsily, 1987; Goovaerts, 1997; Deutsch and Journel, 1998) is based on the RF-model in Eq. (2.7). Here the trend is not a function of spatial co-ordinates but a function of secondary variables. Note that data on the secondary variables need to be available at the prediction points. Universal kriging incorporating secondary variables has been evaluated in several comparative studies, for example Ahmed and de Marsily (1987), Denby et al. (2005), Attorre et al. (2007), Brus and Heuvelink (2007), Coulibaly and Becker (2007), Hengl (2007), and Bargaoui and Chebbi (2009). Heuvelink et al. (2007) described its application in digital soil mapping.

Kriging with a guess field (Delhomme, 1978; Ahmed and de Marsily, 1987), *regression kriging* (Odeh et al., 1994, 1995, model B), (Hengl et al., 2004, 2007) or *residual kriging* (Mardikis et al., 2005) are similar methods based on the RF-model in Eq. (2.7). First, a trend surface or ‘guess field’ is constructed. This guess field may result from a numerical model (Delhomme, 1978; Ahmed and de Marsily, 1987). The guess field is subtracted from the observations on the primary variable, and the residuals are interpolated by ordinary kriging. Spatial predictions of the primary variable are obtained by adding the kriged residuals to the guess field. Kriging with a guess field is related to *Simple kriging with varying local means* (Goovaerts, 1997; Li and Heap, 2008) in which the stationary mean m in Eq. (2.4) is replaced with known varying means that depend on secondary information. The guess field can also result from a regression model (Odeh et al., 1994, 1995; Hengl et al., 2004, 2007; Mardikis et al., 2005) explaining the primary variable from secondary variables. After fitting the regression model, the regression residuals are interpolated by simple kriging. Spatial predictions of the primary variable are obtained by adding the kriged residuals to the regression predictions. Problems related to estimating the residual variogram in regression kriging are addressed by Lark et al. (2006), who present universal kriging with restricted maximum likelihood (REML-E-BLUP) to estimate the spatial variance model. Hengl (2007) applied regression kriging to indicator variables, using continuous memberships that are linearized using the logit transformation. Pebesma et al. (2005) combined Poisson regression (a Generalized Linear regression Model, GLM) and (co)kriging of residuals to map sea bird densities over the North Sea, and assessed temporal changes by comparing spatial

aggregates of consecutive years. Regression trees (CART, see below) can also be applied in regression kriging (Bishop and McBratney, 2001; Erxleben et al., 2002; Li and Heap, 2008). Bishop and McBratney (2001) also combined a Generalized Additive regression Model (GAM) with kriging. Hengl et al. (2009) combined point pattern analysis, Ecological Niche Factor Analysis (Hirzel et al., 2002, ENFA) and regression-kriging to interpolate occurrence-only data.

Regression methods

If the variable of interest is related to one or more auxiliary variables for which exhaustive high resolution data are available, then a regression model describing this relationship can be used in spatial interpolation, see, e.g., Chapter 3 in Denby et al. (2005). An example of such an auxiliary variable is ground surface elevation, exhaustive data of which are available in a Digital Elevation Model (DEM). It should be noted, however, that the regression residuals are assumed to be spatially independent. If this assumption is too strong cokriging or one of the previously discussed combinations of regression and kriging is advised. Odeh et al. (1994) applied a multiple linear regression model in the spatial prediction of soil variables. Wilks (2008) applied local weighted regression in the spatial interpolation of weather generator parameters. The weights are determined by the distances between the interpolation point and the locations of the training data. *Regression trees* (CART) (Li and Heap, 2008) or binary decision trees use binary recursive partitioning whereby the data of the primary variable are successively split along the gradient of the explanatory variables into two descendent subsets or nodes. The data are split in a way that at any node the difference between two split groups is maximized. The mean value of the primary variable in each node can then be used to map the variable across the region of interest. For a detailed description of regression methods, including GAM, Ridge-regression, LASSO and artificial neural networks we refer to Hastie et al. (2009).

Other methods

In *classification* (Li and Heap, 2008) an area is divided into subareas or strata using choropleth maps such as soil maps, vegetation maps, or maps with administrative areas. Next these subareas are characterized by the mean and variance of the attribute measured at locations within the area of interest. This method shares the same assumptions as regression methods on the absence of spatial structure in the residuals. In *Stratified global mean estimation* (Brus et al., 1996; Hernandez-Stefanoni and Ponce-Hernandez, 2006) the uncertainty about the true global mean can be quantified if *block kriging* is applied, the strata being blocks, see Subsection 2.1.1. See Chapter 6 for the use of block kriging in upscaling. Borak and Jasinski (2009, PCM) estimated per-class means to replace missing observations, in this way using global estimates as local estimates. Laplacian smoothing splines can also be applied within strata (Brus et al., 1996).

The *Bayesian Maximum Entropy (BME) method* (Christakos, 2000; Brus and Heuvelink, 2007; Brus et al., 2008) characterizes our uncertainty about spatial variables with probability distribution functions. The basic idea is to choose probability distribution functions that have maximum entropy, while satisfying a number of constraints. The entropy of a random variable is a measure of its uncertainty: the

larger the entropy, the larger the uncertainty. Under the constraints that the mean, variance and spatial correlation of the resulting probability distribution are known and fixed, BME yields a normal distribution and the results are identical to those of kriging. However, BME can also handle different and additional constraints and thus is more flexible than kriging, but the price paid for this is an increased numerical complexity. The two main steps in BME are first to compute the unconditional probability distribution of the variable using a numerical technique known as iterative scaling, and second to condition the distribution on the available observations. The BME method can be applied to both numerical and categorical variables.

As kriging and BME, the *Markov random field (MRF) approach* (Besag, 1974; Norberg et al., 2002; Wu et al., 2004; Kasetkasem et al., 2005; Hartman, 2006; Brus and Heuvelink, 2007) aims to characterize random spatially distributed variables with probability distribution functions. The starting point of MRF is defined in terms of *conditional* probability distributions, in which case the probability of occurrence of the variable of interest at some location is defined conditional to the value of the variable at neighbouring locations. The key property of the MRF approach is that it assumes that the local neighbourhood contains all information necessary to characterize the probability distribution of the variable. In addition, it uses numerical approaches, in particular Markov Chain Monte Carlo simulation, to compute predictions and simulations of the random variable. MRF is not as well developed as kriging and involves advanced mathematical statistical theories, but it appears a promising technique that has recently drawn increased attention, simultaneously with the development of Markov Chain Monte Carlo methods. As BME, the MRF method can be applied to both numerical and categorical variables.

Barber and Gelfand (2007) formulated a log-linear model of coregionalization in a Bayesian hierarchical framework to interpolate tree population sizes.

2.1.3 Methods incorporating process knowledge

A possible way to incorporate process knowledge in spatial interpolation is to construct a guess field using a physical-mechanistic model, and next to interpolate the residuals (see *kriging with a guess field* in the previous subsection and, e.g., Delhomme (1978); Ahmed and de Marsily (1987)). Denby et al. (2005) applied radial basis functions and Inverse Distance Weighting in interpolating the residuals of a guess field constructed by physical-mechanistic models for prediction of atmospheric concentrations. They also mention a Bayesian approach for combining measured and modelled data, which distinguishes hard (measured) and soft (modelled) data, that can be applied for spatial interpolation (Denby et al., 2005, p. 30). Matthijsen and Visser (2006) interpolated particulate matter concentrations (PM₁₀) using the model OPS (Van Jaarsveld, 2004), and mapped the local uncertainties on the basis of an uncertainty analysis.

2.2 Methods that do not quantify uncertainty

2.2.1 Methods without use of ancillary information

Methods based on Inverse Distance Weighting

Inverse Distance Weighting methods (IDW) are based on the assumption that the similarity of values of a spatially distributed numerical variable z decreases with distance d or a power p of the distance. This decline of similarity is incorporated in the interpolation as

$$\hat{z}(\mathbf{s}_0) = \frac{\sum_{i=1}^n \frac{z(\mathbf{s}_i)}{d_i^p}}{\sum_{i=1}^n \frac{1}{d_i^p}}, \quad (2.18)$$

in which \mathbf{s}_0 indicates the location to be interpolated to, and $\mathbf{s}_i, i = 1 \dots n$ indicate the n locations where z has been observed. Figure 2.5 (left) gives an example of interpolation by IDW.

Inverse distance weighting in its most simple form with $p = 1$ has been compared with alternative interpolation algorithms by Zimmerman et al. (1999), Caruso and Quarta (1998), Schloeder et al. (2001), Erxleben et al. (2002), Jones et al. (2003), Pebesma (2004), Denby et al. (2005), He et al. (2005), Mardikis et al. (2005), Hernandez-Stefanoni and Ponce-Hernandez (2006), Coulibaly and Becker (2007), Hengl (2007), Luo et al. (2008) and Spadavecchia and Williams (2009). The performance of inverse squared distance weighting ($p = 2$) has been compared with the results of alternative interpolation algorithms by Brus et al. (1996).

Several authors tailored the IDW-algorithm for application in specific cases: Detrended inverse distance weighting (D-IDW; Attorre et al. (2007)); Gradient Plus Inverse Distance Squared (Mardikis et al., 2005); Angular distance weighting (ADW; Hofstra et al. (2008)); Anisotropic Inverse Distance Weighting (Tomczak, 2003); Association rule mining (ARM) based spatial interpolation (IDW, Teegavarapu (2009)), and Association rule mining (ARM) based spatial interpolation (modified inverse-distance weighting method, Teegavarapu (2009)).

A refinement of the IDW method is natural neighbour interpolation (NNI; Jones et al. (2003), Hofstra et al. (2008) and Li and Heap (2008)). In NNI the weights depend not only on distance, but also on topological factors. For a description of natural neighbour interpolation we refer to Webster and Oliver (2007).

The nearest neighbour algorithm

As in inverse distance weighting methods, the basic assumption is that values of a spatially distributed variable at short distance are more similar than at larger distance. In nearest neighbour methods the value of z at the nearest observation point is assigned to z at the prediction point, \mathbf{s}_0 . In fact, it is IDW interpolation with the power p in Eq. (2.18) going to infinity. The pattern resulting from this method is also referred to as ‘Thiessen polygons’. Nearest neighbour algorithms can be applied to numerical as well as to categorical variables. Comparative studies in which nearest neighbour algorithms are evaluated are reported by Brus et al. (1996), Denby et al. (2005), He et al. (2005), Stahl et al. (2006) and Li and Heap (2008).

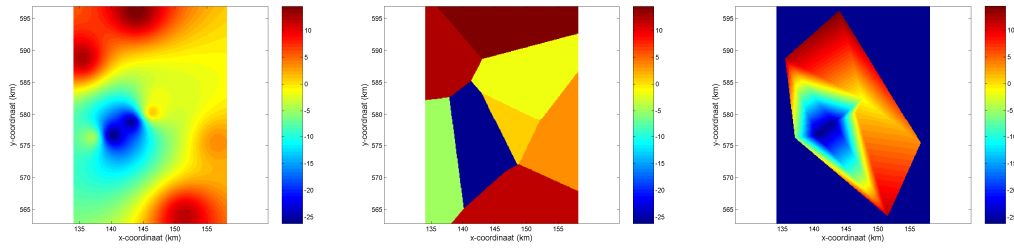


Figure 2.5: Interpolation of temporal change in ground surface elevation in the ‘Wadden Sea’ (see also Figure 2.3). Left: Inverse Distance Weighting. Center: Thiessen polygons. Right: Triangular Irregular Network.

Other methods

There are many, less general, interpolation methods that do not quantify uncertainty and that do not make use of ancillary information. We mention them briefly here. The *Triangular irregular network* (TIN), also referred to as bilinear interpolation, is the two-dimensional equivalent of linear interpolation (Denby et al., 2005; Li and Heap, 2008). Teegavarapu (2009) applied *association rule mining (ARM) based spatial interpolation* (coefficient of correlation weighting) to estimate missing precipitation records. A method known from soil surveys is *representative profile description* (Brus et al., 1996), which is applicable to numerical and categorical variables. To each unit of the soil map a ‘representative’ soil profile is assigned on the basis of expert knowledge. Caruso and Quarta (1998) compared *Hardy’s Multiquadric Method* and the *Tension Finite Difference Method* with inverse squared distance weighting and kriging. Luo et al. (2008) applied *local polynomial interpolation* to interpolate continuous wind speed in England and Wales. Perry and Niemann (2008) applied *Empirical Orthogonal Function (EOF) interpolation* to generate soil moisture patterns.

2.2.2 Methods using ancillary information

Methods based on stratification

Prior information such as soil maps or landuse maps can be used to divide an area into subareas or strata. Next, interpolation algorithms can be applied within these strata, adapted to the characteristics of variable to be interpolated within these strata. Examples of deterministic methods in which stratification is applied are:

- Moving average (stratified) (Brus et al., 1996).
- Nearest neighbour algorithm (stratified) (Brus et al., 1996).
- Inverse squared distance (stratified) (Brus et al., 1996).

Other methods

Falke and Husar (1998) and Denby et al. (2005) described a deterministic method to improve interpolations of observations on a variable z by using a more densely

observed ancillary variable y , which is based on the following algorithm:

$$\hat{z}(\mathbf{s}_0) = \left(\frac{\sum_{i=1}^n w_i \frac{z(\mathbf{s}_i)}{y(\mathbf{s}_i)}}{\sum_{i=1}^n w_i} \right) \cdot y(\mathbf{s}_0), \quad (2.19)$$

where $z(\mathbf{s}_i)$ is the measured value in measuring points $\mathbf{s}_i, i = 1 \dots n$, $y(\mathbf{s}_i)$ is the ancillary variable in the measuring points \mathbf{s}_i , $y(\mathbf{s}_0)$ is the ancillary variable in the interpolation point \mathbf{s}_0 , and w_i is the weight that depends on the distance of points $\mathbf{s}_i, \mathbf{s}_0$. Eq. (2.19) differs slightly from the equation given by Denby et al. (2005), which obviously contained an error.

