

Aggregation of ecological indicators for mapping aquatic nature quality

Overview of existing methods and case studies

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Abstract

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Indicators for aquatic nature quality are calculated using ecological monitoring data from individual sampling stations. For reporting purposes, these results need to be aggregated and scaled up to higher levels (catchment area, country). This report provides an overview of different existing spatial aggregation methods for this purpose, including an evaluation of their suitability for aquatic ecological indicators. So-called 'model-based' methods, consisting of some sort of 'kriging' step followed by calculation of the arithmetic mean, appeared to be the most appropriate. Application of these methods to multimetric indicators of aquatic macroinvertebrates in two Dutch subcatchment areas confirmed their suitability. However, the methods that were used were based on aggregation (using kriging) over Euclidian (straight), distances. It is recommended to conduct further research on the suitability of interpolation through stream networks, i.e., through the waterways themselves.

Key words: ecological indicators, aquatic nature values, spatial aggregation, upscaling, spatial correlation, surface water, (sub) catchment areas, stream networks

Referaat

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Indicatoren van de aquatische natuurkwaliteit worden berekend op basis van ecologische monitoringsgegevens van individuele locaties. Deze resultaten dienen t.b.v. hun rapportage geaggregeerd en opgeschaald te worden naar een hoger niveau (stroomgebied, landelijk). Dit rapport geeft een overzicht van verschillende bestaande ruimtelijke aggregatiemethoden voor dit doel, inclusief een beoordeling van hun geschiktheid voor aquatische ecologische indicatoren. Het meest geschikt blijken zogenaamde modelgebaseerde methoden, bestaande uit een interpolatie door een nader te kiezen soort 'kriging' gevolgd door berekening van het rekenkundig gemiddelde. Toepassing van deze methoden op multimetrische indicatoren van macrofauna uit twee Nederlandse deelstroomgebieden bevestigde hun geschiktheid. De gebruikte methoden waren echter gebaseerd op aggregatie (met kriging) over 'Euclidische' (rechte) afstanden. Aanbevolen wordt om nog nader onderzoek te doen naar de geschiktheid van interpolatie door stroomnetwerken, d.w.z. via de loop van de waterwegen zelf.

Trefwoorden: ecologische indicatoren, aquatische natuurwaarden, ruimtelijke aggregatie, opschalen, ruimtelijke correlatie, oppervlaktewater, (deel) stroomgebieden, stroomnetwerken

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Woord vooraf

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Inhoud

Woord vooraf	5
Summary	9
Samenvatting	11
1 Introduction	13
1.1 Background	13
1.2 Aggregation & upscaling	13
1.3 Scaling of processes & indicators	14
1.4 Objectives	14
1.5 How to read this report?	14
2 Study design & methods	15
2.1 Literature survey	15
2.2 Criteria for evaluation	15
2.3 Available data & indicators	15
2.4 Case studies	17
3 Results	19
3.1 Literature survey	19
3.2 Aggregation methods	19
3.3 Selection of appropriate methods	21
3.4 Case studies	24
3.4.1 Introduction	24
3.4.2 Sub-catchment area Rhine-East	25
3.4.3 Sub-catchment area Rhine-West	28
4 Discussion	31
5 Conclusions & recommendations	33
References	35
Annex 1	37

Summary

The Netherlands Environmental Assessment Agency (PBL) is developing a set of indicators for aquatic nature quality of surface waters, i.e., the occurrence of rare species and so-called 'nature target species'. The results of these indicators need to be aggregated and to be scaled up to the level that is important to Dutch policy makers and the general public, i.e., the level of catchment areas and the national level. This study is the first step towards such aggregation and upscaling methods.

The aim of the present study was (1) to provide an overview and classification of the different methods that exist for the aggregation of local information on aquatic nature quality to the regional (catchment) and national level, (2) to provide (ecological) criteria for spatial aggregation and upscaling, (3) to evaluate existing methods based on these criteria and on their particular advantages and disadvantages, and (4) to recommend on the most suitable methods to use for aggregation and upscaling of indicators for aquatic nature quality calculated using existing monitoring data.

The study consists of two parts, (1) a literature survey of existing methods for aggregating and upscaling of aquatic ecological indicators and (2) case studies for trial and demonstration of selected methods.

Based on the literature survey a classification of possible methods was made. The methods were evaluated using criteria such as suitability for hydrological systems, ecological realism, complexity/simplicity of the method, data requirements, necessary software and computer capacity and possibilities to quantify uncertainty. The evaluation showed that an approach consisting of (1) interpolation by kriging (or a related method) followed by (2) arithmetic averaging was the best choice. The reasons for this were (a) that it is required to assess the uncertainty of the aggregated values and (b) that a 'design-based' method was not possible because aquatic monitoring stations in The Netherlands are not selected by probability sampling. This left 'model-based' aggregation methods as the only solution and most of these use some sort of kriging. An additional advantage of interpolation methods such as kriging is that hot spot locations and spatial patterns are also identified. This facilitates taking appropriate policy and management measures to improve the nature quality of surface waters.

Recently, multimetric indicators (MMIs) for nature quality of aquatic macro invertebrate assemblages were developed in commission of PBL. Two selections were used in the current study to try and demonstrate spatial aggregation methods: polder ditch data from the area between the island of Texel and the North Sea Canal in the Rhine-West sub-catchment and data on stream macro fauna from the eastern Rhine-East sub-catchment. In both case studies, analysis of the spatial variation based on Euclidian (straight) distances showed a clear spatial correlation. This confirmed that geostatistical methods based on Euclidian distances are appropriate in these cases.

The assessment of the spatial correlation of aquatic nature quality data or indices should be further investigated using different methods that are based on hydrological distance between sampling stations such as stream network kriging (with and without connectivity and/or stream hierarchy). The results of these methods for indicators of different types of aquatic taxonomical groups should be compared and the most appropriate method for each

taxonomical group, i.e., that best describe the spatial distribution and or correlation for each indicator, should be selected.

On the basis of the selected methods a decision tree for the appropriate aggregation steps and methods can be established. This tree also needs to include the order in which different aggregations steps need to be done (aggregation in time, between taxonomical groups, between different types of surface waters, and spatial aggregation).

Samenvatting

Het Planbureau voor de Leefomgeving (PBL) ontwikkelt een set indicatoren voor de beoordeling van de aquatische natuurkwaliteit van oppervlaktewateren, gebaseerd op het voorkomen van zeldzame soorten en natuurdoelsoorten. De resultaten van deze indicatoren dienen uiteindelijk geaggregeerd en opgeschaald te worden tot het niveau dat van belang is voor beleidsmakers en het publiek, het niveau van stroomgebied of heel Nederland. Deze studie is een eerste stap in de richting van een dergelijke aggregatie en opschaling.

Het doel van de studie was (1) om een overzicht te genereren van de verschillende bestaande methoden voor het aggregeren van lokale informatie betreffende de aquatische natuurkwaliteit tot op het niveau van stroomgebied en het nationale niveau, (2) om (ecologische) criteria op te stellen voor ruimtelijke aggregatie en opschaling, (3) om bestaande methoden te evalueren op basis van deze criteria en de specifieke voor- en nadelen van de methoden en (4) om aanbevelingen te doen voor de meest geschikte methoden voor het aggregeren en opschalen van indicatoren voor de aquatische natuurkwaliteit, gebruikmakend van bestaande monitoringsgegevens.

De studie bestond uit twee delen: (1) een literatuurstudie naar bestaande methoden voor het aggregeren en opschalen van aquatische ecologische indicatoren en (2) case studies om de geselecteerde methoden uit te proberen en te demonstreren.

Op basis van de literatuurstudie werd een classificatie van de mogelijke methoden opgesteld. De methoden werden geëvalueerd met criteria zoals hun geschiktheid voor watersystemen, ecologisch realisme, complexiteit/eenvoud van de methode, benodigde gegevens, benodigde software en computercapaciteit en de mogelijkheden om onzekerheid te kwantificeren. De evaluatie wees uit dat een benadering door middel van (1) interpolatie met 'kriging' (of een verwante methode) gevolgd door (2) berekening van het meetkundig gemiddelde de beste methode was. De redenen hiervoor waren (a) dat er behoefte is aan het bepalen van de onzekerheid van geaggregeerde waarden en (b) dat een ontwerpgebaseerde methode niet mogelijk is omdat in Nederland locaties voor aquatische monitoring niet worden geselecteerd met kanssteekproeven. Hierdoor bleven modelgebaseerde aggregatiemethoden over als de enige mogelijkheid en de meeste van deze methoden maken gebruik van een enige soort van 'kriging'. Een bijkomend voordeel van interpolatiemethoden zoals kriging is dat hiermee 'hot spot' locaties en ruimtelijke patronen worden opgespoord. Dit vergemakkelijkt het nemen van de juiste beleidsbesluiten en maatregelen om de natuurkwaliteit van oppervlaktewateren te verbeteren.

