Mathematical Modeling of Marine Environment Contamination Using Fuzzy Set Theory

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Dedicated to my Parents, and to my

sisters and brothers: Amani, Abdullah, Mariam, Sarah and Mohammad

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Chapter 1

Introduction

Two marine environmental regions will be introduced in this chapter which shall be the focus of this study. Our general aim is to mathematically model an environmental region with respect to metal distribution.

1.1 Environmental Regions

As an introduction, two environmental regions from which the studying blocks for this research were obtained are presented. The regions, Liverpool bay and Morecambe bay, were selected based on the domain expert's scientific knowledge of both regions.

1.1.1 Liverpool bay

Liverpool bay is an area within the Irish Sea whose precise limits have not been defined. At most times it is often used to describe that part of the Irish Sea limited to the south by the North Wales coast, east of Great Ormes Head, and to the east by the Lancashire coast as far north as the estuary of the Ribble River (Figure 1.1). The seaward boundaries are not precise but are generally taken to be some 50 kilometres to the north and west of the two coasts [15] which can be considered as the general description of the bay. As for a precise description, Liverpool bay is

Figure 1.1: Study area including depth contours(m). The waste disposal sites in Liverpool bay are indicated by SI (sewage and industrial wastes), Y and Z (dredged spoil sites). The polygon off the Mersey and the North Wales coast indicates the perimeter of the sampling grid.

considered to be a relatively shallow, semi-enclosed water body. Most of the area is seen to lie within the 40m isobath, whereas the depth over the sewage disposal area (site SI [1]) is said to be between 25 and 30m. To help in interpreting the results, an understanding of some of the geophysical and industrial activities that occur in Liverpool bay may be needed.

First, we shall look the geophysical aspects that characterize the bay. The discharges into Liverpool bay are mainly from the rivers Mersey, Ribble, Dee and Clwyd. The influences of these freshwater discharges upon the waters of Liverpool bay have been found to vary seasonally, with considerable enhancement during the winter months and with higher precipitation and fluvial discharges than the summer. Although water circulation in the bay, in general, depends on several factors such as tides, winds, and freshwater inputs, there is a well established estuarine-like circulation induced by the low-density freshwater inputs from the rivers, the Mersey in particular, and by higher density seawater from the Irish Sea. In this circulation, low-density water moves offshore on the surface and high-density water moves inshore near the bottom. This density-driven inshore movement of bottom water, coupled with tidal asymmetry producing stronger flood than ebb tides induces, a net sediment transport directed east and south-east toward the Mersey. The direction of net sediment transport has been confirmed by studies using sea-bed drifters, radio-labelled sewage and by the grain-size distribution in the bay.

According to a number of studies [16, 15], Liverpool bay is considered to be an area of sandy sediments, although irregular patches of mud have been found in some places. Another important characteristic is the net directional transportation of sediments. There exist two directions of sediment transport in Liverpool bay, one from NW to SE and another from west to east. Very fine sand (62.5 to 125.0 μm) is the fraction more easily transported in the easterly direction whereas coarser sediment (fine sand, 125-250 μm) is preferentially moved towards the south-east (see Camacho-Ibar,1992). In summary, there is a general trend to observe in the

[1] Site SI includes stations: K8-K11, L10-L12 and J9

Figure 1.2: Location of stations in Liverpool bay in which superficial sediment samples were taken for study.

distribution of fine sediments, with intermediate values between 5-10 percent in the northern region of the sampling grid that decreases towards the North Wales Coast where they reach values less than one percent. The distribution of muddy deposits was seen to be erratic throughout the region, although muddy banks near the Burbo Bight (10-20 percent) appeared to be a permanent feature.

A wide range of commercial and leisure activities is carried out in Liverpool bay. These activities include fishing, gravel extraction, sailing and boating, swimming and the use of amenity beaches, and most importantly, the bay is used as a site for the disposal of sewage sludge and dredged spoil. Disposal activities of sewage sludge in Liverpool bay started after the construction of the first sewage treatment plants near Manchester and Salford in the early 1890s. Sludge disposal has continued until 1998[2] inclusively at a designated area (site SI) shown in Figure 1.2. Disposal of industrial wastes has taken place at the same site since the late 1960s. The bay also receives direct discharges of domestic and industrial wastes from coastal outfalls, and indirectly from the discharges of effluents into the rivers flowing into Liverpool bay. These discharges are mainly organic in composition, with metallic compounds included in its inorganic content, and its constituents are present both in suspension and in solution [1]. The main riverine contributions are from the rivers Mersey, Dee, and Ribble.

All of these disposal operations occur inside an area licensed by the Ministry of Agriculture, Fisheries and Food (MAFF). This Ministry is responsible for the control of disposal of wastes at sea, including the licensing of all disposal operations. MAFF does the predischarge control on wastes, enforces the licensing conditions, and carries out surveys of the areas licensed for the disposal of wastes to ensure that the marine environment and its resources are being protected. [14]

[2]Reference: personal communication

1.1.2 Morecambe bay

Morecambe bay is a large macro-tidal estuary with important wildlife resources. It is located on the eastern shore of the Irish Sea, north-west of England. Of particular relevance in the bay are the Grange and Heysham Channels at the landward end of the Lune Deep (itself an interesting feature of glacial origin) and other channels lying between Yeoman Wharf, Furness Bank and Mort Bank. Also of particular interest is the dredged access channel leading to the port of Barrow-in-Furness. Figure 1.3 shows the stations of the sampled area from Morecambe bay taken in 1988.