A spatial model based on classification, such as a traditional soil map, can be seen as a special form of interpolation (Heuvelink and Webster, 2001; Hengl, 2007) for categorical data.

2.2.3 Methods incorporating process knowledge

Analogous to the methods mentioned in Subsection 2.1.3 a guess field can be constructed using a physical-mechanistic model, see Denby et al. (2005) for a review. The interpolations can possibly be improved by interpolating the residuals using a deterministic algorithm as described in Subsection 2.2.1, and adding them to the guess field.

Chapter 3

Interpolation in time

3.1 Methods that quantify uncertainty

3.1.1 Methods without use of ancillary information

Methods based on kriging

The kriging methods described in Subsection 2.1.1 can also be applied for interpolation in time. Examples are given in the case study described in Section 8.1. In modelling the temporal dependence structure, e.g. a variogram, it is important to be aware of the specific character of processes developing in time. In particular, when secondary variables are used in the model (see subsection 3.1.2) causality should be considered.

ARIMA modelling

Time series models can be used for data filling, which can be seen as a form of interpolation in time. We discuss time series modelling briefly here, with a focus on data filling.

The state of many phenomena in nature changes with time. This temporal variation can be described by time-series models. One general class of models is that of time-series models as described by Box and Jenkins (1976) and Hipel and McLeod (1994).

A process is said to be *stationary* if its statistical properties do not change with time. Stationarity can only be assumed, given the length of the period and the length of time intervals. *Strong* or *strict stationarity* means that all statistical properties are time-independent, so they do not change after time shifts. It is often sufficient to assume *weak stationarity of order k* , which means that the statistical moments up to order k only depend on differences in time and not on time as such. *Second-order stationarity* means that the mean, the variance and the autocorrelation function of the process are time-independent. This is also called *covariance stationarity*.

We now consider a discrete-time second-order stationary stochastic process. Suppose that we have an equidistant time series of n observations, $z_1, z_2, z_3, \dots, z_n$. The

process cannot be exactly described, so z_t is considered to be a realization of a stochastic process Z_t . For many environmental processes it is likely that the state at a particular time is correlated with the state at previous times. These processes are referred to as *autoregressive (AR) processes*. An autoregressive process of order 1, an AR(1) process or Markov process, is given by

$$Z_t - \mu = \phi_1(Z_{t-1} - \mu) + \epsilon_t , \quad (3.1)$$

where μ is the mean level, ϕ_1 is the AR parameter, and ϵ_t is the error term with zero mean and variance σ_ϵ^2 . ϵ_t is assumed to be identically and independently distributed (IID), so

$$E[\epsilon_t \epsilon_{t-k}] = \begin{cases} \sigma_\epsilon^2 & \text{if } k = 0 \\ 0 & \text{if } k \neq 0 \end{cases} \quad (3.2)$$

for all t . Using the backward shift operator B , Eq. (3.1) can be written as

$$Z_t - \mu = \phi_1(BZ_t - \mu) + \epsilon_t , \quad (3.3)$$

where $BZ_t = Z_{t-1}$. Eq. (3.3) can also be written as

$$\phi(B)(Z_t - \mu) = \epsilon_t , \quad (3.4)$$

with $\phi(B) = 1 - \phi_1 B$.

An *autoregressive process of order p , an AR(p) process*, is given by

$$Z_t - \mu = \phi_1(Z_{t-1} - \mu) + \phi_2(Z_{t-2} - \mu) + \dots + \phi_p(Z_{t-p} - \mu) + \epsilon_t , \quad (3.5)$$

or using the backward shift operator:

$$\phi(B)(Z_t - \mu) = \epsilon_t , \quad (3.6)$$

where $\phi(B) = 1 - \phi_1 B - \phi_2 B^2 - \dots - \phi_p B^p$ is the autoregressive operator of order p . To obey the assumption of stationarity, the values of the AR parameters are restricted. For an AR(1) process, this restriction is $|\phi_1| < 1$.

In *moving average processes* the state at a certain time depends on a random shock at that time and a random shock which occurred at one or more previous times. A first-order moving average process, MA(1), is given by

$$Z_t - \mu = \epsilon_t - \theta_1 \epsilon_{t-1} . \quad (3.7)$$

Here ϵ_t and ϵ_{t-1} are random shocks which form part of a white noise process with zero mean and finite and constant variance. Using the backward shift operator, Eq. (3.7) can be written as

$$Z_t - \mu = \theta(B)\epsilon_t , \quad (3.8)$$

where $\theta(B) = 1 - \theta_1 B$ is the MA operator of order one. The process is invertible if $|\theta_1| < 1$. For the meaning of invertibility we refer to Box and Jenkins (1976, p. 49-51) and Hipel and McLeod (1994, p. 104). The process is stationary for all values of θ_1 since ϵ_t is stationary. Note that if $|\theta_1| > 1$, the current event $Z_t - \mu$ depends more on events that happened further in the past. This can be avoided by the invertibility constraint $|\theta_1| < 1$.

An MA(q) process is given by

$$Z_t - \mu = \epsilon_t - \theta_1 \epsilon_{t-1} - \theta_2 \epsilon_{t-2} - \dots - \theta_q \epsilon_{t-q} , \quad (3.9)$$

or

$$Z_t - \mu = \theta(B)\epsilon_t , \quad (3.10)$$

where $\theta(B)$ is the MA operator of order q . The process is stationary for all values of the MA parameters.

A time series may contain properties of an autoregressive process as well as a moving average process. An *autoregressive moving average ARMA(1,1) process* is given by

$$Z_t - \mu = \phi_1(Z_{t-1} - \mu) + \epsilon_t - \theta_1\epsilon_{t-1} . \quad (3.11)$$

The ARMA(p, q) process is given by

$$\phi(B)(Z_t - \mu) = \theta(B)\epsilon_t , \quad (3.12)$$

where $\phi(B)$ and $\theta(B)$ are the AR(p) and the MA(q) operator, respectively.

Calculating differences allows a trend to be removed from a series:

$$\nabla Z_t = (Z_t - \mu) - (Z_{t-1} - \mu) \quad (3.13)$$

$$\nabla^2 Z_t = \nabla Z_t - \nabla Z_{t-1} \quad (3.14)$$

and so on, until a series of differences is obtained with a constant mean in time.

Basically, an *Autoregressive Integrated Moving Average (ARIMA) model* is an ARMA model for stationary differences:

$$\nabla^d Z_t - \mu = \frac{\theta(B)}{\phi(B)}\epsilon_t . \quad (3.15)$$

A form of nonstationarity often encountered in environmental processes is periodicity (e.g. seasonality or daily fluctuation). Besides periodicity in the mean, the variance itself may also have periodic behaviour. For example, shallow water tables in the wet season may vary more than deep water tables in the dry season, due to reduced storage capacity of the unsaturated zone in the wet season. If the variance varies in time, i.e., there is heteroscedasticity, the variance should be made constant by an appropriate deseasonalization procedure or by a Box–Cox transformation of the time series (Hipel and McLeod, 1994).

In the case of a *seasonal autoregressive moving average process*, differences are calculated for the so-called seasonal distance, with the aim of removing a seasonal trend. For example, the seasonal distance for monthly values is twelve. The general notation of a SARIMA(p, d, q) \times (P, D, Q) model is

$$\nabla^d \nabla_s^D Z_t - \mu = \frac{\theta(B)\Theta(B^s)}{\phi(B)\Phi(B^s)}\epsilon_t , \quad (3.16)$$

where s indicates the seasonal lag.

ARIMA modelling is based on equidistant time series. In this context interpolation can be seen as *data filling*, i.e. replacing missing values by estimates. Data filling techniques are *back forecasting*, *seasonal adjustment* and *intervention analysis*. For a description of back forecasting and seasonal adjustment we refer to Hipel and McLeod (1994). The climatological method of data filling described by Borak and Jasinski (2009) (TC) is similar to seasonal adjustment. Data filling by intervention

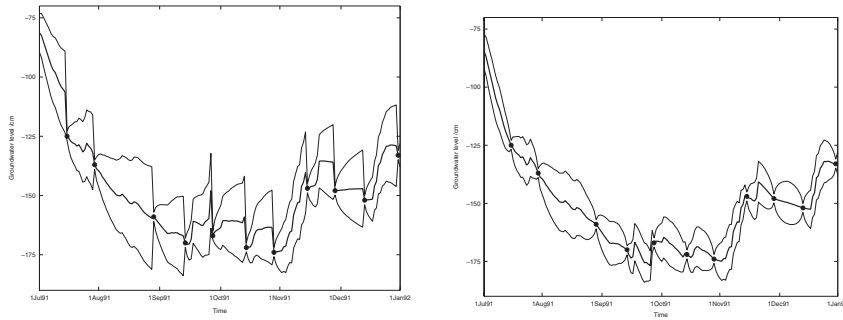


Figure 3.1: Left: Kalman filtering. Right: Kalman smoothing of groundwater levels. Dots are observations, fat line represents prediction and thin lines the limits of the 95 per cent prediction interval. Variance of measurement error = 1 cm².

modelling will be described below. This method can be seen as a special form of transfer function-noise (TFN) modelling. Statistical packages like Genstat (Payne, 2000) which estimate ARIMA model parameters by maximum likelihood or least squares procedures provide also estimates for missing values. It should be noted that the percentage of missing values should not be too large (say, not more than 10%), and that the missing values should not follow a systematic pattern in time.

State-space approach and Kalman filtering

In the *state-space approach* a stochastic residual is added to a deterministic model to represent model error. Observations of the state are used in conjunction with the dynamic behaviour of the system to make predictions at unobserved points in time. Two equations are considered: the state equation and the measurement equation. The state equation has the following general form (according to Heuvelink and Webster (2001)) (note the similarity with an AR(1) process):

$$Z_t = g \{Z_{t-1}\} + \epsilon_t, \quad (3.17)$$

and the measurement equation is

$$Y_t = h \{Z_t\} + \eta_t, \quad (3.18)$$

where Y_t is the measurement, and η_t is the measurement error. The state equation (Eq. (3.17)) is used to predict Z_t . The accuracy of the prediction depends on the variance in Z_{t-1} and on the variance in the system noise ϵ_t . If an observation Y_t with known accuracy is available, the original prediction can be updated in a way that optimally weighs the uncorrected prediction with the observation. This procedure is referred to as Kalman filtering (Kalman, 1960). In Kalman *smoothing* the present state is predicted from past, present and future observations. Important advantages of the state-space approach are 1) that irregularly observed series can be modelled, and 2) that physically-mechanistic models can easily be incorporated into the system (see Subsection 3.1.3). Figure 3.1 gives examples of Kalman filtering and Kalman smoothing.

Minimum mean absolute error linear interpolator (MMAELI)

Lu and Hui (2003) developed a *minimum mean absolute error linear interpolator (MMAELI)* for missing data in time series which is less influenced by some atypical observations than maximum likelihood and least squares procedures.

3.1.2 Methods using ancillary information

Methods based on kriging

The cokriging methods and combinations of regression and kriging described in Subsection 2.1.2 can also be applied in temporal interpolation. However, the specific character of processes developing in time, in particular causality, should be considered.

Transfer function-noise (TFN) modelling

(After De Gruijter et al. (2006)). A class of time-series models which describe the linear dynamic relationship between one or more input series and an output series is that of the transfer function model with added noise (TFN) developed by Box and Jenkins (1976). For applications to environmental series, we refer to Hipel and McLeod (1994) and Heuvelink and Webster (2001).

If one input series $\{X_t\}$ is considered, the TFN model is defined as

$$Z_t = Z_t^* + N_t, \quad (3.19)$$

where

$$Z_t^* = \sum_{i=1}^r \delta_i Z_{t-i}^* + \omega_0 X_{t-b} - \sum_{j=1}^s \omega_j X_{t-j-b} \quad (3.20)$$

is the transfer component, and

$$N_t - \mu = \sum_{i=1}^p \phi_i (N_{t-i} - \mu) + \epsilon_t - \sum_{j=1}^q \theta_j \epsilon_{t-j}, \quad (3.21)$$

is the noise component. The *subscript* b is a pure delay, which is the number of time steps after which a reaction to an input change is observed in the output. The extension to more input series is straightforward.

The transfer component in Eq. (3.19) can be written as

$$\begin{aligned} Z_t^* &= \nu_0 X_{t-b} + \nu_1 X_{t-1-b} + \nu_2 X_{t-2-b} + \dots \\ &= \nu(B) X_{t-b}. \end{aligned} \quad (3.22)$$

The weights $\nu_0, \nu_1, \nu_2, \dots$ form the impulse-response function $\nu(B)$:

$$\nu(B) = \frac{\omega(B)}{\delta(B)} = \frac{\omega_0 - \omega_1 B - \omega_2 B^2 - \dots - \omega_s B^s}{1 - \delta_1 B - \delta_2 B^2 - \dots - \delta_r B^r}. \quad (3.23)$$

The theoretical impulse–response function reflects the same autoregressive and moving average characteristics as the theoretical autocorrelation function.

We refer to Bierkens et al. (1999) for an application of the Kalman filter algorithm in TFN modelling of irregularly observed series of water table depths.