Recent werden in opdracht van het PBL multimetrische indicatoren ontwikkeld voor de natuurkwaliteit van aquatische macrofaunagroepen. Twee datasets uit dit werk werden in de huidige studie gebruikt om enkele geselecteerde ruimtelijke aggregatiemethoden uit te proberen en te demonstreren: gegevens van poldersloten uit het gebied tussen Texel en het Noordzeekanaal uit het Rijn-West-deelstroomgebied en gegevens van macrofauna in beken uit het oostelijke deel van het Rijn-Oost-deelstroomgebied. In beide casussen werd door analyse van de ruimtelijke variatie op basis van Euclidische (rechte) afstanden een duidelijke ruimtelijke correlatie vastgesteld. Dit bevestigde dat geostatistische methoden op basis van Euclidische afstanden geschikt waren voor deze casussen.

De geschiktheid van verschillende methoden ter bepaling van de ruimtelijke correlatie van aquatische natuurwaarden en -indices gebaseerd op de hydrologische afstand tussen monitoringslocaties, zoals stroomnetwerk kriging, dient nader onderzocht te worden (met en zonder connectiviteit en/of stroomhiërarchie). De resultaten van deze methoden voor indicatoren van verschillende aquatische taxonomische groepen dienen onderling vergeleken te worden, zodat voor iedere taxonomische groep de meest geschikte methode, dat wil zeggen de methode die de ruimtelijk verspreiding en correlatie het best beschrijft, geselecteerd kunnen worden.

Op basis van de geselecteerde methoden kan een beslisboom voor het kiezen van de meest geschikte aggregatiestappen en -methoden worden vervaardigd. Deze beslisboom dient ook de volgorde te bevatten waarin de verschillende aggregatiestappen plaats vinden (aggregatie in de tijd, tussen taxonomische groepen, tussen verschillende soorten oppervlaktewater en ruimtelijke aggregatie).

1 Introduction

1.1 Background

In order to evaluate the efficacy of policies and to inform policy makers and the general public about new developments and trends the Netherlands Environmental Assessment Agency (PBL) publishes a yearly report on the state of natural areas and landscapes in The Netherlands, the 'Nature Balance'. The Nature Balance summarises data from studies and monitoring exercises conducted by a wide variety of different Dutch institutions and presents these in a comprehensive way, easily understandable to lay-people.

The PBL is currently developing a set of indicators for aquatic nature quality of surface waters, i.e., the occurrence of rare species and so called 'nature target species'. These indicators are based on the routine ecological data gathered by Dutch water boards. Nature target species are species that are characteristic of 'nature target types' that represent different natural habitats (Bal *et al.*, 2001). The occurrence of these species can be used to evaluate the effectiveness of nature conservation on the spot. The indicators provide information on the status of different taxonomical groups (macrophytes, aquatic invertebrates and fish) and express nature quality on a scale from 0 to 1. In 2009 indicators were developed for aquatic macroinvertebrates in two types of Dutch surface waters, polder ditches and streams (Verdonschot & Verdonschot, 2010).

The results of these indicators need to be aggregated and to be scaled up to the level that is important to Dutch policy makers and the general public, i.e., the level of catchment areas and the national level. However, a method for this purpose has not yet been established. This study was conducted as a first step in order to fill this gap.

1.2 Aggregation & upscaling

In everyday language the term 'scale' is used to refer to two different things, the spatial detail such as the cartographic scale (also 'grain', 'support') or the spatial extent of geographical coverage, e.g., in case of a 'large scale' phenomenon (Atkinson & Tate, 2000). The grain or support is the largest area (or time interval) for which the property of interest is considered homogeneous (Bierkens *et al.*, 2000). Some authors opt to use the first type of definition (e.g., Pebesma & Heuvelink, 1999; Bierkens *et al.*, 2000), others explicitly the second (e.g., Atkinson & Tate, 2000).

In this report we use the term scale for the size of the grain/support. Hence, upscaling is the process of increasing the size of the support (Bierkens *et al.*, 2000). This can be done both in space (increasing the area of evaluation) and in time (increasing the time interval). In landscape ecology 'upscaling' is most often used to describe the translation or extrapolation of information from local scales to landscape and regional scales (King, 1991). The term aggregation is more or less synonymous to upscaling (Bierkens *et al.*, 2000), and we will use the two words interchangeably in this report.

In order to scale up, local information must be aggregated to a higher scale. There are many different methods to do this (see Chapter 3). Aggregation requires integration of the finer-grained heterogeneity of the lower scale and how to do this is the biggest challenge of scaling up (King, 1991). The opposite processes of aggregation and upscaling are disaggregation and downscaling respectively. This requires a different approach yet again (Bierkens *et al.*, 2000).

1.3 Scaling of processes & indicators

Scale is a crucial concept for understanding and describing patterns and processes in nature. At different scales, different ecological patterns and processes are important and in ecology much effort has been devoted to the study of scaling ecological and environmental processes and phenomena (see Van Gardingen *et al.*, 1997; Turner *et al.*, 2001; Storch *et al.*, 2007). Well known examples include species-area relationships in biodiversity studies and scaling up photosynthesis from the level of leaves to canopies and further up to the forest level. Aggregation/upscaling of processes often involves the use of ecological models to describe the process at different scales and aggregation is done to reduce model complexity (Rastetter *et al.*, 1992). And when aggregating, for example from point support to block (area) support, the order in which the aggregation and modelling steps take place is important, particularly for non-linear processes and models (Pebesma & Heuvelink, 1999).

However, upscaling of processes needs to be distinguished from upscaling of data or indicators (Stein *et al.*, 2001). For the first topic it has to be identified how processes interact at different scales, whereas for the second issue one only has to find useful ways of aggregation/upscaling parameter values. This is coined “post-processing” by Van Beurden & Douven (1999), as opposed to pre-processing (spatial data modelling) and environmental modelling. One of the possible aims of post-processing is “to produce a simple aggregated presentation to decision and policy makers” (Van Beurden & Douven, 1999). This is also the subject of the present study.

1.4 Objectives

The aim of the present study was:

1. to provide an overview and classification of the different methods that exist for the aggregation of local information on aquatic nature quality to the regional (catchment) and national level,
2. to provide (ecological) criteria for spatial aggregation and upscaling,
3. to evaluate existing methods based on these criteria and on their particular advantages and disadvantages, and
4. to recommend on the most suitable methods to use for aggregation and upscaling of indicators of aquatic nature quality that are calculated using existing monitoring data.

The focus of the study was mostly on spatial aggregation and upscaling, i.e., not on the aggregation of data and indicators in time and not on the aggregation of different taxonomical groups and different types of surface water although these issues are also briefly discussed.

1.5 How to read this report?

After the general introduction in this Chapter 1, Chapter 2 describes the study design and methods: (1) the data that are available to assess aquatic nature quality in The Netherlands, (2) the way this information is used to calculate recently developed indicators based on a metric approach, and (3) the way our study was conducted, with a literature survey and a limited case study. Chapter 2 also contains the criteria that were applied for the evaluation of the different existing aggregation/upscaling methods. The results of the study are given in Chapter 3 gives a short description of various methods for aggregation and upscaling of aquatic ecological data as well as an overview of the possibilities and limitations of these methods. The second part of Chapter 3 deals with two case studies on the interpolation of Multimetric Indicator (MMI) values for aquatic macroinvertebrates in two Dutch sub-catchment areas. Chapter 4 provides a general discussion of our findings and Chapter 5, finally, summarises the most important conclusions and recommendations of the study.

2 Study design & methods

The study consists of two parts, a literature survey of existing methods for aggregating and upscaling of aquatic ecological indicators and case studies for trial and demonstration of selected methods.

2.1 Literature survey

We screened the scientific literature for publications on the aggregation and upscaling of spatially distributed ecological data. The survey was performed using the on-line search facilities of Scopus[®] and ISI Web of KnowledgeSM, available through the library of Wageningen UR, and the Wageningen library catalogue. The search included key words such as 'upscaling' '(spatial) aggregation', 'catchment', 'watershed', 'map', 'aquatic', 'water', 'nature', 'ecology'. A second more targeted search was conducted on the aggregation of data from 'stream networks' and in 'catchments'. The first source for the study was the peer-reviewed scientific literature. In addition to this, the internet was quickly searched for any existing Dutch grey literature on the topic (reports etc.).

2.2 Criteria for evaluation

Based on the literature research and our own experience we deduced a classification of the various existing methods for aggregating and upscaling of aquatic ecological indicators for surface water nature quality. For each class of methods the possibilities and limitations are briefly described. The methods were further evaluated using the following criteria:

1. *Suitability for hydrological systems*. For example, it might be relevant to account for the spatial configuration, connectivity, hierarchy and directionality of sites in a stream network.
2. *Ecological realism* (use of ecological knowledge). Estimates might be improved by incorporating ecological knowledge in the procedure of spatial aggregation.
3. *Complexity/simplicity*. We strive for scientifically sound methods that are preferably easy to apply.
4. *Data requirements*. Some methods, for example, require a certain data configuration or a minimum number of data.
5. *Necessary software and computer capacity*. More complicated aggregation techniques may require special software and for extended analysis in GIS extra calculation capacity may be needed.
6. *Possibilities to quantify uncertainty*. This information is of interest in estimating the differences in status between catchment areas, in estimating temporal trends in ecological surface water quality, and in testing against standards.