Data filling using intervention models

Methods accounting for serial correlation include the intervention models, described by Hipel and McLeod (1994). Intervention models form a special class of TFN models. The general form of an intervention model is

$$Z_t = I_{i,t} + Z_{j,t}^* + N_t, \quad i = 1, \dots, m, \quad (3.24)$$

where $t = 1, \dots, n$ indicates the t -th element of a series of length n , Z_t is the process of interest, $I_{i,t}$, $i = 1 \dots m$ is the intervention component, $Z_{j,t}^*$, $j = 1 \dots n$ are possible n transfer components (see before) and N_t is a noise component describing the part of Z_t that cannot be explained from the intervention and the transfer component. The noise component is usually taken as an ARMA model, see (3.12). The intervention component I_t is a transfer function with the following general form:

$$I_t = \delta_1 I_{t-1} + \delta_2 I_{t-2} + \dots + \delta_r I_{t-r} + \omega_0 S_{t-b}^{(T)} - \omega_1 S_{t-1-b}^{(T)} - \dots - \omega_m S_{t-m-b}^{(T)}, \quad (3.25)$$

where $\delta_1 \dots \delta_r$ are autoregressive parameters up to order r , $\omega_0 \dots \omega_m$ are moving average parameters up to order m , b is a pure delay parameter and T indicates the time at which the intervention takes place. Using the backward shift operator B , (3.25) can be written as

$$I_t = \frac{\omega(B)}{\delta(B)} B^b S_t^{(T)}, \quad (3.26)$$

with $B^k z_t = z_{t-k}$ and k is a positive integer.

If $S_t^{(T)}$ is an input series indicating a step intervention, then

$$\begin{aligned} S_t^{(T)} &= 0 & \text{if } t < T, \\ S_t^{(T)} &= 1 & \text{if } t \geq T. \end{aligned} \quad (3.27)$$

Step interventions influence processes in different ways, which can be expressed by different forms of the transfer function in Eq. (3.26), see Hipel and McLeod (1994) for details. The intervention model can also be used for data filling. In this case T is the time for which a value is missing, $S_t^{(T)} = 0$ if $t \neq T$ and $S_t^{(T)} = 1$ if $t = T$. The intervention model for data filling reduces then to

$$I_t = \omega_0 S_t^{(T)}. \quad (3.28)$$

An estimate for the missing value at T is $-\omega_0$.

Other methods

Dekkers and Heisterkamp (2004) described a class of time series models based on Bayesian statistics. As compared to ARIMA models and TFN models these *Bayesian*

time series models can be applied to relatively short time series having a length of 8 to 10 observations. The computer program NPbats of Dekkers and Heisterkamp (2004) can automatically estimate missing data and the model accounts for changes in variation (heteroscedasticity). NPbats is applied to detect trends, to describe relationships between time series and to analyse the influence of governmental policy on people and environment.

A *structural time-series model* (Visser, 2002, 2005) has the following basic structure:

$$y_t = \text{trend}_t + \text{cycl}_t + (\text{influence of explanatory variables})_t + \text{noise}_t. \quad (3.29)$$

The parameters of structural time-series models can be estimated with the Kalman filter algorithm, see Subsection 3.1.3 for a brief description. For details of the estimation procedure we refer to Visser (2002) and Visser (2005).

Dijkema et al. (2007) applied an *additive mixed model* which is basically a linear regression + an ARMA model for the residuals. The model has similarities with the structural time series model of Visser (2002) and Visser (2005).

3.1.3 Methods incorporating process knowledge

Time series models can have a physical basis, e.g. the ARMA model for annual streamflow described by Salas and Smith (1981), the AR(1) model for soil water content described by Parlange et al. (1992), the physically based TFN model for the relationship between precipitation surplus and water table depth described by Knotters and Bierkens (2000) (with Kalman filter application for fitting to irregularly observed series), and the continuous-time transfer function-noise model (PIRFICT) described by Von Asmuth and Knotters (2004).

3.2 Methods that do not quantify uncertainty

3.2.1 Methods without use of ancillary information

All interpolation algorithms described in Subsection 2.2.1 can also be applied in the time domain, as will be demonstrated in Section 8.1. Borak and Jasinski (2009) applied *temporal linear averaging* and *temporal cubic splines* to replace missing data in time series of leaf area indices.

3.2.2 Methods incorporating process knowledge

Physical-mechanistic models can be applied to replace missing data in environmental time series. Stauch and Jarvis (2006) combined multidimensional semi-parametric spline interpolation with an assumed but unstated dependence of net CO₂ flux on light, temperature and time.

Chapter 4

Interpolation in space and time

4.1 Methods that quantify uncertainty

4.1.1 Methods without use of ancillary information

Three basic approaches can be distinguished: 1) time series models with a spatial extension, 2) geostatistical models with a time extension, and 3) hybrid models combining time series modelling and geostatistical modelling, such as time series models with regionalized parameters.

The first category includes the *STARMA* (*space-time ARMA model*) (Cliff and Ord, 1975; Pfeifer and Deutsch, 1980), which is an extension to the univariate ARMA model, accounting for correlations between time series observed at various locations. Dalezios and Adamowski (1995) applied STARMA models in spatiotemporal precipitation modelling. Epperson (2000) applied STARMA models to represent theoretical models for ecological variation.

The second category includes the geostatistical approach to space-time (ST) modelling, based on the following RF-model, described for example by Kyriakidis and Journel (1999), Heuvelink and Webster (2001), Hengl (2007) and Spadavecchia and Williams (2009):

$$Z(\mathbf{s}, t) = m(\mathbf{s}, t) + R(\mathbf{s}, t), \quad (4.1)$$

where $m(\mathbf{s}, t)$ is a deterministic function of the space-time coordinates \mathbf{s} and t , and $R(\mathbf{s}, t)$ is a zero-mean stochastic component describing the space-time fluctuations around $m(\mathbf{s}, t)$, with the following autocovariance function:

$$C(\mathbf{h}_S, \mathbf{h}_T) = \text{Cov} [R(\mathbf{s}, t), R(\mathbf{s} + \mathbf{h}_S, t + \mathbf{h}_T)] . \quad (4.2)$$

Spadavecchia and Williams (2009) compared ST-simple kriging, ST-ordinary kriging and ST-kriging with an external drift using a residual variogram with spatiotemporal lags in the interpolation of meteorological variables. Because of basic differences between processes causing temporal variation and processes causing spatial variation, the residual $R(\mathbf{s}, t)$ will usually have space-time anisotropies. To overcome this problem the Bilonick or metric model might be applied. The stochastic component $R(\mathbf{s}, t)$ is divided in a S part $R_S(\mathbf{s})$, a T part $R_T(t)$ and a ST part $R_{ST}(\mathbf{s}, t)$. Assuming that these three components are second-order stationary and mutually

independent, the semivariogram of $R(\mathbf{s}, t)$ is the sum of three components:

$$\gamma(\mathbf{h}_S, \mathbf{h}_T) = \gamma_S(\mathbf{h}_S) + \gamma_T(\mathbf{h}_T) + \gamma_{ST}(\mathbf{h}_{ST}), \quad (4.3)$$

in which the ST lag \mathbf{h}_{ST} is obtained by introducing a geometric anisotropy ratio α :

$$\mathbf{h}_{ST} = \sqrt{\mathbf{h}_S^2 + \alpha \mathbf{h}_T^2}. \quad (4.4)$$

The metric model has the advantage that its component can be interpreted physically. Estimation of the model parameters is complicated, however. Snepvangers et al. (2003) compared ST-ordinary kriging and ST-kriging with an external drift model of soil water content, using the metric model for spatiotemporal structure, and Jost et al. (2005) applied these methods to soil water storage in a forest ecosystem. A possible way to account for temporal trends is to include time, for instance Julian day number, as a secondary variable into the trend component $m(\mathbf{s}, t)$ in Eq. (4.1) (Hengl, 2007). The *multivariate geostatistical model* introduced by Rouhani et al. (1992) and discussed by Denby et al. (2005) is based on a multi-scale temporal approach. The observations are considered as realizations of separate, but correlated random variables. This collection of one-dimensional random variables can be considered as a set of correlated random functions. A disadvantage of this multivariate geostatistical method is that a large number of variograms and covariance functions need to be estimated. In the *spatiotemporal random field*, introduced by Christakos and Vyas (1998) and discussed by Denby et al. (2005), the assumption of stationarity is not necessary, in contrast to the multivariate geostatistical method.

The third category consists of hybrid models combining time series modelling and geostatistical modelling. An example is the study on space-time estimation of grid-cell hourly ozone levels by Meiring et al. (1998), in which ARMA-parameters, mean field and prewhitened residuals are interpolated spatially. This method shows some similarities with the Bayesian approach for spatiotemporal interpolation described by Riccio (2005).

The *fractal interpolation* of rain rate time series, described by Paulson (2004) does not fit into one of the three categories described above. This stochastic numerical method is developed to interpolate point rain rate time series to shorter sampling periods while conserving the expected first- and second-order statistics, and should be applicable to the temporal interpolation of radar-derived rain rate maps.

4.1.2 Methods using ancillary information

Analogous to universal kriging, kriging with an external drift or kriging with a trend model in the spatial context described in Subsection 2.1.2, the trend component $m(\mathbf{s}, t)$ in Eq. (4.1) can be a function of secondary variables. Snepvangers et al. (2003), Jost et al. (2005) and Spadavecchia and Williams (2009) refer to this method as to *ST-kriging with an external drift*. Hoogland et al. (2008, 2010) applied this method recently to the interpolation of fluctuation characteristics of water table depths in the Netherlands. Kyriakidis et al. (2004) developed the *hybrid model*, combining a model for temporal trend and regression with cokriging of residuals using secondary variables, to simulate daily precipitation at regional scales. This is basically a *regionalized time series model*. The *Bayesian Maximum Entropy approach (BME)*, briefly described in Subsection 2.1.2, can be extended to the space-time context (Christakos et al., 2001).

4.1.3 Methods incorporating process knowledge

The *state-space approach* described in Subsection 3.1.3 can be extended to space-time, as described for example by Heuvelink and Webster (2001), Denby et al. (2005), Heuvelink et al. (2006) and Wu et al. (2008). Large computational efforts are needed to solve the Kalman filter equations, however, because of the large vectors and variance-covariance matrices. Knotters and Bierkens (2001) incorporated physical knowledge into *regionalized time series models*, by first constructing guess fields of time series model parameters using the physical relationships described by Knotters and Bierkens (2000), and next interpolating residuals by ordinary kriging. Bierkens et al. (2001) and Knotters and Bierkens (2002) embedded the physically based regionalized time series model in a ST-Kalman filter.

Optimal interpolation (Denby et al., 2005; Sen et al., 2006; Tombette et al., 2009) shows similarities with kriging in calculating interpolation weights, and is equivalent to data assimilation based on variational methods and the Kalman filter, which are now considered to be more flexible and easier to apply. *Variational methods* (Denby et al., 2005; Wu et al., 2008) are based on the minimization of a cost function for the difference between model predictions and observations (Lorenz, 1986). Variational methods are less flexible than Kalman filtering techniques, but the computational effort is much lower.

4.2 Methods that do not quantify uncertainty

4.2.1 Methods incorporating process knowledge

Process models (also referred to as physical-mechanistic and deterministic models) can be used for space-time interpolation of environmental variables. Numerous examples can be given. An example is given by Hoogland et al. (2006), who used a process model for groundwater flow in interpolating water table depths. Global information on the accuracy, such as space-time root mean squared interpolation errors, can be obtained by validation.

Chapter 5

Summary of interpolation methods

Tables 5.1 to 5.3 summarize the interpolation methods described in the previous chapters. The table indicates how the methods meet the criteria listed in Chapter 1. The conditions on the size of the data set are, if possible, given by a minimum number of observations needed to interpolate. The minimum of 100-150 observations for kriging methods is recommended by Webster and Oliver (1992) to fit a model of spatial structure. If such a model is already available, then the minimum number of observations needed for kriging is much lower. In time series modelling, the observation period should amply cover the correlation length in univariate modelling (e.g., ARIMA models), or the response time in transfer function-noise modelling, see De Gruijter et al. (2006, Chapter 13) for more details on the sampling aspects of time series modelling.

Table 5.1: Classification of interpolation methods. - -: very easy to apply. -: easy to apply. +: some expert knowledge needed in application, in general well documented in literature and standard software available. ++: complex algorithm, specific expertise needed in application. +++: very complex algorithm, specific knowledge needed in application.

Method	Space, time, space-time	Numerical/Categorical	Quantified uncertainty	Ancillary information	Process knowledge	Conditions on size of data set	Complexity	Software available?
Simple kriging, Ordinary kriging, Kriging in the presence of a trend, Block kriging	space, time	numerical	yes	no	no	> 100-150	+	yes
Indicator kriging	space, time	numerical, categorical	yes	no	no	> 100-150	+/+++	yes
Disjunctive kriging, Multi-Gaussian kriging, Lognormal kriging	space, time	numerical	yes	no	no	> 100-150	++	yes
Trans-Gaussian kriging	space, time	numerical	yes	no	no	> 100-150	++	yes
Factorial kriging	space, time	numerical	yes	no	no	> 100-150	++	yes
Geostatistical classification and class kriging, Poisson kriging, Bayesian kriging, Robust kriging, Variation decomposition + kriging with a relative variogram and non-stationary residual variance, Detrending combined with kriging, Neural network residual kriging, Modified residual kriging, Compositional kriging, Topological kriging, Kriging with hydrologic distances	space, time	numerical	yes	no	no	> 100-150	+++	no
Thin plate (smoothing) splines	space, time	numerical	yes	no	no	> 100-150	+++	yes
Bayesian automating fitting functions, Hierarchical Bayesian models	space, time	numerical,	yes	no/yes	no	?	+++	no
Trend surface analysis	space, time	numerical	yes	no	no	> ca. 10	-	yes

Table 5.2: Classification of interpolation methods (continued).

Method	Space, time, space-time	Numerical/ Categorical	Quantified uncertainty	Ancillary information	Process knowledge	Conditions on size of data set	Complexity	Software available?
Stratified kriging	space, time	numerical	yes	yes	no	> 100-150	++	no
Simple cokriging, Ordinary cokriging, Collocated cokriging	space, time	numerical	yes	yes	no	> 100-150	++	yes
Cokriging with trend models, Modified residual cokriging	space, time	numerical	yes	yes	no	> 100-150	+++	no
Principal component kriging	space, time	numerical	yes	yes	no	> 100-150	++	no
Kriging with uncertain data	space, time	numerical	yes	yes	no	> 100-150	+	no
Kriging with an external drift	space, time	numerical	yes	yes	no	> 100-150	++	yes
Kriging with a guess field	space, time	numerical	yes	yes	yes	> 100-150	+	no
Regression trees (CART)	space, time	numerical, categorical	yes	yes	yes	≥ 2	+	yes
Classification	space, time	numerical	yes	yes	yes	≥ 2	-	no
Global mean (stratified)	space, time	numerical	yes	yes	yes	≥ 4	-	no
Laplacian smoothing splines (stratified)	space, time	numerical	yes	yes	no	≥ 2	+++	yes
Bayesian maximum entropy estimator	space, time, space-time	numerical, categorical	yes	no/yes	no	?	+++	yes
Markov random field (MRF)	space, time	numerical, categorical	yes	no/yes	no	?	+++	no
Inverse distance weighting	space, time	numerical	no	no	no	no	--	yes
Nearest neighbour algorithm	space, time	numerical, categorical	no	no	no	no	--	yes
Triangular irregular network (TIN)	space	numerical	no	no	no	≥ 3	--	yes
Linear interpolation	space, time	numerical	no	no	no	≥ 2	--	yes
Moving average (stratified), Inverse squared distance (stratified)	space, time	numerical	no	yes	no	≥ 2	--	yes
Nearest neighbour algorithm (stratified)	space, time	numerical, categorical	no	yes	no	≥ 2	--	yes
(S)ARIMA-modelling, intervention models	time	numerical	yes	no	no	> correlation length	+	yes
MMABLL	time	numerical	yes	no	no	> correlation length	+++	no
TFN-modelling, intervention models	time	numerical	yes	yes	no	> response time	+	yes
Bayesian time series models (NPBats)	time	numerical	yes	yes	no	$\geq 8 - 10$	++	yes
Structural time series models	time	numerical	yes	yes	no	> correlation length	+	yes
Physically based ARMA models	time	numerical	yes	no	no	> correlation length	+	no
Physically based TFN models	time	numerical	yes	yes	no	> correlation length	+	no

Table 5.3: Classification of interpolation methods (continued).

Method	Space, time, space-time	Numerical/ Categorical	Quantified uncertainty	Ancillary information calibration	Process knowledge	Conditions on size of data set	Complexity	Software available?
Process models	space, time space-time	numerical	no	yes	yes	no, unless in calibration	+-++++	yes
STARMA models	space-time	numerical	yes	no	no	> correlation length	+++	no
Space-time kriging, multivariate geostatistical model, spatiotemporal random field	space-time	numerical	yes	no	no	> 100-150	+++	no
Regionalized time series model (ARIMA, hybrid model)	space-time	numerical	yes	no	yes	space: > 100-150 time: > correlation length	++	no
Space-time kriging with an external drift	space-time	numerical	yes	yes	yes	> 100-150	+++	no
Regionalized time series model (TFN, hybrid model)	space-time	numerical	yes	yes	yes	space: > 100-150 time: > response time	++	no
State-space approach	time, space-time	numerical	yes	yes	yes	?	+++	yes
Optimal interpolation	space-time	numerical	yes	yes	no	?	+++	no
Variational methods	space-time	numerical	yes	yes	yes	?	+++	no

Chapter 6

Aggregation and disaggregation

6.1 Aggregation

Aggregation, also referred to as *upscaling*, involves transferring information from a smaller (detailed) scale to a larger (coarse) scale. Here, 'scale' refers to the 'support' as it is known in geostatistics, i.e. the size, volume and shape of entities over which is aggregated. For example, point observations of Cadmium concentration in the topsoil inform at a point scale. To inform about the Cadmium concentration at a field scale these point observations need to be aggregated in some way. The most simple way is to compute the arithmetic average of the values observed in the field. It should be noted, however, that this will result in unbiased estimates of the areal mean only if the locations have been selected by Simple Random Sampling (Cochran, 1977). In all other situations the observations should be weighted in some way to obtain unbiased and optimal estimates of the areal mean. When locations or sampling rounds have been selected following a probability-based sampling design, then the weights are determined by the sampling design. For an overview of designs for probability sampling we refer to Cochran (1977) and De Gruijter et al. (2006). For a decision support system on up- and downscaling we refer to Bierkens et al. (2000).

If the observations have been collected at purposively selected locations or sampling rounds, then the observed values need first to be interpolated and next the interpolated values can be aggregated. In the interpolation a model of spatial structure can be applied for weighing the observed values. For instance, the spatial correlation structure can be described by a semivariogram, see Chapter 2 for details and Chapter 8 for applications. Basically, all interpolation methods described in Chapter 2 to 4 can be used in aggregation of purposively selected observations. A possible way to aggregate from point scale to, e.g., field scale, is as follows:

1. Interpolate the observed values to a dense grid of interpolation points covering the area of interest. In case of a geostatistical approach: construct a model of the spatial structure of the variable, e.g., a semivariogram, and use this model for weighing the observations. Eqs. (2.5) and (2.6) show how the weights are calculated in Simple Kriging. For backgrounds on calculation of kriging weights we refer to Isaaks and Srivastava (1989), Cressie (1993) and Goovaerts (1997);

2. Aggregate the interpolated values. For instance, an areal mean can be obtained by arithmetic averaging of the interpolated values.

If the accuracy of the aggregated value needs to be quantified, the following geostatistical approach can be followed:

1. Obtain an independent realisation of values for a dense grid covering the area of interest, by conditional geostatistical simulation;
2. Aggregate the simulated values, (e.g., arithmetic averaging to obtain an areal mean);
3. Repeat steps 1 and 2 a large number of times (say 500). The mean of the 500 aggregated values is a final estimate, the standard deviation is a measure of its accuracy.

Conditional geostatistical simulation as used in step 2 above is a variant of kriging, whereby the purpose is not to compute the best estimate at an unobserved location but instead to generate a possible value from its conditional probability distribution. Many algorithms have been developed over the past decades, such as Cholesky decomposition and sequential Gaussian simulation (Goovaerts, 1997).

In Section 2.1.1 *block kriging* was mentioned as a method that can be applied if the target quantity is the average value over a block of specific dimensions, for example the average Cd concentration over a 1-hectare field if remedial measures are applied to 1-hectare areas (Goovaerts, 1997). It was mentioned that the block can have any size or shape. In fact, block kriging aggregates point values to averages over areas or volumes. *Global kriging* (Goovaerts, 1997) is a special case of block kriging. In global kriging the block size equals the entire study area, and the block estimate is an estimate of the global mean of the target variable over the study area. However, according to Goovaerts (1997) it is not advised to apply the block kriging system to estimate the global mean directly from the data for the following three reasons:

1. The covariance function can seldom be assumed to be stationary over the study area.
2. Estimates of covariance values for large lag distances are inaccurate, since often a few pairs of observations are separated by such large distances.
3. Using all data in estimation causes long computation time and a risk of an unstable kriging matrix.

For these reasons Goovaerts (1997) advised a two-step procedure. First the study area is discretized into small blocks and average values are estimated for each of these blocks. Next the global mean is estimated as a linear combination of these block estimates, weighting them proportional to the areal sizes of the blocks. Alternatively, a declustered mean of the data can be computed, see also Isaaks and Srivastava (1989, Chapter 10). Global kriging has been applied by Hofstra et al. (2008) in the field of climate research. Global kriging is typically applied to estimate a global mean if data locations have been selected purposively and if the number of observations is large enough to fit a variogram (say, at least 100-150 observations, Webster and Oliver (1992)). The term *global kriging* might be confusing, since this term is also widely used to distinguish kriging using all data from kriging using data from a restricted neighborhood (referred to as *local kriging*).

6.2 Disaggregation

In disaggregation, or *downscaling*, the variation of a variable at a small (detailed) scale is reconstructed, given the value at a larger (coarse) scale. The many ways of disaggregation can be divided on the basis of answers to the following two questions (Bierkens et al., 2000):

1. Is there ancillary information that can be used to explain some of the unknown temporal or spatial variation of the property at the small scale within the larger scale?
2. Is there a mechanistic model describing this (unknown) temporal or spatial variation?

If the answer to both questions is no, then information can be disaggregated using *empirical functions*. If the average value at the larger scale is exactly known *deterministic empirical functions* or *conditional stochastic functions* can be applied in disaggregation. Examples of deterministic empirical functions are splines, linear functions and general additive models. For a discussion and examples of the application of conditional stochastic functions in disaggregation we refer to Bierkens et al. (2000, Subsection 3.2.2). If only the probability function of the average value at the larger scale is known, then *unconditional stochastic functions* can be applied in disaggregation. The unknown variation at the smaller scale is described with a stochastic function with parameters such as mean, variance and semivariogram. Next realisations are generated at the smaller scale, and these realisations are averaged over the larger scale. The parameters of the stochastic function are adjusted such that the averages resemble the probability distribution of the property at the larger scale.

Mechanistic models and fine scale ancillary information can be used in deterministic and conditional and unconditional stochastic functions for disaggregation. For a discussion and examples we refer to Bierkens et al. (2000, Sections 3.3 and 3.4), respectively.

Disaggregation is relatively often applied in climate research, to generate weather conditions at a more detailed temporal and spatial scale than the scale at which observations are collected. For example, Mezghani and Hingray (2009) combine generalized linear models (GLM's) and K -nearest neighbour resampling to generate multisite hourly time series of precipitation and temperature from daily observed weather data, see also Buishand and Brandsma (2001) for the application of nearest neighbour resampling. Marani and Zanetti (2007) use a stochastic point process model in disaggregating daily rainfall observations to an hourly or subhourly scale. For a review of stochastic disaggregation methods for climate data we refer to Srikanthan and McMahon (2001).

Chapter 7

Brief overview of software

This chapter gives a brief overview of both commercial and open-source software for interpolation. Mentioning the trade name is only for technical information, not to endorse the software products. The software packages are arranged in alphabetic order.

ArcGIS, ArcGIS Geostatistical Analyst

ArcGIS is an integrated collection of GIS software products that enables spatial analysis, data management, and mapping. The ArcGIS Geostatistical Analyst (www.esri.com) provides tools for exploring the data (e.g., histograms and trend analysis), modelling the semi-variogram/covariance, geostatistical interpolation, cross-validation (leave-one-out), map comparison, and mapping probabilities of exceeding critical thresholds.

$E\{Z\}$ -kriging

In education, $E\{Z\}$ -kriging, developed by Dennis Walvoort, can be used to explain the principles of ordinary point kriging, block kriging and the semi-variogram. The software is available for free at www.ai-geostats.org. Figure 2.2 shows how $E\{Z\}$ -kriging demonstrates the calculation of kriging weights in ordinary kriging.

Genstat

The statistical package Genstat (Payne, 2000) provides tools for regression analysis, analysis of the spatial correlation structure, geostatistical interpolation and time series modelling. Regression analysis in Genstat includes simple and multiple linear regression, polynomial regression, cubic smoothing splines, generalized linear models and nonlinear regression. Geostatistical analysis in Genstat includes fitting of semi-variograms and ordinary point kriging. Time series analysis includes ARIMA modelling and transfer function-noise modelling.

ISATIS

ISATIS is a comprehensive geostatistical software tool developed by Geovariances in France. It comprises modules for exploratory spatial data analysis, variogram modelling, many of the kriging varieties described in this report, and conditional and unconditional geostatistical simulation. It is shipped with a graphical user interface and is available for several platforms.

GSLIB

GSLIB (Geostatistical Software LIBrary) is a collection of geostatistical programs developed at Stanford University over the past 15 years (Deutsch and Journel, 1998). Programs are available for variogram modelling, geostatistical interpolation, simulation and cross-validation. The kriging methods in GSLIB include simple kriging, ordinary kriging, kriging with a trend model, kriging with an external drift, factorial kriging, cokriging, lognormal kriging, multiGaussian kriging, disjunctive kriging, indicator kriging and indicator cokriging, indicator principle component kriging and block kriging. GSLIB is freely available as open source software at www.gslib.com.

ILWIS

ILWIS (Integrated Land and Water Information System) is a stand-alone integrated GIS package developed at the International Institute of Geoinformation Science and Earth Observations (ITC), Enschede, the Netherlands. The interpolation possibilities in ILWIS enable variogram modelling, analysis of anisotropy in the data, interpolation by ordinary kriging and cokriging (with one covariable), universal kriging with coordinates as predictors and linear regression. For a description and illustration of application in spatial interpolation we refer to Hengl (2007). ILWIS is freely available as open source software at <http://www.ilwis.org>.

MATLAB[®]

MATLAB[®] is a high-level technical computing language and interactive environment for algorithm development, data visualization, data analysis, and numeric computation. It is produced by 'The MathWorks' (www.mathworks.com). Several (user-written) toolboxes on geostatistics for MATLAB[®] are available. MATLAB[®] also provides procedures for time-series analysis and state-space modelling.