2.3 Available data & indicators

Information on the chemical and ecological status of surface waters in The Netherlands is routinely gathered by the 26 water boards, the regional Dutch water authorities that are responsible for the management of waterways (including barriers and adjacent roads), water quantity and water quality. Each water board has its own particular monitoring network. In the past, different water boards even used different methods, but the implementation of the European Water Framework Directive (WFD) in 2000 has led to more harmonisation of the

methods and reporting (Torenbeek & Pelsma, 2008). Most monitoring data on ecological quality of surface waters, collected by the water boards, are gathered in a single national database, the so-called 'Limnodata Neerlandica' (www.limnodata.nl). This database contains data on biota (phytoplankton, diatoms, zooplankton, macrophytes and aquatic invertebrates). Fish data are collected in the 'Piscaria' database, which is also accessible through the Limnodata website.

In addition to establishing the ecological status of Dutch surface waters for the WFD, the ecological information in these databases may also be used to assess the nature quality of surface waters. However, many of the target species for nature conservation policy are by definition very rare and seldom found during routine ecological monitoring of freshwater bodies. So although these species represent nature values, their low numbers do not allow their use as indicators on a regional or national scale. This discrepancy has led to a new approach for the development of suitable indicators, the use of proxies (Verdonschot & Verdonschot, 2010). Proxies for target species are indicators based on sufficiently abundant species that are characteristic, functionally relevant and/or sensitive to environmental stress and thus may represent the rarer species. Without collecting the target species, the aquatic nature value may be estimated using such proxies once they have been established.

Verdonschot & Verdonschot (2010) recently developed proxies for the nature quality of aquatic macroinvertebrates in Dutch polder ditches and in streams. They evaluated assemblages of species along gradients of nature quality (nutrients in the case of ditches, general state of degradation in streams) and determined which indicators best described these gradients. On the basis of the analysis two proxies were established, each based on the indicators that correlated most: the first multimetric index (MMI) for ditches and the MMI2 for streams. Each proxy includes four types of metrics: metrics for sensitivity/tolerance, species composition, diversity/richness and functional traits (Table 1). MMI values are expressed on a scale from 0 to 1.

Table 1. Individual metrics that make up the multimetric indices (MMIs) for the nature quality of polder ditches and streams in The Netherlands (from Verdonschot & Verdonschot, 2010).

Polder ditches (MMI)			Streams (MMI2)		
Metric	Type of metric		Metric	Type of metric	
	Contribution ¹	Class ²		Contribution ¹	Class ²
Proportion of taxa preferring fresh water	+	ST	Proportion of oligosaprobic taxa (2 sources)	-	ST
Proportion of taxa preferring a eutrophic habitat	-	ST	Number of Diptera taxa (without Chironomidae)	-	COM
Proportion of limnophilic taxa	-	ST	Proportion of individuals D+DH+H ³	+	FUN
Number of Gastropod families	-	COM	Proportion of taxa preferring a macrophyte habitat	+	FUN
Proportion of individuals preferring silt	-	FUN	Proportion of Trichopteran taxa	-	COM
Number of Trichopteran families	+	DIV	Number of Hirudinean taxa	+	DIV
Number of Gastropod individuals	-	COM	Number of Heteropteran taxa	+	DIV
Proportion of individuals preferring sediment	+	FUN			
Number of detritivorous taxa	+	FUN			
Proportion of Hirudinean genera	-	COM			
Number of Heteropteran genera	+	DIV			

¹ +/- positive or negative contribution to the multimetric indicator

² ST metric of sensitivity/tolerance

COM metric of composition

FUN metric of functional properties

DIV metric of richness/diversity

³ D= detritivore, DH=detriti-herbivore, H= herbivore

The data used by Verdonschot & Verdonschot (2010) included 223 macroinvertebrate samples in ditches and 453 in streams taken over 20-year period. The original data were first selected and used by Nijboer *et al.* (2003) and Verdonschot *et al.* (2004) in order to establish typologies for Dutch polder ditches and Dutch streams. These days they have become part of the Limnodata Neerlandica. At the end of their exercise Verdonschot & Verdonschot (2010) calculated and mapped the values of the MMI1 and MMI2 indices for ditches and streams respectively. The same data were also made available for use in the present study.

2.4 Case studies

The sampling locations used by Verdonschot & Verdonschot (2010) are not evenly distributed over all areas in The Netherlands. Freshwater polder ditches are characteristic of the lower areas in the west and north of the country whereas streams are mainly found on the grounds in the east and south. Because of the varying taxonomic quality of identifications and differences in sampling effort, not all water boards are represented in the dataset. As a consequence it contains gaps for certain geographical areas.

For this study we therefore selected two areas from the macroinvertebrate data of Verdonschot & Verdonschot (2010) for trial and demonstration purposes: polder ditch data from the area between the island of Texel and the North Sea Canal in the Rhine-West sub-catchment and data on stream macrofauna from the eastern Rhine-East sub-catchment.

A GIS layer with surface waters was extracted from the digital TOP10vector topographical map of The Netherlands. The files with the selected data were prepared using the ArcGIS 9.3.1 program. Surface waters in the database are defined either as lines (streams and ditches narrower than 6 m) or as polygons (lakes, streams, rivers and ditches broader than 6 m). From both layers, the waters situated in the Rhine-East and Rhine-West (excluding Texel and the Rhine-West area south of the North Sea Canal) sub-catchments were selected. Both layers were converted to a raster with an output cell size of 20×20 m using the 'Polygon/Polyline to Raster' tool from the ArcGIS 'Spatial Analyst' toolbox. Then, raster files were converted to points using the 'Raster to Point' tool. Coordinates and sub-catchment names were assigned to each point. For coordinates the 'Calculate Geometry' dialog box was used. Texel and the areas south of the North Sea Canal were removed from the Rhine-West area. In order to assign sub-catchments to each point, the layer with the allocated Rhine-East and Rhine-West areas sub-catchments was intersected (Analysis Toolbox) with each of the point layers containing the topography of the surface waters.

3 Results

3.1 Literature survey

The first more general literature search for aggregation and upscaling methods for ecological indicators yielded more than 40 papers and five books. These publications were all screened. The majority of these publications originated in the geosciences and in terrestrial environmental sciences such as soil science and landscape ecology. The publications are testimony of the progress made over the past 20 years in these fields and the number of possible methods to aggregate landscape data over surface areas seems sheer endless (e.g., King, 1991; Rastetter *et al.*, 1992; Heuvelink & Pebesma, 1999; Van Beurden & Douven, 1999; Atkinson & Tate, 2000; Stein *et al.*, 2001; Vermaat *et al.*, 2005; Vereecken *et al.*, 2007).

Hardly any of the publications found explicitly dealt with the freshwater environment. Freshwater bodies are a special case for aggregation and upscaling because many of them are line objects such as ditches and streams or isolated entities as in the case of ponds and lakes. Traditional aggregation and upscaling methods over surfaces on the bases of Euclidian (straight) distances may therefore be less readily applicable. Instead, one may have to deal with aggregation over 'hydrological' distances, i.e., through the waterways themselves. The additional search on aggregation in stream networks and within catchment areas came up with some ten additional papers on this topic that proved to be very useful for our overview and classification (see Section 3.2).

3.2 Aggregation methods

In this section we present the results of the literature search on methods for spatial aggregation of data on ecological quality of surface waters. Bierkens *et al.* (2000) provided a classification of upscaling methods for environmental research and criteria for selection of the most appropriate methods. We used this classification to make an overview of possible aggregation methods for the purpose of this study (see Chapter 1) and added descriptions and examples from our literature survey.

A scientific description of the selected methods with the appropriate references is given in Annex 1. Here we summarize the most important characteristics of the methods, i.e., the characteristics that are most important for the final choice of a specific method for a specific indicator.

A first important distinction is the one between aggregation/interpolation methods that allow the user to quantify the uncertainty. This choice depends on the requirements of the end user of the methods. When aggregate indicator values for areas need to be compared to the values for other areas, or when indicator values are compared to fixed values such as environmental quality criteria for surface waters, it is wise to assess the uncertainty of the interpolated and aggregated indicator values in order to analyse if any observed differences are statistically significant or not. Methods that do not quantify uncertainty include relatively simple and well-known interpolation techniques used in GIS such as Inverse Distance Weighting (IDW) and related techniques (see Annex 1, bullet 2). On the other hand, when uncertainty needs to be quantified one has to apply either so-called 'design-based' methods or 'model-based' methods, depending on the type of data.

Design-based methods (Annex 1, bullet 1.a) can only be used when the data points are chosen randomly. For aquatic sampling this would mean that all the biological sampling stations in a particular database must have been selected by a random (statistical) sampling procedure. Several random sampling designs can be applied. The aggregate values for larger areas can be calculated as the average value for all sampling stations, accounting for the applied random selection method. But when the sampling stations are not randomly selected, unbiased statistical estimates based on the sampling design are not possible and the only solution left for interpolation and aggregation consists of model-based methods. An example of a design-based environmental monitoring strategy, including ecological water quality, is the Environmental Monitoring and Assessment Program (EMAP) (US-EPA, 2002). For the selection of monitoring stations in this program, an intricate random selection method is applied.