R

R (www.r-project.org) is a free software environment for statistical computing and graphics. It runs on a wide variety of UNIX platforms, Windows and MacOS. Many packages are available for spatial statistics, for instance *gstat* (www.gstat.org),

geoR (leg.ufpr.br/geoR), geoRglm, (gbi.agrsci.dk/5fch/geoRglm), fields (www.image.ucar.edu/GSP/Software/Fields), RandomFields, sgeostat, and spatial. In addition, R also contains packages for time-series analysis and state-space modelling.

SAGA GIS

SAGA (System for Automated Geoscientific Analyses) is an open source GIS developed in Germany (Universität Göttingen, and since 2007 Universität Hamburg). It contains modules for semivariogram analysis, ordinary kriging, universal kriging, and spline interpolation. It can be downloaded from www.saga-gis.org.

Surfer

Surfer contains interactive tools for variogram analysis and kriging. It is produced by Golden Software (www.goldensoftware.com) and ships with a graphical user interface.

S+

S+ is a commercial implementation of the S programming language sold by TIBCO Software Inc. (spotfire.tibco.com). Like its open source counterpart R, it has packages for spatial statistics and time-series analysis.

Vesper

Vesper (Variogram Estimation and Spatial Prediction plus ERror) is a program for variogram estimation/modelling and kriging. It is capable of performing kriging with *local* variograms in an automatic way. Vesper runs on Windows, and has a graphical user interface. It is available for free from the site of the Australian Centre for Precision Agriculture (www.usyd.edu.au/agriculture/acpa/software/vesper.shtml).

Chapter 8

Case studies

8.1 Temporal interpolation of indicators for ecological water quality

8.1.1 Data

Ecological water quality is summarized in multimetric scores, ranging from 0 to 1. The ecological water quality is indicated by these scores, to which we refer as ‘indicators’. Eight irregularly spaced time series of unequal length have been observed in the district water board “Regge en Dinkel” in the eastern part of the Netherlands. Table 8.1 summarizes the dataset. Figure 8.1 shows the time series plots of the indicators.

8.1.2 Application of interpolation methods

From the set of eight series we selected a series of short, intermediate and extensive length: 611, 400 and 643, respectively. To these series we applied the following selection of interpolation methods:

- Inverse distance weighting (IDW) with powers $p = 1, 2$ and 3 (see Eq. (2.18)), as examples of interpolation methods that do not quantify uncertainty;
- The following kriging methods, as examples of interpolation methods that quantify accuracy:
 - Ordinary kriging on untransformed data;
 - Ordinary kriging on data after logit-transformation;
 - MultiGaussian kriging (normal-score transform);
 - Simple kriging with a known varying mean (a seasonal trend).

Kriging was performed using the GSLIB software (Deutsch and Journel, 1998). The time series models described in Section 3.1 are not considered, because the sampling intervals are of irregular length.

Table 8.1: Summary of dataset of indicators for ecological water quality in “Regge en Dinkel”.

Location	Start date	End date	Number of observations
400	11-4-1983	8-10-2007	20
611	12-10-1992	7-5-2008	6
623	5-11-1981	1-10-2008	42
637	8-3-1982	8-10-2007	29
638	16-9-1980	15-10-2007	19
640	6-8-1980	1-10-2008	42
643	21-4-1981	20-10-2008	44
644	6-12-1982	15-10-2007	22

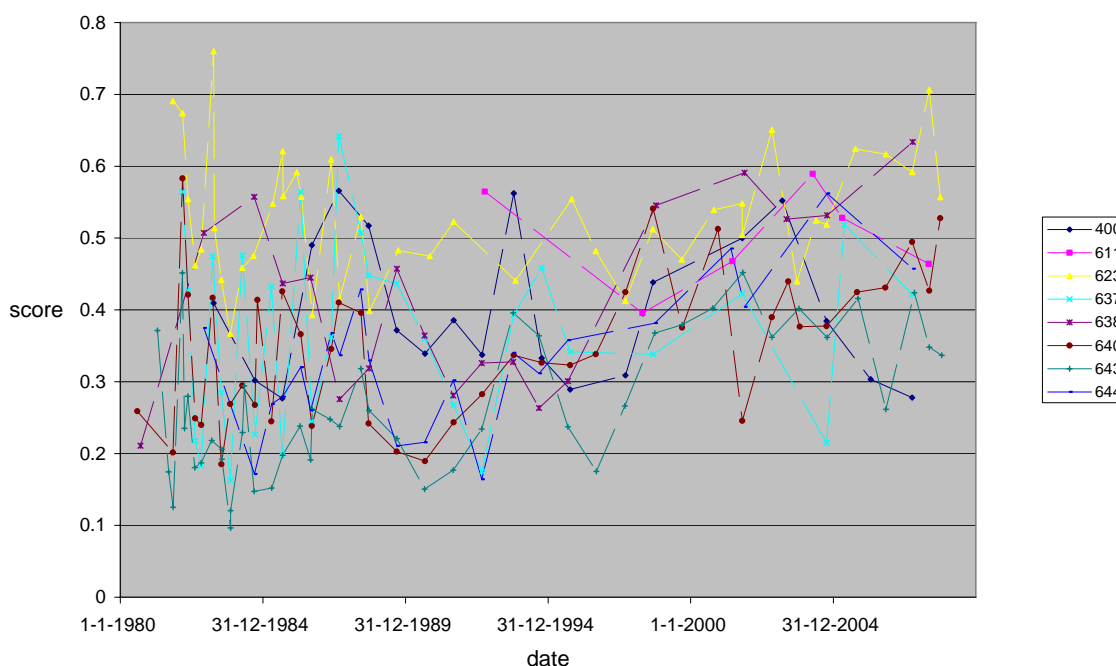


Figure 8.1: Time series plots of indicators for ecological water quality in “Regge en Dinkel”.

8.1.3 Results

Figure 8.2 shows results of IDW for series 611, for $p = 1, 2$ and 3 (see Eq. (2.18)). The pattern for $p = 1$ is rather spiky, which might not reflect reality. The larger the power, the more smooth is the interpolated pattern, because observations at short distance become more important.

Series 400 was interpolated by *ordinary kriging*. First, the temporal structure was analyzed by plotting a sample semivariogram, and next the temporal structure was modelled. Figure 8.3 shows the sample semivariogram and the fitted model of temporal structure. Because sample semivariogram does not reflect a temporal structure, a pure nugget model was fitted. *Ordinary kriging* using a pure nugget model and all data (i.e., global kriging) results in the mean level of the data as predicted values, see Figure 8.4. Although ordinary kriging has the advantage that uncertainty can be quantified, the results in Figure 8.4 are unsatisfying since the interpolated pattern

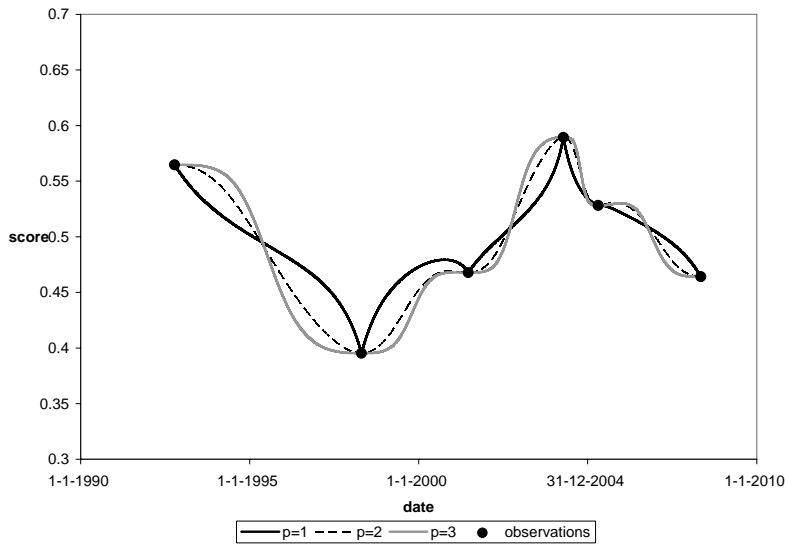


Figure 8.2: Interpolation by Inverse Distance Weighting for location 611, with power $p = 1$, 2 and 3 (see Eq. (2.18)).

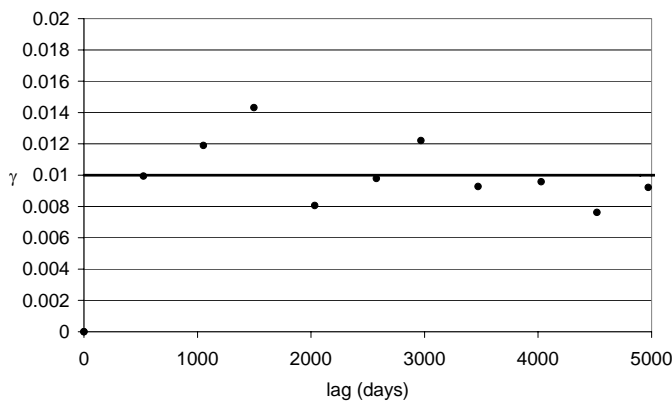


Figure 8.3: Sample semivariogram for the time series observed at location 400, and fitted pure nugget model.

does not reflect reality. It is well known that kriging has a smoothing effect. If a pure nugget variogram is applied this smoothing effect is most extreme.

We applied several kriging methods to interpolate the time series observed at location 643. First, we applied *ordinary kriging* to the untransformed data. Figure 8.5 shows the sample semivariogram and the fitted model. Due to the limited number of observations the results of automatic fitting of a semivariogram were unsatisfying. Therefore, we fitted the following exponential model manually to the sample semivariogram:

$$\gamma(h) = 0.003 + 0.007 \cdot \left[1 - e^{\left(-\frac{h}{1400}\right)} \right], \quad (8.1)$$

with h being the lag distance in days. All 44 data were used in the interpolation, i.e. *global* kriging. Figure 8.6 shows the results of interpolation of untransformed scores by ordinary kriging. The interpolated values are clearly *smoothed*. The irreg-

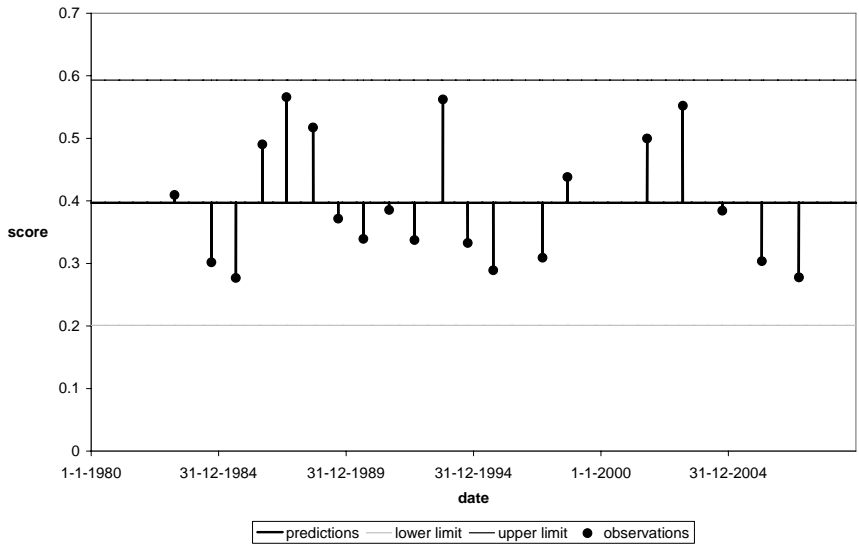


Figure 8.4: Interpolated values for location 400, obtained by ordinary kriging using the pure nugget semivariogram in Figure 8.3. Predicted values, lower and upper limits of the 95% prediction interval.

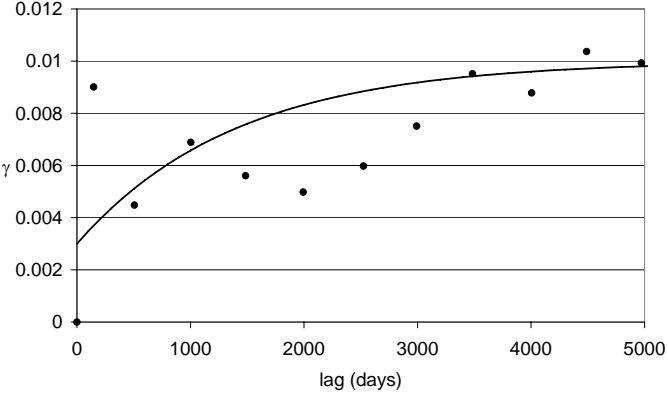


Figure 8.5: Sample semivariogram for the time series observed at location 643, and fitted exponential model.

ular pattern of the 95% prediction intervals can only be explained from numerical artefacts such as roundings.