Model-based methods are used when sampling stations are selected purposively. In that case unbiased estimates based on the sampling design only are not possible. To interpolate and aggregate the data, one needs a model that describes the spatial correlation structure of the data.

Model-based methods often include some sort of 'kriging'. Kriging refers to interpolation methods that belong to the family of linear least squares estimation algorithms, also used in familiar statistical techniques such as analysis of variance (ANOVA) and linear regression. In kriging a so-called semivariogram is used that shows the distance between sampling points (or 'lag' distance) on the x-axis and the measure of spatial dissimilarity (called ' γ ') on the y-axis. Usually spatial dissimilarity between points increases with increasing lag distance between points. This can be modelled by, for instance, an exponential, Gaussian or spherical curve. The mathematic formulas for the semivariogram and examples from the case studies are provided in Chapter 4.

Several kriging methods are available to be used for aggregation of aquatic nature indicators (see Annex 1, bullets 1.b.i-1.b.vi). The most appropriate model of spatial correlation can be identified by fitting several models and determining which model best describes the spatial correlation. But one may also look at the expected type of spatial interdependency. One important distinction between the different model-based methods described in Annex 1 is that between methods that apply models based on 'straight line distance' (also called 'Euclidean' distance) and models based on hydrological distance. The difference is illustrated in Figure 1. The straight line distance is the distance as the crow flies. The hydrological distance is the distance between two points in a stream network as measured through the streams themselves. Two points may be separated by a straight line distance of, say, 100 m, but by 200 m hydrologically when the stream meanders strongly.

Kriging methods based on symmetric and asymmetric hydrological distance have been developed recently for interpolation of variables on chemical water quality (Cressie *et al.*, 2006; Peterson & Urquhart, 2006; Peterson *et al.*, 2006; Ver Hoef *et al.*, 2006; Peterson *et al.*, 2007). These methods were applied to locate environmentally impaired stream segments, within the framework of the Clean Water Act in the USA.

Besides methods based on hydrological distance, several other kriging methods for interpolation within stream networks were recently developed. For a brief overview we refer to Annex 1. In Section 3.3 we justify why model-based methods must be used for the aggregation of the aquatic nature indicators considered here. Because the application of kriging methods for stream networks is rather complicated (see Ver Hoef *et al.*, 2006) and standard software is not available, we decided to apply conventional kriging methods based on straight line distance only during this pilot study.

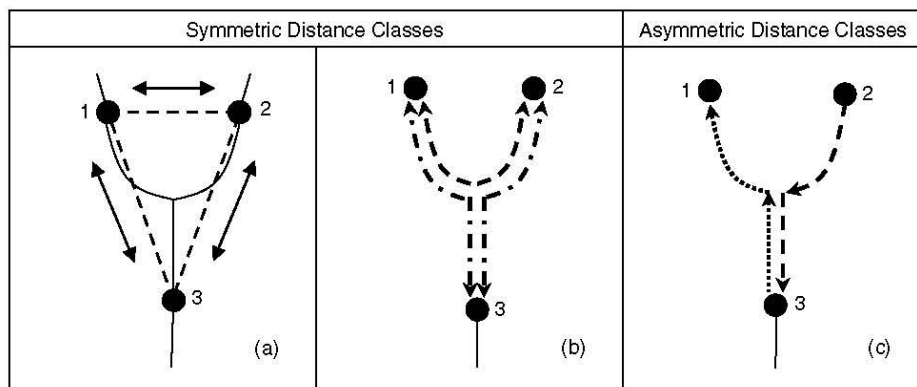


Figure 1 a) Straight line distance between observation points (Euclidian distance), b) Symmetric hydrologic distance, and c) Asymmetric hydrologic distance. The stream network is represented by a solid line, while distance measurements are represented with dotted lines. Sites 1, 2, and 3 are all neighbours to one another when straight line distance and symmetric hydrologic distance measures are used. Asymmetric distance classes (c) include upstream and downstream asymmetric hydrologic distance. Sites 1 and 2 are neighbours to site 3, but not to each other. From: Peterson *et al.*, 2006.

3.3 Selection of appropriate methods

A detailed evaluation of the different methods described in Section 3.2 and Annex 1 according to the criteria from Section 2.2 is shown in Table 2. Here we summarise the most important findings. We applied the decision support system given by Bierkens *et al.* (2000) to choose an appropriate method of spatial aggregation. In this procedure the following questions were answered:

- *Is there a model involved?* (Bierkens *et al.*, 2000, p. 20, Figure 11) The scores to be aggregated are not used as input of a model in a later stage, so the answer is: no. The scores are determined from observations on plant and fauna species. Aggregation is realised by estimating a spatial average of the scores.
- *Is the information exhaustive?* (Bierkens *et al.*, 2000, p. 29, Figure 18) No. Scores are determined for a limited number of locations.
- *Auxiliary information explains part of the spatial information?* The spatially information can be explained partly from information on the water type, i.e., stream or ditch. This information can be used in stratification of the area of interest. Within these strata or subareas no further auxiliary information is available.
- *Are space/time samples (to be) taken at random?* No. The observation sites have been selected purposively. This implies the use of geostatistical methods or deterministic functions in spatial aggregation.
- *Are there sufficient samples to estimate the variogram?* Webster & Oliver (1992) advise to estimate the variogram from 100-150 sampling locations. If the number of locations is less than 100-150, Bierkens *et al.* (2000) advise to apply deterministic functions such as Inverse Distance Weighting or Thiessen polygons in spatial aggregation. In our case studies, scores were available for 171 locations in the streams of sub-catchment area Rhine-East, at 41 locations in the ditches of sub-catchment area Rhine-East and at 59 locations in the ditches of sub-catchment area Rhine-West north of the North Sea Canal (excluding the isle of Texel).

In summary, for our purpose a design-based approach can not be applied because the data are not collected according to a probability-based sampling design. To be able to quantify the

accuracy of the aggregated measure, we decided to estimate variograms, to apply a geostatistical (kriging) approach based on straight line distances (Method 1.b.i in Annex 1), and to test this approach in practice in the case studies, even though the number of observations in ditches of Rhine-East and Rhine-West was lower than the minimum of 100-150 advised by Webster & Oliver (1992). In this way we are at least able to quantify the uncertainty about the aggregated measure. It should be noted, however, that uncertainty about the model of spatial structure itself, i.e. the variogram, is not accounted for in the geostatistical approach. In other words, the uncertainty about the aggregated measure is quantified, but only in the context of the specific model of spatial structure used. A different variogram model might result in a different estimate of uncertainty. The variogram model itself is a source of uncertainty, which is generally not accounted for. If the variogram model has been modelled on the basis of a large number of observations, however, uncertainty about the variogram model is expected to be negligible.

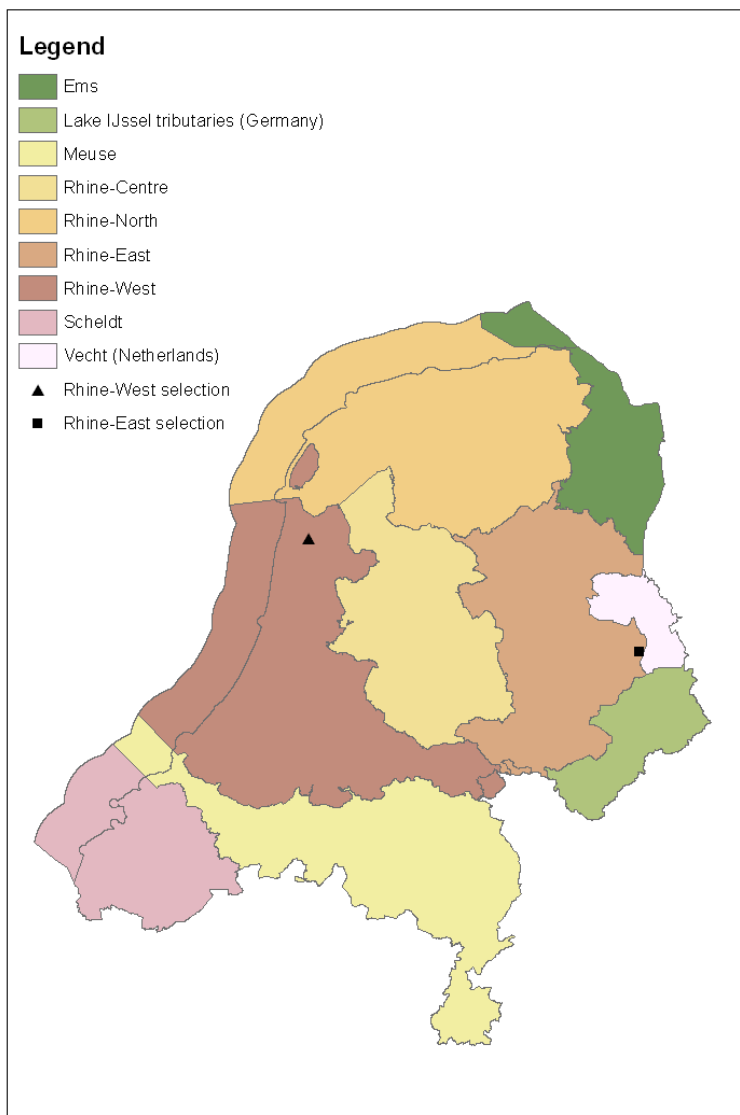


Figure 2. Study areas. The locations of the sections of the sub-catchment area Rhine-West (dark brown) in Figure 6 and of the sub-catchment area Rhine-East (light brown) in Figure 8 are indicated by a square and a triangle, respectively.