Because the indicators range from 0 to 1, the limits of the 95% prediction intervals can theoretically fall outside this range if kriging is applied to the untransformed data. To prevent for this we applied a logit-transformation to the scores, and next interpolated the transformed values and calculated the 95% prediction intervals. Finally the interpolated values and the lower and upper limits of the 95% prediction interval were back-transformed. The logit-transformation is given by

$$z^* = \ln \left(\frac{z}{1-z} \right), \tag{8.2}$$

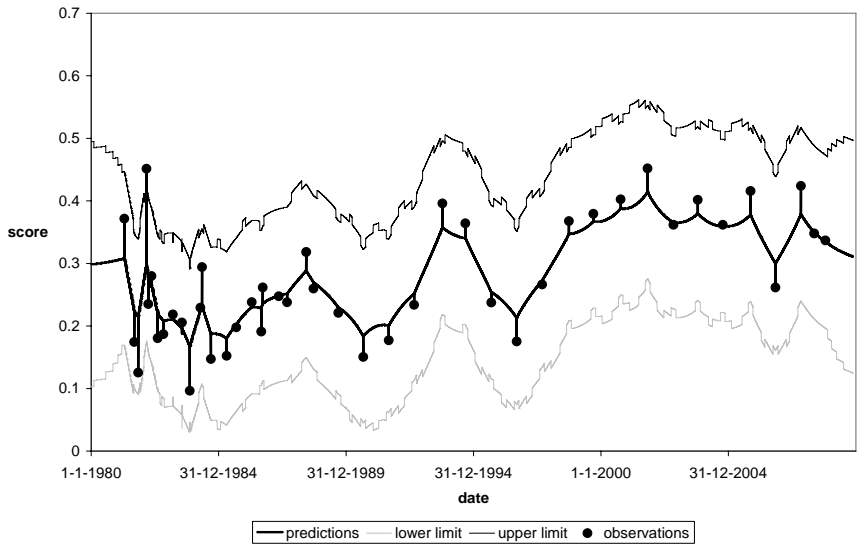


Figure 8.6: Interpolated values for location 643, obtained by ordinary kriging using the exponential semivariogram in Figure 8.5 and Eq. (8.5). Predicted values, lower and upper limits of the 95% prediction interval.

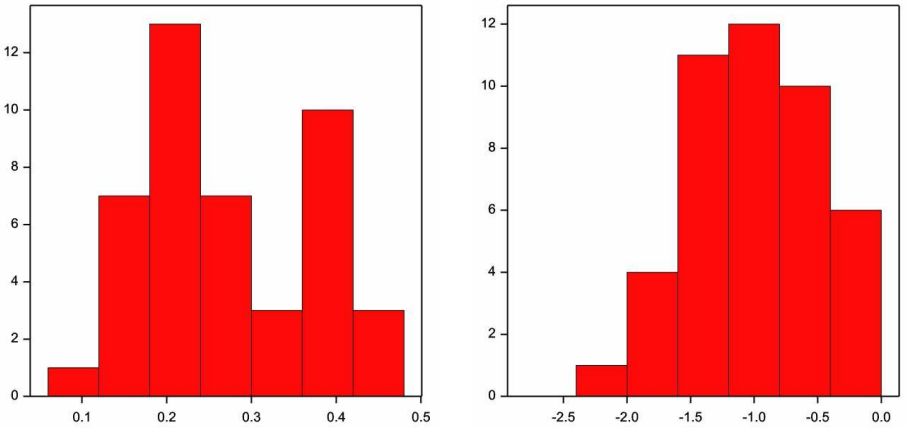


Figure 8.7: Histograms of indicators for ecological water quality at location 643, before logit-transformation (left) and after (right).

and the back-transformation to the original scale by

$$z = \frac{e^{z^*}}{1 + e^{z^*}}. \tag{8.3}$$

Figure 8.7 shows histograms of the untransformed and transformed scores.

Figure 8.8 shows the sample semivariogram of the logit-transformed scores, and the exponential model that was manually fitted. The next exponential model was used in ordinary kriging:

$$\gamma(h) = 0.1 + 0.15 \cdot \left[1 - e^{\left(-\frac{h}{1400}\right)} \right]. \tag{8.4}$$

Figure 8.9 shows the interpolated series and 95% prediction intervals, obtained by

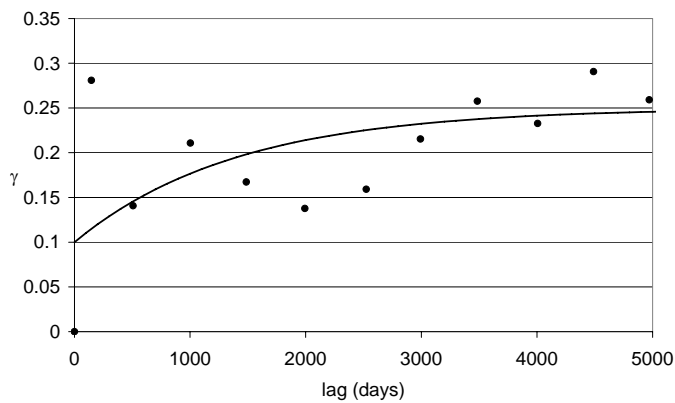


Figure 8.8: Sample semivariogram for the time series observed at location 643 after logit-transformation, and fitted exponential model.

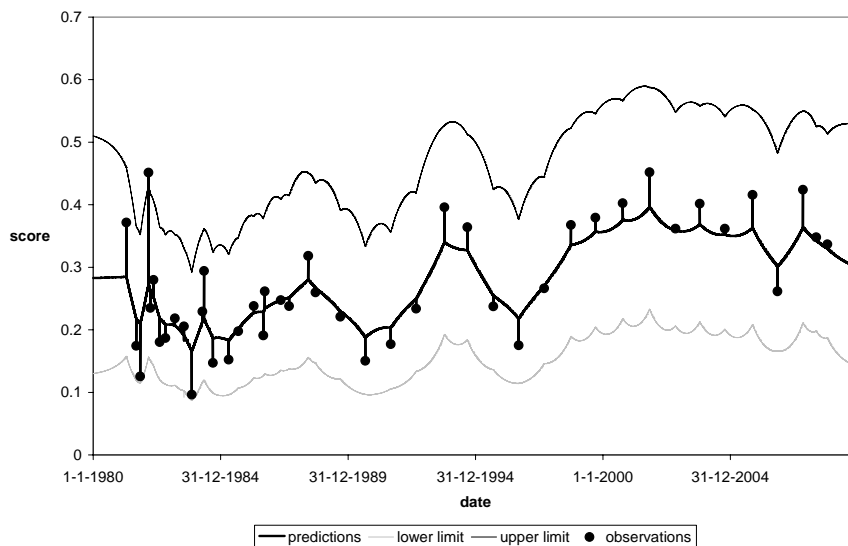


Figure 8.9: Interpolated values for location 643, obtained by ordinary kriging of logit-transformed indicators, using the exponential semivariogram in Figure 8.8 and Eq. (8.4). Predicted values, and lower and upper limits of the 95% prediction interval, after backtransformation to the original scale.

ordinary kriging of logit-transformed scores. The results are very similar to those obtained by ordinary kriging of the untransformed scores, see Figure 8.6. However, it should be noted that the 95% prediction intervals are not symmetric, in particular in the left hand side of the graph in Figure 8.9. The interpolated values are *median unbiased* at the original scale, see De Oliveira (2006).

A possible way to interpolate non-Gaussian data is *multi-Gaussian kriging* (Goovaerts, 1997; Deutsch and Journel, 1998), see Subsection 2.1.1. First the original data are transformed into values with a standard normal histogram (the so called *normal score transform*). Next, the transformed values can be interpolated to any unvisited location by simple kriging, ordinary kriging or kriging with a trend model. Figure 8.10 illustrates the normal score transform of the indicators observed at location 643. Figure 8.11 shows the sample semivariogram of the transformed

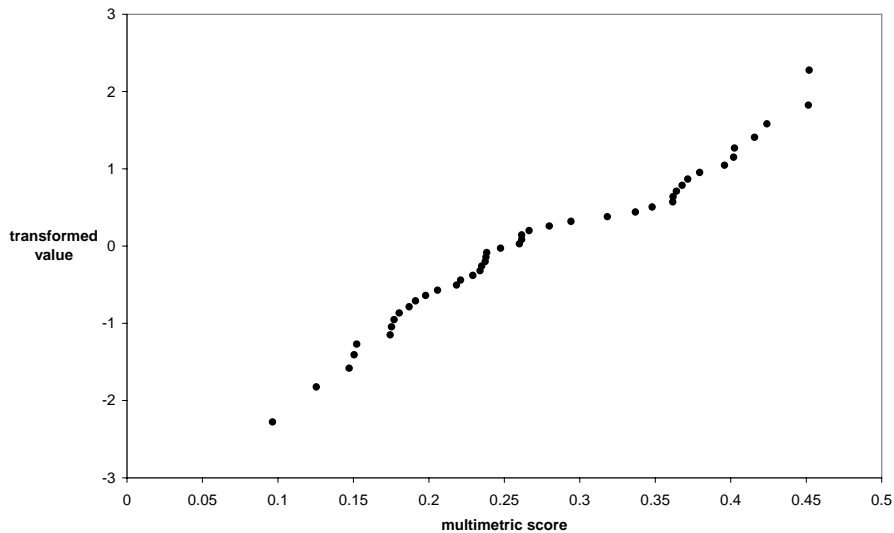


Figure 8.10: Normal score transform of the multimetric scores observed at location 643 in ‘Regge en Dinkel’

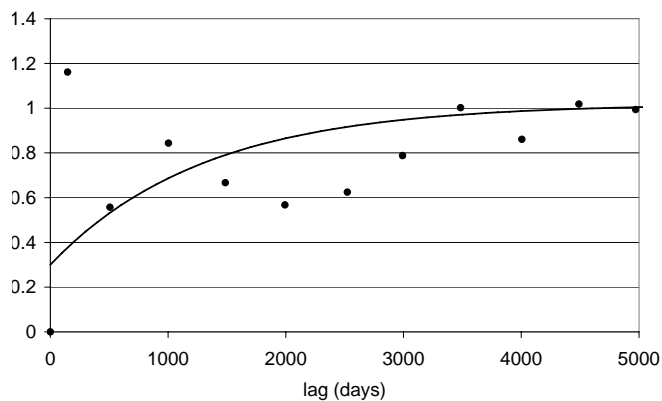


Figure 8.11: Sample semivariogram for the time series observed at location 643 after normal-score transformation, and fitted exponential model.

data and the fitted exponential model:

$$\gamma(h) = 0.3 + 0.72 \cdot \left[1 - e^{-\frac{h}{1300}} \right]. \quad (8.5)$$

Figure 8.12 shows the interpolated series and 95% prediction intervals, obtained by ordinary kriging of indicators after normal score transformation. In back-transformation, linear interpolation is applied between the values in Figure 8.10. For the upper tail extrapolation by a hyperbolic model with $\omega = 1.5$ is applied (Deutsch and Journel, 1998). It is clear that extrapolation results in unrealistic values of the upper limit of the 95% prediction interval.

It is known that the indicators vary following a seasonal pattern. This seasonal trend can be described as a deterministic component in the following random function model:

$$Z(t) = m(t) + R(t), \quad (8.6)$$

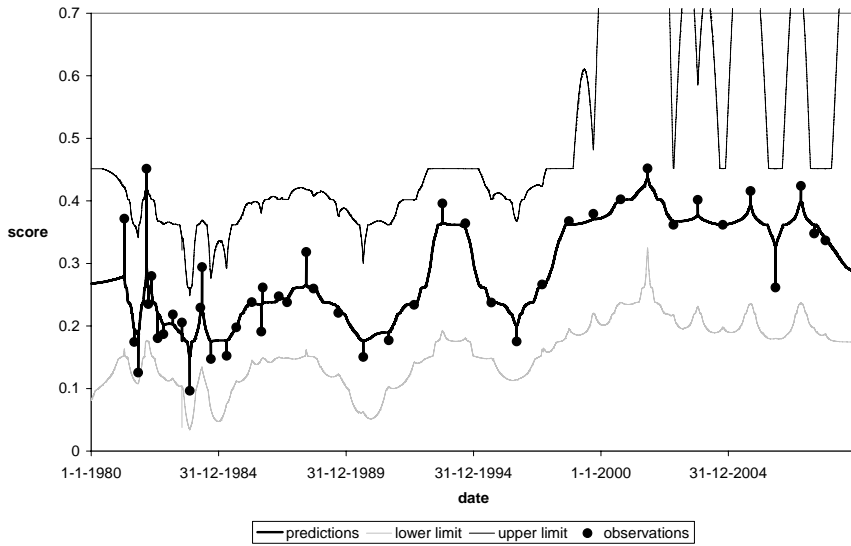


Figure 8.12: Interpolated values for location 643, obtained by ordinary kriging of multimetric scores after normal score transformation, using the exponential semivariogram in Figure 8.11 and Eq. (8.5). Predicted values, and lower and upper limits of the 95% prediction interval, after backtransformation to the original scale.

with t indicating the day number, $Z(t)$ the variable of interest, i.e., indicator of ecological water quality, $m(t)$ the seasonal trend and $R(t)$ the temporally correlated residual component. We fitted the following regression model, describing the seasonal trend in the data (standard errors in parentheses):

$$m(t) = \begin{matrix} 0.2870 & +0.05759 \cdot \sin(\frac{2\pi}{365} \cdot t + 1.311) \\ (0.0164) & (0.0308) & (0.232) \end{matrix}, \quad (8.7)$$

The percentage of variance accounted for is 8.7%. The residuals $R(t)$ are correlated. Figure 8.13 shows the semivariogram describing the temporal correlation structure. The following exponential model has been fitted:

$$\gamma(h) = 0.002 + 0.006 \cdot \left[1 - e^{(-\frac{h}{1400})} \right]. \quad (8.8)$$

Next, simple kriging with varying local means (Sects. 2.1.1, 2.1.2) is applied using the semivariogram given in Eq. (8.8) and Figure 8.13. Figure 8.14 shows the results of interpolation. The seasonal trend clearly dominates the interpolated pattern.