Table 2. Evaluation of methods for aggregation and upscaling of aquatic nature quality indicators according to the criteria from §2.2.

Criterion	(1) Methods that quantify uncertainty			(2) Methods that do not quantify uncertainty (Inverse Distance Weighting, Thiessen polygons)	
	(1a) Design-based methods	(1b) Model-based methods			
		(1bi) Methods based on straight line distance	(1bii) Methods based on symmetric hydrologic distance	Methods based on (1biii) weighted asymmetric hydrologic distance, (1biv) geostatistical method incorporating landscape characteristics in an adjusted distance metric, (1bv) topological kriging, or (1bvi) on the physiographical space	
1. Suitability for hydrological systems	+ Suitable for all hydrological systems	± Depends on spatial distribution of taxa	+ Connectivity of water bodies is accounted for	++ Connectivity, hierarchy and direction of current of water bodies is accounted for	- Hydrology not taken into account
2. Ecological realism (use of ecological knowledge)	+ Ecological knowledge can be used in the sampling design (e.g. stratification according to aquatic habitat)	± Depends on spatial distribution of taxa, Stratified kriging according to aquatic habitat. Suitable for organisms that disperse through air	+ Probably suitable for aquatic organisms that disperse actively through water	++ Probably suitable for aquatic organisms that disperse passively through water, i.e., with the current	± Ecological knowledge can be used in the sampling design (e.g. stratification according to aquatic habitat)
3. Complexity/simplicity	++ Inference is very simple	+ Inference is relatively simple	- Modelling of spatial structure is relatively complex	-- Modelling of spatial structure is very complex	++ Inference is very simple
4. Data requirements	- Probability-based sampling design required. At least 5-10 observations	- At least 100-150 observations required. Spatial coverage preferred	- At least 100-150 observations required. Spatial coverage preferred	- At least 100-150 observations required. Spatial coverage preferred	- Spatial coverage preferred
5. Necessary software and computer capacity	++ No requirements	+ Standard geostatistical software can be applied	-- Special software required	-- Special software required	+ Standard GIS software can be used
6. Possibilities to quantify uncertainty	++ Valid estimates of accuracy	+ Model-based quantification of uncertainty	+ Model-based quantification of uncertainty	+ Model-based quantification of uncertainty	-- No quantified uncertainty

++ very positive property, + positive property ±, property neither positive nor negative, - negative property, -- very negative property

3.4 Case studies

3.4.1 Introduction

In this subsection we describe the spatial aggregation of scores (proxies) in two areas: the sub-catchment area Rhine-East and the part of the sub-catchment area Rhine-West that is situated north of the North Sea Canal (excluding the isle of Texel).

We applied a geostatistical kriging method of spatial aggregation based on straight line distance to data collected in streams and ditches in the sub-catchment area Rhine-East (Subsection 3.2.2), and to data collected in ditches in the part of the subcatchment area Rhine-West situated north of the North Sea Canal (excluding the isle of Texel) (Subsection 3.2.3). Figure 2 (p. 22) shows the location of the study areas. Analysis of spatial structure and interpolations are performed using GSLIB software (Deutsch & Journel, 1998).

The geostatistical approach of aggregation followed in the two cases has the following steps:

1. Construct a model that describes the spatial correlation structure of the scores (i.e., a semivariogram);
2. Discretise the waters in the catchment area to a dense network of points (say, 20 m separation distance);
3. Interpolate scores to the dense network of points (see step 2) in the catchment area by ordinary point kriging, using the model of spatial structure obtained in step 1;
4. Calculate the aggregated score for the catchment area by linear averaging of the *interpolated* values, obtained in step 3.

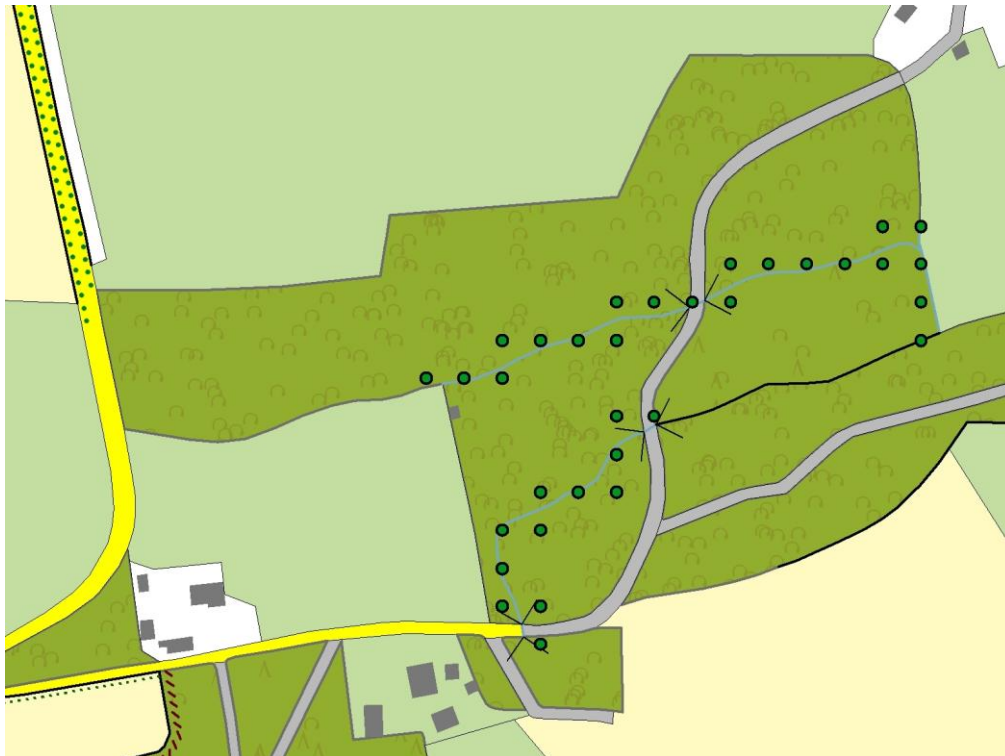


Figure 3. Example of discretised waters. The blue lines indicate streams. The dots indicate the discretised locations to which the scores were interpolated. Note the black line segment, indicating a trench that has not been discretised.

These steps are explained and illustrated in the following subsections. If uncertainty needs to be quantified, simulation instead of interpolation should be performed. However, software to simulate to irregular networks of interpolation points was not available and developing new software was beyond the scope of this study. We restrict ourselves to a brief description of the simulation procedure. If the accuracy of aggregated score needs to be quantified, then steps 3 and 4 should be replaced by:

3. Obtain an independent realisation of scores for the discretised waters in the catchment area by conditional geostatistical simulation, using the model of spatial structure obtained in step 1;
4. Average the simulated values to an aggregated score for the catchment area;
5. Repeat steps 3 and 4 a large number of times (say 100). The mean of the 100 scores is a final estimate, the standard deviation is a measure of its accuracy.

Figure 3 shows an example of the discretised waters. Line elements were discretised to points separated by distances of 20 m. It should be noted that some segments of streams or ditches were digitised as ‘trenches’ or as boundaries between parcels. This explains that the pattern of discretised waters is interrupted in some parts of the area.

3.4.2 Sub-catchment area Rhine-East

Figure 4 shows the semivariogram for the scores observed in both streams and ditches in the sub-catchment area Rhine-East. The semivariogram reflects the ‘dissimilarity’ of observations as a function of distance between observations: the larger the distance between two observations, the less similar will their values be. The variogram is defined by

$$2\gamma(\mathbf{h}) = \text{Var} \left[Z(\mathbf{u} + \mathbf{h}) - Z(\mathbf{u}) \right],$$

with γ being the semivariance, Z the variable of interest (indicator score), \mathbf{u} indicating the location at which Z has been observed, and \mathbf{h} the distance between two locations at which Z has been observed.

We assumed *isotropy* instead of *anisotropy*, i.e. it is assumed that the spatial correlation structure does not depend on direction. This may not be entirely true if organisms disperse with the current in streams such as many macroinvertebrates. However, the number of observations is relatively small to model anisotropy accurately, especially in ditches (41). Alternatively, an anisotropic semivariogram model can be constructed using expert knowledge on dispersion patterns of organisms. This would be an interesting topic for future research.

The semivariogram shows a clear spatial structure: the similarity of scores decreases with increasing distance between the locations at which the scores were observed. Observations that are separated with distances larger than about 16 km are not correlated, as the semivariogram in Figure 4 shows.

We fitted a spherical model to the semivariogram:

$$\gamma(\mathbf{h}) = c_0 + c \cdot \left[1.5 \frac{\mathbf{h}}{a} - 0.5 \left(\frac{\mathbf{h}}{a} \right)^3 \right], \text{ if } \mathbf{h} \leq a,$$

$$\gamma(\mathbf{h}) = c_0 + c, \text{ if } \mathbf{h} > a,$$

with c_0 being the 'nugget' parameter, representing observation errors and variation at short distances, $c_0 + c$ the 'sill' parameter, representing the maximum level of spatial variation, and a the range parameter, being the distance up to which the scores are spatially correlated. If there is no spatial correlation, the values of a and c go to zero and the semivariogram model is a horizontal line at level c_0 . The more spatial correlation, the larger the values of a and of c relative to c_0 .

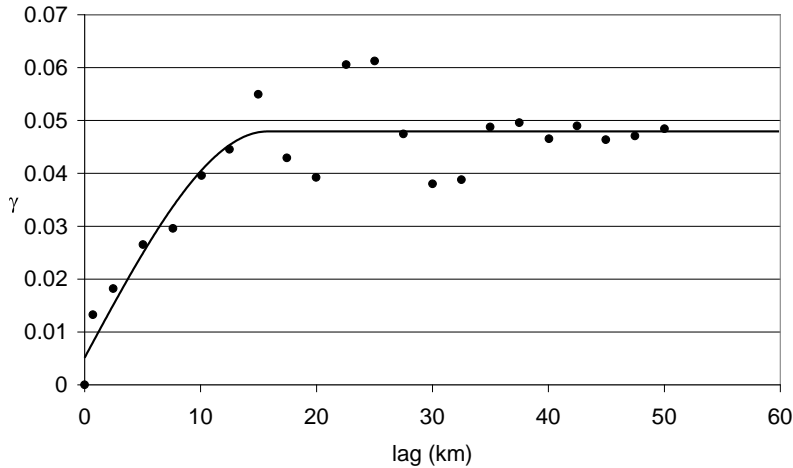


Figure 4. Dots: Sample semivariogram of scores observed in streams and ditches, in the sub-catchment Rhine-East. Line: the spherical model that has been fitted to the sample semivariogram, with $c_0=0.005$, $c_1=0.043$, and $a=15.776$ km.

We analysed the spatial structure of scores also for streams and ditches separately. Figure 5 shows the semivariogram for scores observed in streams in the sub-catchment Rhine-East. Note that the semivariogram in Figure 5 is very similar to the semivariogram for both ditches and streams in Figure 4. This can be explained from the relatively large number of observations in streams compared to the observations in ditches (171 vs. 41).

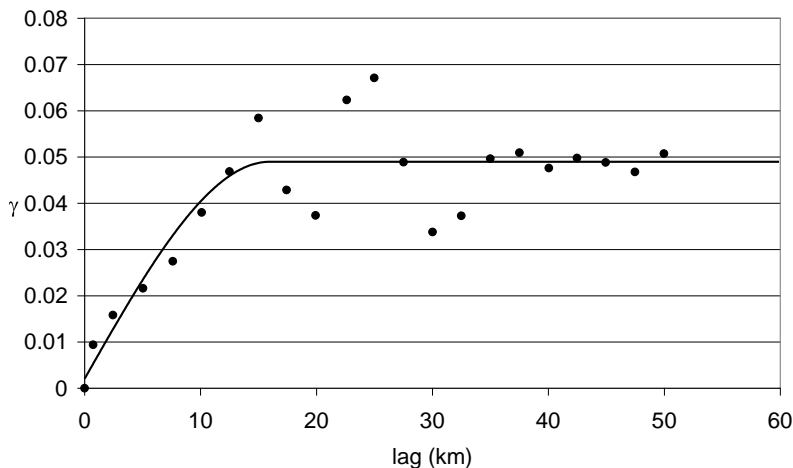


Figure 5. Dots: sample semivariogram of scores observed in streams, in the sub-catchment Rhine-East. Line: the spherical model that has been fitted to the sample semivariogram, with $c_0=0.002$, $c_1=0.047$, and $a=15.955$ km.

Figure 6 shows the semivariogram for scores observed in ditches in the sub-catchment Rhine-East (based on 41 observations). Spatial correlation seems to be absent. Furthermore, the level of the sill is low as compared to the semivariogram for streams in Figure 5. In summary, the scores in ditches seem to be spatially uncorrelated and relatively constant. This corresponds with our common ecological knowledge about macroinvertebrates ditches in sandy areas such as the Rhine-East sub-catchment where ditches are much less connected (Piet Verdonshot, personal comment).

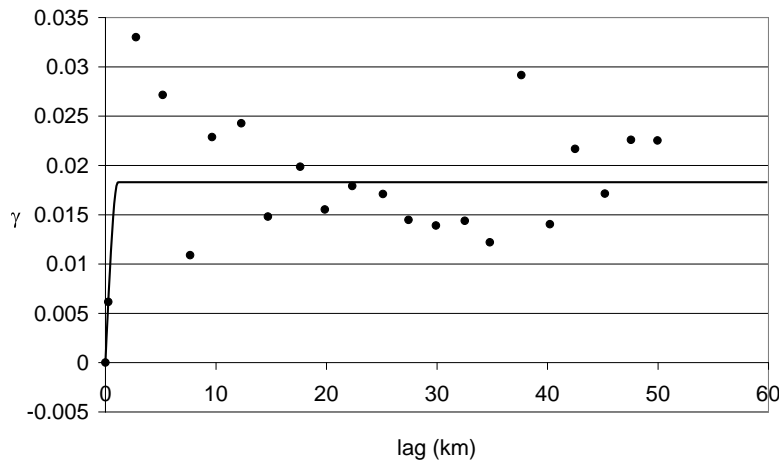


Figure 6. Dots: sample semivariogram of scores observed in ditches, in the sub-catchment Rhine-East. Line: the spherical model that has been fitted to the sample semivariogram approximates the pure nugget model, i.e. absence of spatial structure.

The scores that were determined for 212 locations in streams and ditches were interpolated to the discretised waters by ordinary point kriging (Deutsch & Journel, 1998), using the semivariogram presented in Figure 4 and with a neighbourhood of 59 observation points, the maximum number for which stable calculations were possible with the software used. Figure 7 shows the results of the interpolation for a part of the area. Besides a map with interpolated values (left), we constructed a map of kriging standard deviations (right), reflecting the accuracy of the interpolated values. Figure 7 (right) confirms that inaccuracy (uncertainty) increases with distance to the observation points.

The aggregated score for the catchment area 'Rhine-East' is estimated by calculating the areal mean of the interpolated scores, which equals 0.41. If spatial correlation is neglected the aggregated score estimated by the arithmetic mean of the observations equals 0.46. However, neglecting spatial correlation is not justified, given the semivariogram in Figure 4 that shows a clear spatial correlation structure. Accounting for spatial correlation results in a smaller estimate for the overall score in the catchment area 'Rhine-East'.

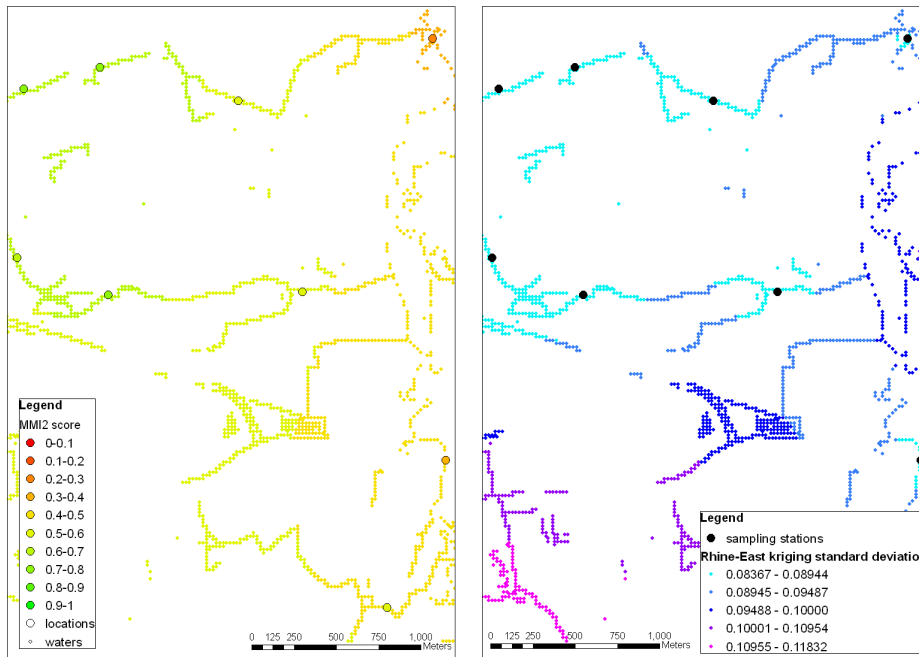


Figure 7. Results of interpolation for a section of catchment area 'Rhine-East'. Left: interpolated scores. Right: kriging standard deviations.