8.1.4 Discussion

This case study shows only a small selection of a large number of interpolation methods that can be applied for interpolation in time. The time series models described in Section 3.1 could not be applied because of the irregular interval lengths. The application of geostatistical methods was limited to series with sufficient data to estimate the model of temporal correlation accurately. The various interpolation methods lead to quite different results, which confirms that choosing an appropriate interpolation method is important. For a discussion on the plausibility of results

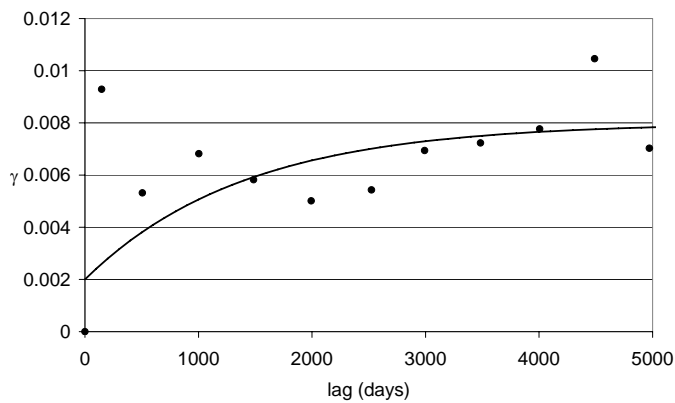


Figure 8.13: Sample semivariogram for the residual term in Eq. (8.6).

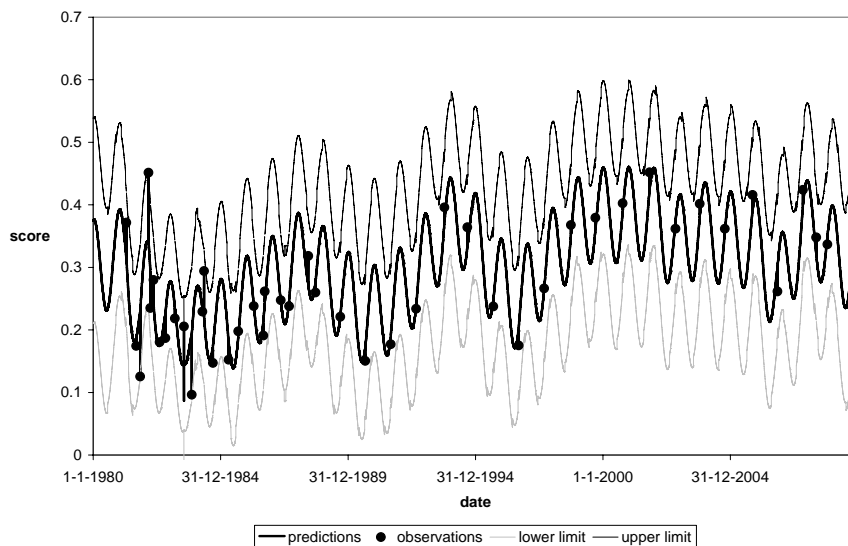


Figure 8.14: Interpolated values for location 643, obtained by simple kriging with a varying mean. The varying mean is described by a regression model of the seasonal variation in multivariate scores. Predicted values, and lower and upper limits of the 95% prediction interval.

more knowledge of the underlying ecological processes is needed. It would be interesting to validate the accuracy of the interpolation by using a set of independent validation data or by cross-validation.

8.2 Spatio-temporal interpolation and aggregation of pesticide concentrations in Dutch surface waters

This section reports on a methodology and case study that are described in much more detail in Heuvelink et al. (2010).

8.2.1 Objective

The Dutch surface waters are routinely sampled and analysed on the concentration of pesticides and other crop protection chemicals. Several hundreds of locations are sampled several times each year and analysed on hundreds of substances. The data are stored in a common database and partially presented to the public in the ‘bestrijdingsmiddelenatlas’ (www.bestrijdingsmiddelenatlas.nl).

The measurements stored in the database are point observations in space and time, whereas the interest of policy and decision makers is in averages over larger areas and longer time periods. Here, we restrict ourselves to the situation where averages are needed for the growing season (March 1 to October 1) for the whole of the Netherlands. Consequently, the point observations need to be aggregated to the larger support. We present a method that uses a simple method for temporal aggregation and a more complex method for spatial aggregation. The methods are briefly described, with reference to relevant sections in previous chapters and illustrated with results for one substance, ‘metribuzin’.

8.2.2 Interpolation and aggregation methods

Temporal aggregation of point measurements of concentrations during the growing season at measurement locations is done as follows. First, monthly averages are computed by unweighted averaging of all measurements within the given month. Next, these monthly averages are averaged for the growing season by taking their (unweighted) arithmetic mean. This two-step procedure ensures that the influence of clustered measurements within a single month dominates less than would be the case with direct averaging of all measurements. A missing value is generated when three or more months have no measurements. The interpolation may be classified as a temporal interpolation method that does not quantify uncertainty and uses no ancillary information (Subsection 3.2.1) and comes close to ‘temporal linear averaging’.

The so-obtained averages for the growing season are log-transformed and next spatially interpolated with regression kriging (Subsection 2.1.2), whereby first the relationship with explanatory variables, such as water surface type, proportion of area under agriculture and the concentration of the substance as predicted by a deterministic pesticide distribution model, is quantified and used in a linear multiple regression model. Next, the residuals of the regression are interpolated using simple kriging. Here, space-time simple kriging was used because growing season averages are available for a sequence of years and can be both spatially and temporally correlated (i.e. between years). The sum of the regression predictions and kriged residuals is back-transformed by taking the antilog.

Spatial aggregation was done by repeated sampling from the conditional probability distribution of the regression residuals using sequential Gaussian simulation. This yields multiple realizations (‘possible realities’) of the residual. These were added to the regression predictions, back-transformed and averaged over the entire Dutch surface water (using the amount of water at each prediction location (i.e. grid cell) as a weight). If this procedure is done for a sufficiently large number of realizations (say 100 or more), then the histogram of the averages approaches the probability distribution of the average concentration for the Dutch surface water and growing

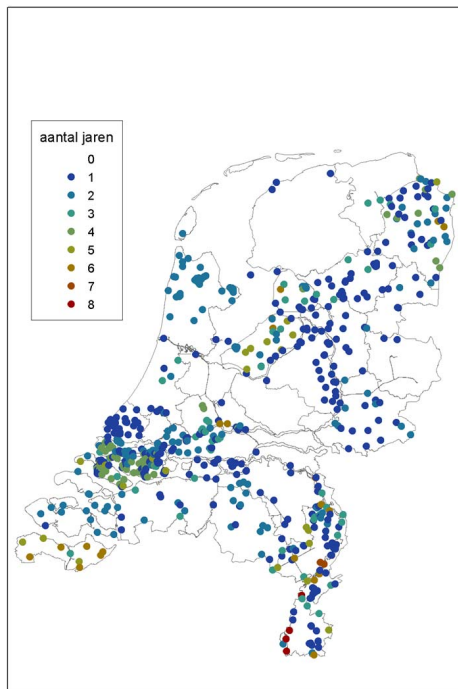


Figure 8.15: Number of years in between 1997 and 2006 for which a growing season average could be computed at measurement locations.

season. Means and lower and upper limits of prediction intervals can be computed from the sample and plotted for a series of years, thus allowing to derive temporal trends in the country and growing season average concentration and quantify their statistical significance.

8.2.3 Results for metribuzin

The space-time interpolation and aggregation was done for metribuzin for the time period 1997 to 2006. Figure 8.15 shows the locations in the Netherlands for which averages of the concentration during the growing season could be computed. It also shows the number of years for which the average was computed. A histogram of all seasonal averages thus computed is presented in Figure 8.16 (left). Note the slightly skewed distribution, even though these are log-transformed seasonal averages. The multiple linear regression that was applied to these data yielded significant correlations with the predictions of the deterministic pesticide distribution model, the year number and several environmental variables (e.g. slope angle, drainage and areal proportion agriculture). The regression explained 37 % of the variation in the log-transformed seasonal average, which was somewhat disappointing. Indeed, the histogram of the regression residuals (Fig 8.16, right) shows a substantial spread, although it is smaller than that of the observations (Figure 8.16, left). Note also that the residuals are more symmetrically distributed.

The space-time experimental semivariogram of the regression residual is given in Figure 8.17 (left). A semivariogram model was fitted to it using a weighted least

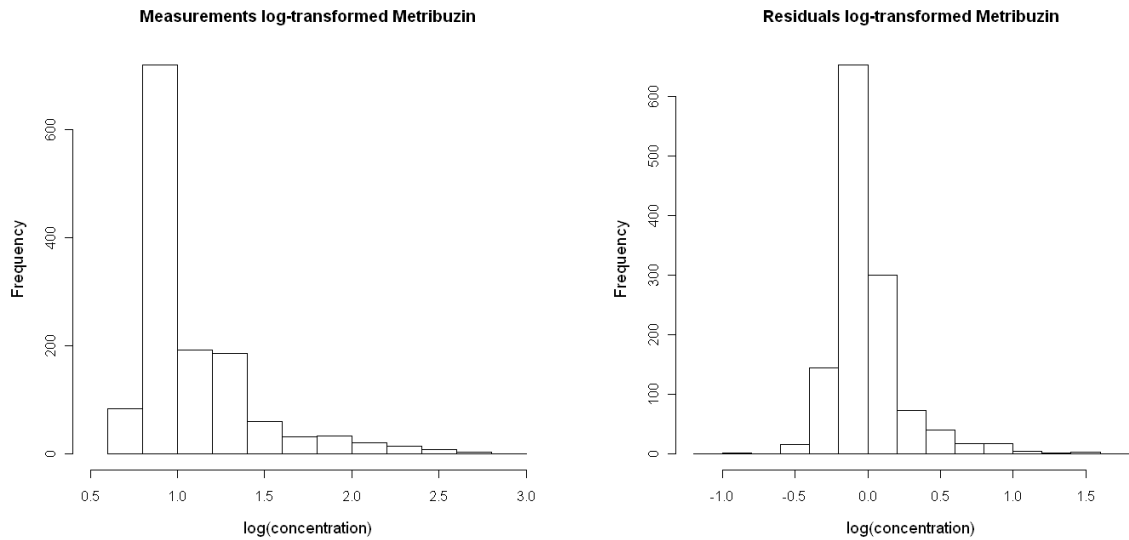


Figure 8.16: Histogram of ‘observed’ seasonal averages of metribuzin (left) and regression residuals (right) during the 1997-2006 period.

squares criterion. The result is given in Figure 8.17 (right). Both spatial and temporal correlation are present, with a spatial range of about 5 km and a temporal range of about 2 years. Regression and space-time interpolation of the residuals was done for all years at a spatial grid resolution of 1 km. Since the type of surface water is also used as an explanatory variable, the results depend on the surface water category too. Here, for illustration purposes, only results for 2006 and surface water category 1 (ditches) are presented. The observed residuals for 2006 are shown in Figure 8.18. Figure 8.19 (left) gives the result of regression only, whereas Figure 8.19 (right) shows the result of the regression kriging. The maps are similar, which indicates that the influence of the kriged residual is small compared to that of the regression. Crisp boundaries are apparent. These are caused by crisp boundaries on the map of agricultural regions in the Netherlands, which was one of the explanatory variables used in the regression. The kriging standard deviation map is given in Figure 8.20. It confirms that interpolation errors are small in the neighbourhood of observation locations and large further away from them. Some spotted areas with smaller standard deviations appear that do not correspond with the locations given in Figure 8.18. These areas correspond with locations where observations were taken in the previous year 2005 (and possibly in 2004).

The result of the spatial aggregation is given in Figure 8.21. Most striking is the large predicted average concentration for 1998, and the smaller peak in 2004. Also, the very narrow width of the confidence interval draws attention. Apparently, a large portion of the variability (and uncertainty) at point locations average out when spatial aggregates are computed. The narrow band indicates that the computed averages are very accurate and that the peaks in 1998 and 2004 are highly significant.

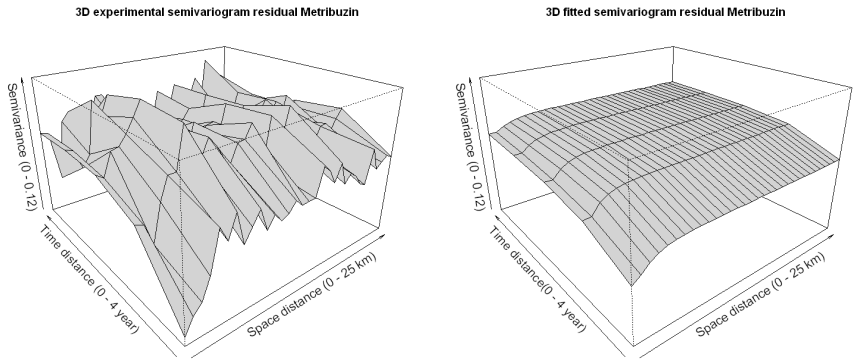


Figure 8.17: Experimental (left) and fitted (right) space-time semivariogram of residual metribuzin.

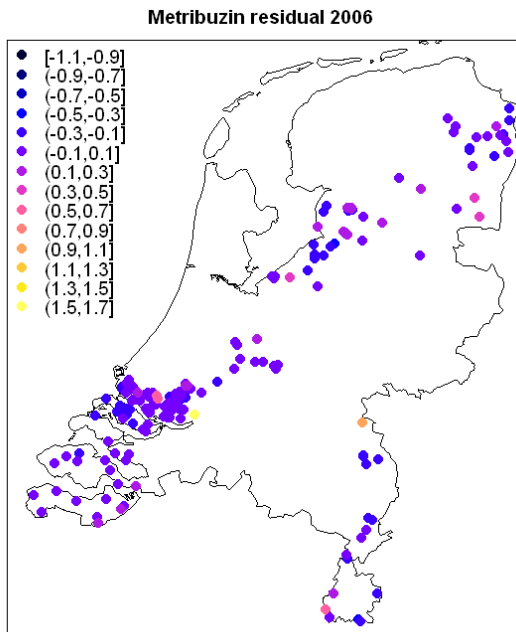


Figure 8.18: Spatial plot of metribuzin residuals in 2006.