3.4.3 Sub-catchment area Rhine-West

We analysed the spatial structure in a set of 59 scores observed in ditches, north of the North Sea Canal, excluding the isle of Texel. The sample semivariogram in Figure 8 shows a spatial structure, that was modelled with a spherical model.

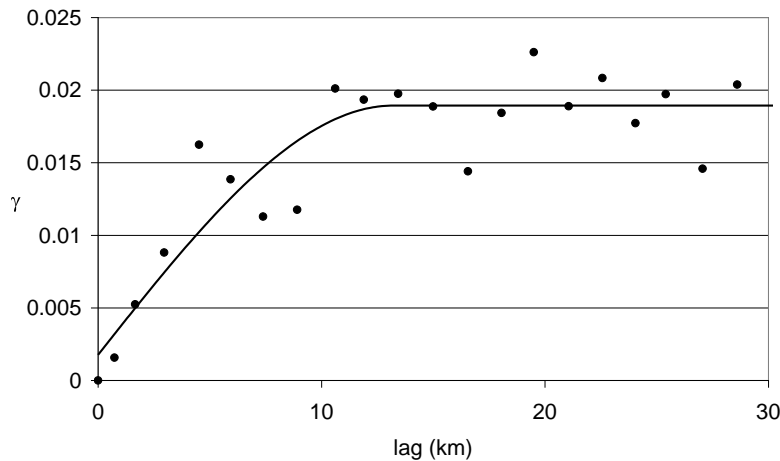


Figure 8. Dots: sample semivariogram of scores observed in ditches, in the sub-catchment Rhine-West, north of the North Sea Canal. Line: the spherical model that has been fitted to the sample semivariogram, with $c_0=0.002$, $c_1=0.017$, and $a=13.216$ km.

The scores that were determined for 59 locations in ditches (there are no streams in the area) were interpolated to the discretised waters by ordinary point kriging, using the semivariogram presented in Figure 8 and all data points. Figure 9 shows the results of the interpolation for a part of the area.

The aggregated score for the catchment area 'Rhine-West' north of the North Sea Canal, excluding the isle of Texel, is estimated by calculating the areal mean of the interpolated scores, which equals 0.44. If spatial correlation is neglected the aggregated score estimated by the arithmetic mean equals 0.41. Accounting for spatial correlation results in a higher estimate for the overall score in the catchment area 'Rhine-East'. Note again that neglecting spatial correlation is not justified, given the semivariogram in Figure 8.

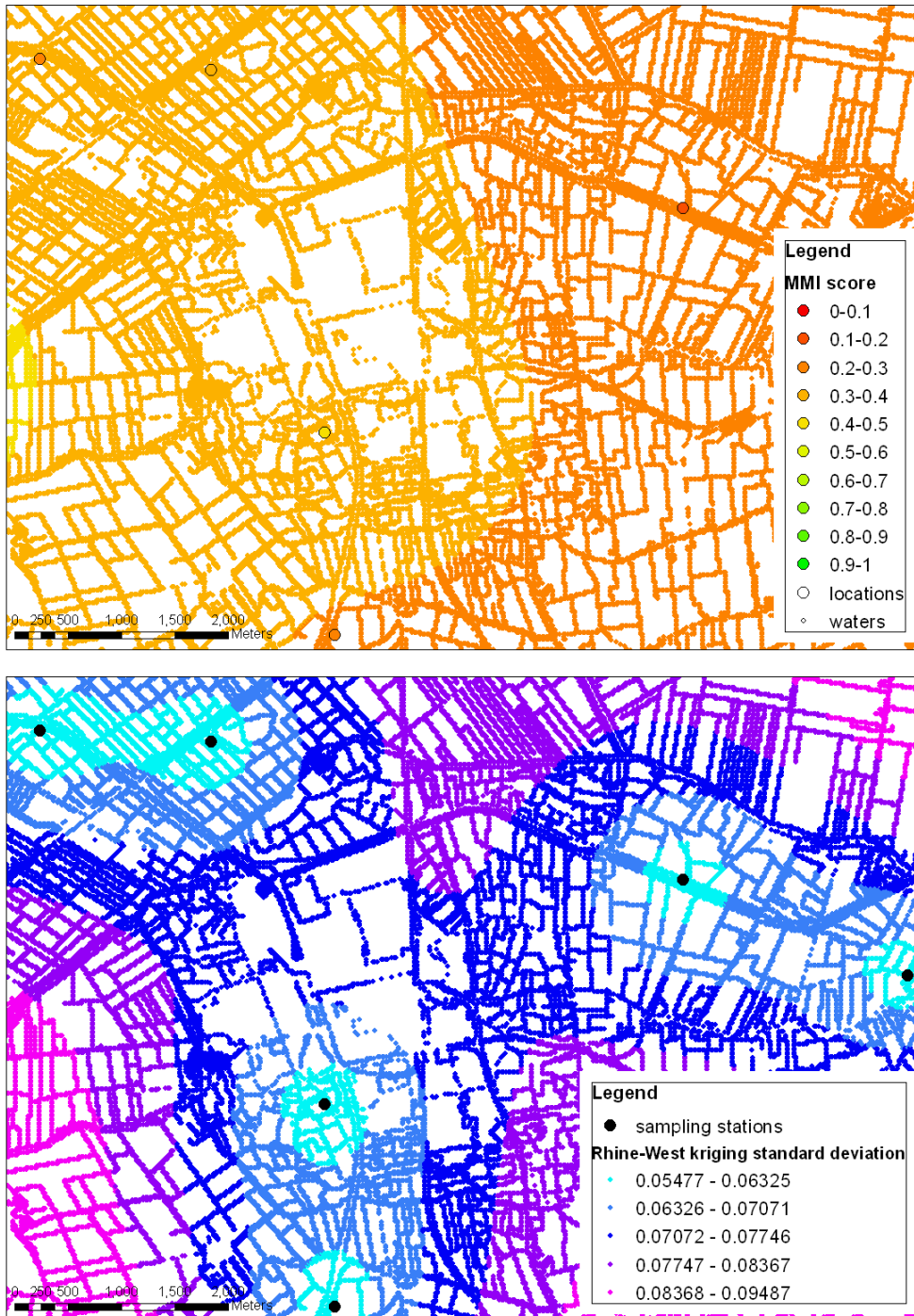


Figure 9. Results of interpolation for a section of catchment area 'Rhine-West'. Top: interpolated scores. Bottom: kriging standard deviations.

4 Discussion

The evaluation of the different methods reviewed in this study showed that the model-based approach consisting of (1) interpolation by kriging (or a related method) followed by (2) arithmetic averaging was the best choice (§3.2, Table 2). The reasons for this were (a) that it is required to assess the uncertainty of the aggregated values and (b) that a design-based method was not possible because aquatic monitoring stations in The Netherlands are not selected by probability sampling. This leaves model-based aggregation methods as the only solution and most of these use some sort of kriging (see §3.2). The use of interpolation methods has one other advantage. When aggregate nature quality indicators are below the threshold, policy and management measures need to be taken in order to improve the situation. In that case it will be necessary to determine where in the area nature quality is worst and thus where taking measures will be most successful for improving the (aggregate) nature quality of surface waters. Interpolation methods such as kriging are necessary once you want to identify such hot spot locations and to assess spatial patterns.

The case study demonstrated that the spatial correlation observed using ordinary kriging based on straight line distances (SLD) while assuming isotropy was suitable to describe the spatial structure of the multimetric nature quality indices for macroinvertebrates. There was spatial correlation at distances up to c. 16 km in the Rhine-East sub-catchment, dominated by streams, and up to c. 12 km in Rhine-West, dominated by polder ditches. These correlation distances may partially reflect (dis)similarities in water quality and landscape factors between adjacent surface waters. However, since most aquatic species move through water, it may be worthwhile to investigate if interpolation methods based on hydrological distance could yield an even better description of the spatial correlation required for interpolation and aggregation of nature quality indices.

This study explicitly deals with spatial aggregation and upscaling of ecological indicators. However, when ecological census data are gathered on a routine basis at the same site, the information also needs to be aggregated taxonomically, for different types of surface waters, and in time.

When different indicators are used for different taxonomical groups this can make finding an appropriate method for overall aggregation and integration very complicated, such as the various freshwater quality indicators that have been established for the Water Framework Directive (Herwijnen & Janssen, 2004). However, the indicators that were used in our case study, the multimetric indices for ditches and streams, are to some extent already aggregated taxonomically. The data of relevant macroinvertebrate groups are combined in a single indicator, with a scale from 0 to 1. Similar indicators for other taxonomical groups, such as macrophytes and fish, will probably be developed in the near future.

The use of such similar types of indicators makes it easier to compare but also to aggregate the indicator values for different types of taxa and for different types of surface waters. In the case study of Rhine-East for example, we jointly used macroinvertebrate MMI indicators for ditches and streams for interpolation. Furthermore, a (weighted) average could be used to aggregate these multimetric indicators for different taxonomical groups. Alternatively the worst indicator value among the different taxa at one sampling station or a combination of the worst case principle with averaging could be used (Herwijnen & Janssen, 2004). However, before such aggregations between taxonomical groups can be done, the effect of the spatial scale of correlation should be investigated. For instance, individual fish move over much further distances than macro invertebrates.

If a summary is needed of the ecological water quality in an area during a given period of time, data need to be aggregated in both space and time. The overview of methods for spatial aggregation, given in Section 3.2, can be extended to the space-time context. De Gruijter *et al.* (2006, Chapter 15) describe various design-based and model-based methods to estimate space-time distribution parameters such as space-time means. Knotters *et al.* (2009) applied kriging methods, Thiessen polygons and Inverse Distance Weighting to interpolate between time instances at which multimetric scores for ecological water quality were determined. These methods can also be applied to aggregate in time, analogous to aggregation in space.

The order in which different aggregations steps are done may affect the outcome, especially when non-linear models or relationships are involved (Pebesma & Heuvelink, 1999; Bierkens *et al.*, 2000). Once (multimetric) nature quality indicators for all aquatic taxonomical groups have been developed, the right order of aggregation should be established. Usually model calculations must precede spatial aggregation (Pebesma & Heuvelink, 1999). However this often requires more calculation capacity than the other way round. Under certain conditions, for example linearity, spatial aggregation can be done before modelling. It should also be established if and at what stage aggregation between the indices for different types of surface waters should take place. Different types of surface waters may be under- or overrepresented in certain sub-catchments. This is not only the consequence of natural hydrological and geographic differences but is also caused by bias in the ecological monitoring networks of the Dutch water boards and differences in sampling effort. For future application it would be useful to construct a decision tree for choosing the appropriate aggregation methods and the right order of the aggregation steps.

The selected methods that were applied in the case studies are based on geostatistical models (kriging). In such a model-based approach a minimum of 100-150 observations is recommended by Webster & Oliver (1992) to estimate a model of spatial structure. If global information is required however, such as spatial means or areal fractions, then a design-based approach based on a probability sample can be considered. If local information is required (such as a map) a model-based approach is more appropriate. If less than 100-150 observations can be afforded and only global information is required, then a design-based approach is the best option (for an extensive discussion on the choice between a model-based and a design-based approach we refer to Brus & De Gruijter, 1997). Finally, when there is no need to assess the uncertainty, i.e. when aggregated values are not statistically compared to each other or to a threshold value, simpler interpolation methods can be used (Inverse Distance Weighting or Thiessen polygons).

5 Conclusions & recommendations

Based on evaluation of the available literature on aggregation methods to upscale aquatic nature quality indicators and on our case studies for the sub-catchments Rhine-East and Rhine-West, the following conclusions can be drawn:

- An approach consisting of interpolation (kriging, or a related method) followed by arithmetic averaging is the only option when the uncertainty of the aggregated values must be assessed. Unbiased estimates of spatial means cannot be obtained by averaging of observations according to a design-based inference, because aquatic monitoring stations in The Netherlands are not selected by probability sampling.
- In the case studies, analysis of the spatial variation based on Euclidian distances showed a clear spatial correlation. This confirmed that geostatistical methods based on Euclidian (straight) distances are appropriate for the cases studied, i.e., the newly developed multimetric indices for nature quality based on aquatic invertebrate communities present in polder ditches and streams in two sub-catchment areas in The Netherlands.

This study was conducted in order to provide an overview of the possible methods for aggregation of aquatic nature quality information. One of the most appropriate methods was tested for one type of indicator (macroinvertebrates). In order to build a more extended system for aggregation of such parameters and mapping the aggregated information the following is recommended:

- The spatial correlation of aquatic nature quality data or indices should be further investigated using different methods (with and without connectivity and or stream hierarchy) that are based on hydrological distance between sampling stations such as stream network kriging. The results for these methods for indicators for different aquatic taxonomical groups should be compared and the most appropriate methods, i.e., that best describe the spatial distribution for each indicator, should be selected.
- The procedure can possibly improved by applying ('anisotropic') semivariogram models that have been constructed using expert knowledge on dispersion patterns of organisms.
- On the basis of the selected methods a decision tree for selection of the most appropriate aggregation steps and methods should be established. This tree also needs to include the order in which different aggregations steps need to be performed (aggregation in time, between taxonomical groups, between different types of surface waters, and spatial aggregation).

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Annex 1

Description and classification of spatial aggregation methods for aquatic nature indicators.

1. Methods that quantify uncertainty

- a. **Design-based methods:** sampling units are selected by probability sampling. The sampling design determines the inclusion probabilities of each sampling unit and of pairs of sampling units. The inclusion probabilities of each sampling unit in the target population must be known and be larger than zero. The inference is based on the inclusion probabilities and thus on the sampling design. An example of design-based approaches for quantifying surface water quality is Generalized Random Tessellation Sampling (GRTS, Stevens & Olsen, 2003, 2004). Brus & Knotters (2008) applied a synchronous pattern (with stratified simple random sampling in both time and space) to test space-time mean nutrient concentrations of surface water against legal standards. Synchronous means that a different set of sampling locations is selected for each sampling time, i.e., the sampling locations are not revisited, as contrasted to static sampling in which all sampling takes place at a fixed set of locations (De Gruijter *et al.*, 2006). Design-based methods have several advantages as compared to model-based methods: (1) aggregated measures can be inferred relative simple from the data, and (2) results are valid because they do not depend on the quality of model assumptions. Validity is particularly important in testing against legal standards. A drawback of design-based methods is that the required probability sample is not always available, or cannot be collected for practical reasons (such as inaccessibility of terrains). Data from additional purposive samples can be used to improve the results of design-based procedures, without losing the advantages of a design-based approach (e.g., regression estimators). It should be noted that the data used in the case studies in Section 3.2 are collected by purposive sampling. Therefore a design-based inference is not appropriate in this study.
- b. **Model-based methods:** sampling units can be selected either by probability sampling or by purposive sampling. Typically, sampling units are selected purposively, aiming for minimization of prediction error variance. Inference is based on a model for spatial and/or temporal variation. It should be noted that averaging implies the assumption of a 'pure nugget model', i.e., absence of spatial correlation. A possible way to aggregate is first to interpolate the observed values to a dense grid and next to average the interpolated values. If percentiles of a distribution are required as aggregation measures, then simulation should be performed instead of interpolation.
 - i. **Methods based on 'straight line distance' (SLD, Euclidian distance).** Kriging methods are traditionally based on Euclidian distances, see Knotters *et al.* (2009) for an overview. A model of spatial variation based on Euclidian distances might not be appropriate for interpolation of observations in stream networks, because they do not account for hierarchy and flow. Ancillary information can be incorporated into the kriging system in various ways. An advantage of SLD-based methods is that standard geostatistical software can be applied in interpolation. Handcock (2007) presents a general framework to combine location-specific, contextual, and complete coverage covariates in estimating the distribution of ecological indicators for water quality of riverine systems.

- ii. **Methods based on ‘symmetric hydrologic distance’ (SHD).** The symmetric hydrologic distance is the distance between two points in a stream network, measured along the stream segments connecting these two points. A disadvantage of SHD-based methods is that applying standard models for spatial variation (e.g., the spherical model) may lead to numerical problems (matrices might not be positive definite, resulting in negative variances) (Ver Hoef *et al.*, 2006; Peterson *et al.*, 2007).
 - iii. **Methods based on ‘weighted asymmetric hydrologic distance’ (WAHD).** This distance is unidirectional because movement between sites is restricted to either the upstream or downstream direction (Peterson & Urquhart, 2006). 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. WAHD has the same disadvantage as SHD with respect to the validity of standard models for spatial variation. Ver Hoef *et al.* (2006) showed that standard geostatistical models of spatial variation (spherical, exponential, Gaussian) are not valid when using stream distance (such as SHD or WAHD), and applied moving average constructions to develop valid models for stream networks. In a case study by Peterson *et al.* (2006) SLD appeared to be more appropriate than WAHD in regional geostatistical modelling. Methods based on SHD or WAHD are relatively new and rather complex to apply as compared to methods based on SLD.
 - iv. **Method incorporating landscape characteristics in an adjusted distance metric** (Lyon *et al.*, 2008). 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. Lyon *et al.* (2008) concluded that kriging based on adjusted hydrologic distance outperformed kriging based on Euclidian distance or on symmetric hydrologic distance. They fitted exponential variograms and did not meet the numerical problems mentioned by Ver Hoef *et al.* (2006).
 - v. **Topological kriging (Top-kriging).** Skøien *et al.* (2006) and Skøien & Blöschl (2007) presented a geostatistical method for interpolation in stream networks based on ‘regularisation’ of the variogram from between-point to between-catchment level. They showed that Top-kriging provided more plausible and more accurate estimates than ordinary kriging. The Top-kriging model seems to be less complex than the models based on SHD and WAHD.
 - vi. **Methods based on the physiographical space** (Chokmani & Ouada, 2004; Guillemette *et al.*, 2009). In this approach 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.
2. **Methods that do not quantify uncertainty.** These methods are based on some deterministic model of spatial and/or temporal variation. Examples are Inverse Distance Weighting and Thiessen Polygons (nearest neighbour interpolation). Because quantitative information on uncertainty is required we do not describe deterministic methods in detail. For an overview we refer to Knotters *et al.* (2009).

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2007

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2008

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2009

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