Figure 8.21 also shows the result obtained with 'naive' upscaling, in which simply the unweighted average of all growing season concentrations at measurement locations is taken as a representative of the country average. The patterns of both curves are similar, although meaningful differences occur (particularly in years 2004 and 2005) that cannot be explained by uncertainty about the regression kriging result, since the naive result is not contained within the boundaries of the prediction interval.

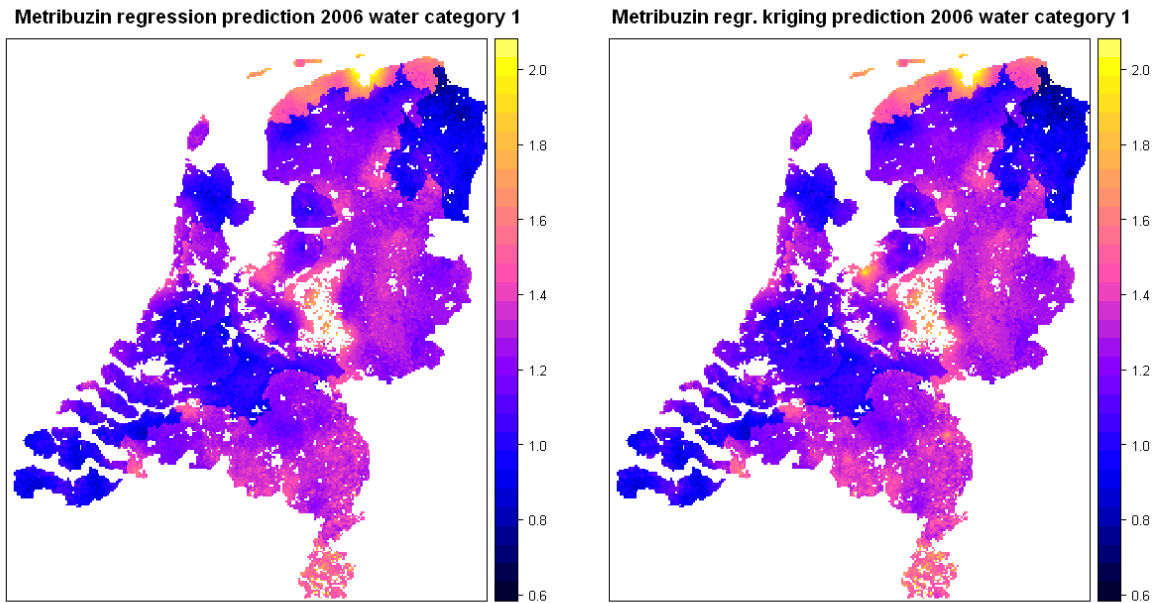


Figure 8.19: Regression predictions (left) and regression kriging predictions (right) of metribuzin for 2006 and watertype category 1.

8.2.4 Discussion

Space-time aggregation of concentrations of pesticides and other crop protection chemicals can be done using space-time regression kriging. Results are meaningfully different from those obtained with 'naive' upscaling, whereby the unweighted average of growing season concentrations at locations is taken. Indeed, 'naive' upscaling may be criticized because it ignores relationships between the dependent and explanatory variables and ignores spatial correlation. Moreover, the locations are not selected with probability sampling and can be highly concentrated in some regions and entirely missing in other regions (e.g. see Figure 8.18).

Space-time regression kriging seems a viable alternative to 'naive' upscaling that has a sound mathematical-statistical basis and can quantify the uncertainty of the interpolated and aggregated values. However, application of the method is cumbersome and requires much expertise. Also, independent validation of the results would be necessary to objectively evaluate the performance of the method. It is important to be aware that regression kriging makes various assumptions, some of which may not be realistic for a given case. For instance, in this case it was assumed that the regression residual is second-order stationary. Assumptions are inevitable when a model-based approach is used, but it is important to critically analyse the assumptions made. In fact, in this study it turned out that several steps in the procedure should be criticized and require modification. For instance, many of the measured concentrations of metribuzin were taken as half the detection limit, in a case where the substance could not be measured in the laboratory. This is all right as long as the detection limit is sufficiently small. However, a substantial part of the

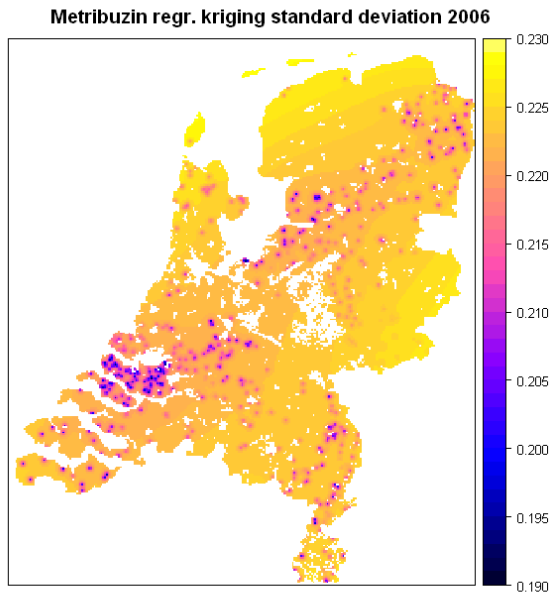


Figure 8.20: Standard deviation of errors in regression kriging predictions of metribuzin for 2006 and watertype category 1.

measurements had very large detection limits. These 'measurements' had a large negative impact on the results of the analysis, which is unrealistic. Also, the data set used to calibrate the regression model did not contain combinations of explanatory variables that were present in the application data set, meaning that extrapolation beyond the ranges of the calibration set were made. Therefore, the results presented here are not the final results and should be treated with caution. Improved results are presented in Heuvelink et al. (2010).

This case study demonstrated that 'naive' upscaling is inappropriate when convenience sampling was employed and resulted in strongly over- or undersampled regions (or regions that are not sampled at all). In such a case, naive upscaling will be biased towards the values at densely measured regions. Since probability sampling was not employed, a model-based alternative (e.g. space-time regression kriging) to interpolation and aggregation was the only viable alternative. However, application of space-time regression kriging is cumbersome and requires specific skills. These problems can partly be resolved by developing a detailed step-by-step procedure and associated software solutions, but expertise and experience remain necessary ingredients to obtain satisfactory results. In particular, expertise and experience are essential for critical analysis of model assumptions and their implications.

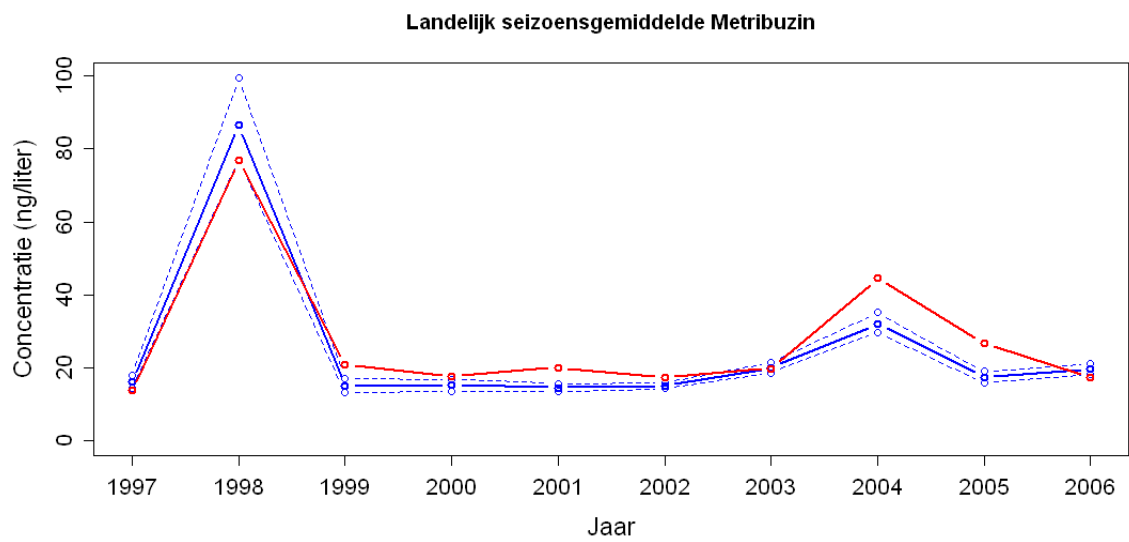


Figure 8.21: Time series of the metribuzin concentration averaged over the growing season and Dutch surface waters. Solid blue line represents the predicted value, dashed blue lines are the boundaries of the 90% prediction interval. Solid red line represents the result obtained with 'naive' upscaling.

Chapter 9

Concluding remarks

9.1 Choosing an interpolation method

In this study a large number of interpolation methods was listed from which environmental scientists can choose. According to the criteria mentioned in Chapter 1 we arranged the methods to interpolation in space, time and space-time. Within each of these three categories we distinguished methods that quantify uncertainty and methods that do not quantify uncertainty. Further distinction was made between methods without use of ancillary information, methods using ancillary information, and methods incorporating process knowledge. This disposition of interpolation methods will help environmental scientists in finding a method that is appropriate to solve their interpolation problem. In the summary table in Chapter 5 the complexity of the methods and the conditions on the size of the data set are indicated. A list of easy-to-use software implementations in Chapter 7 will be of further help in solving the interpolation problem.

Although this disposition can be useful in finding an appropriate interpolation method, more information about the properties of the interpolation methods is needed to support a choice. In particular, more information is needed about the *performance*, i.e. the *accuracy*, of the interpolation methods. Methods are often validated in specific situations, which may not correspond with the problem to be solved. A summary of validation studies and comparative studies such as described by Dubois et al. (2003) and Dubois (2005) will be very helpful. Such a summary will make clear for what situations information on accuracy of interpolation methods is lacking. This can be a starting point for additional validation studies. To this purpose, case studies from the field of environmental scientists at PBL will be very useful. In the next section we discuss validation with respect to the quality of information on accuracy obtained by stochastic interpolation methods.

A valuable next step will be to elaborate the disposition of methods given in this report to a decision tree or decision support system, that guides the environmental scientist to easy-to-use software implementations that are appropriate to solve their interpolation problem. Knowledge of the interpolation problems PBL-workers are facing is crucial in constructing such a tree.

9.2 Information on uncertainty

Statistical information on uncertainty is used in methods from statistical decision theory, e.g., Berger (1985) and Liese and Mieschke (2008), quantitative risk and policy analysis, e.g., Morgan and Henrion (1990), and uncertainty assessment inspired by post-normal science theory (Funtowicz and Ravetz, 1993; Van der Sluijs et al., 2003). Uncertainty in a statistical sense can be defined as the reciprocal of accuracy, while accuracy is defined as the level to which predictions or estimates resemble the true values.

The *overall* or *global* accuracy of results of any interpolation method can be assessed by an independent validation study, in which observations on the ‘field truth’ are preferably selected by probability sampling (Stehman, 1999). *Local* information on accuracy can only be obtained by applying stochastic interpolation methods. The quality of this local information on accuracy depends on model assumptions which cannot always easily be verified.

Perfect information on accuracy (or uncertainty) would imply that the true values are exactly known, which means that there is no need for interpolation. Information on accuracy is based on a limited number of observed differences between true and interpolated values. Thus, information on accuracy or uncertainty is seldom perfect. To assess the usefulness of information on uncertainty in decision making, the quality of this information should be known. If information on *global* accuracy is obtained by validation with an independent probability sample, the quality of this information can easily be quantified. Standard errors of, e.g., map purities or root mean squared errors can be calculated using the inclusion probabilities related to the applied sampling design (De Gruijter et al., 2006). The quality of information on *local* accuracy, such as the kriging variance (Subsection 2.1.1), can be assessed by validation or cross-validation. A possible way is to calculate *reduced residuals* for the n_v validation points (Isaaks and Srivastava, 1989, p. 514):

$$r'(\mathbf{s}_v) = \frac{r(\mathbf{s}_v)}{\hat{\sigma}_K(\mathbf{s}_v)}, \quad (9.1)$$

in which $r(\mathbf{s}_v)$ is the observed difference between the true and the interpolated value at location \mathbf{s}_v , $v = 1 \dots n_v$, and $\hat{\sigma}_K(\mathbf{s}_v)$ is the kriging standard deviation. The standard deviation of $r'(\mathbf{s}_v)$ can be used as a measure of the quality of the kriging variances: if the kriging variances $\hat{\sigma}_K(\mathbf{s}_v)$ are accurate estimates of the true error variances, then the standard deviation of $r'(\mathbf{s}_v)$ should be close to 1.

Studies in which the quality of *local* information on uncertainty has been validated are sparse. We underline the need of such validation studies, the results of which can be used to support a choice from the interpolation methods that quantify uncertainty as described in this report.

9.3 Aggregation and disaggregation

Besides interpolation, aggregation and disaggregation was discussed (Chapter 6). It can be concluded that most interpolation methods can be used in aggregation. Disaggregation is more delicate than aggregation, since assumptions need to be made about the spatial or temporal variation at the smaller scale. Once these assumptions

have been made, many of the interpolation algorithms described in this report can be used for disaggregation. A practical problem is that there is to our knowledge no easy-to-use software for disaggregation. A lot of work on disaggregation techniques has been done in the field of climate research. It would be interesting to extrapolate these techniques to other fields of environmental research.

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