The distribution of mean sediment size was noted by [4] as follows. Within the bay, the bed material is almost exclusively sand, with a mean diameter of approximately 0.1mm (fine sand). Along the Lune Dune, southern region of Morecambe bay, and out into the Irish Sea, some muddy sediments are found. The Morecambe Flats which are exposed at low tide (located along the western boundary of the bay) together with an area extending offshore to the south west, appear to be primarily stoney grounds. The bay is relatively open to wave action from the south-west, and therefore it is likely that waves could play a significant role in suspending material in addition to the tidal flow. On the tidal flats further into the bay, the net transport was found predominantly in a landward direction.

1.2 Research Assignment: General Aim

The dynamic nature of coastal waters presents a severe challenge to environmental assessment of disposal activities in near shore waters. Liverpool bay has received large quantities of sludge-input (industrial waste) on regular basis since the late 1960's. Heavy metal concentrations are measured annually on a grid of locations in order to detect and monitor the changes in the ecological structure of Liverpool bay. On the other hand, unlike Liverpool bay, Morecambe bay with its important wildlife resources is not extensively used for such industrial activities. The geographical locations of the two regions are shown in Figure 1.4.

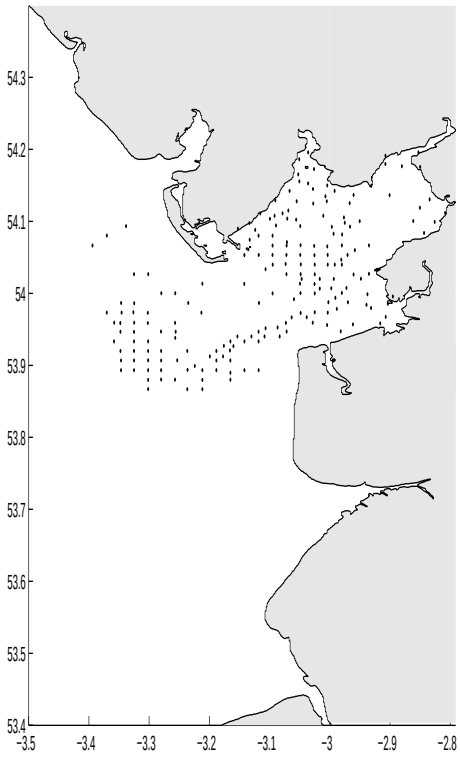


Figure 1.3: Location of stations in Morecambe bay in which superficial sediment samples were taken for study.

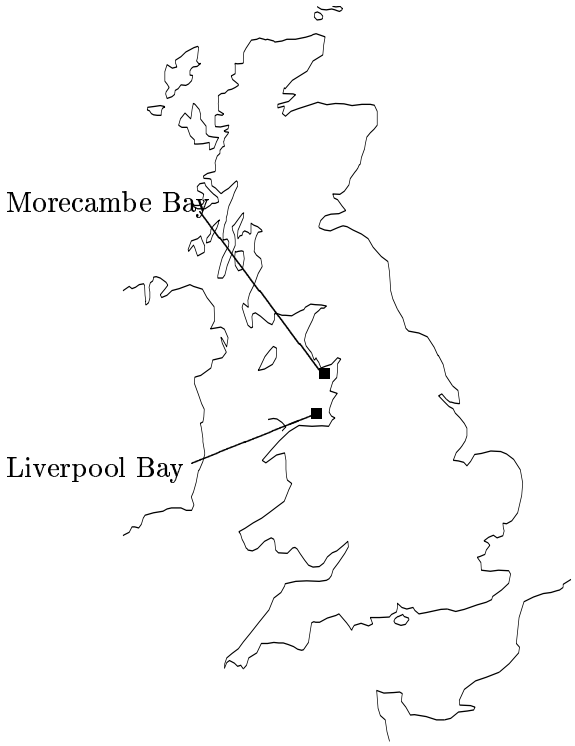


Figure 1.4: Liverpool Bay and Morecambe Bay location in the United Kingdom

Both regions are of importance with respect to the presence of heavy metal concentrations. Morecambe bay is assumed to contain lower levels of metal concentrations compared to Liverpool bay. Therefore, Morecambe bay was suggested as a benchmark for a *relatively clean* marine region. An important difference between Morecambe bay and Liverpool bay is that metal concentrations within Liverpool bay are "point-wise" (i.e., there is a designated disposal site), whereas Morecambe bay obtains a diffused input. See [17, 18] for additional information on monitoring and surveillance of contaminants in the aquatic environment. Liverpool bay also receives heavy metal discharges from continuous sources (Mersey and Dee Estuaries) as well as through erosion [14].

1.2.1 Heavy metals

'Heavy metals' is a general collective term applying to the group of metals and metalloids with an atomic density greater than 6 g/cm^3. Although it is scientifically only taken to be a loosely defined term, it is widely recognized and usually applied to the elements such as Cd, Cr, Cu, Hg, Ni, Pb and Zn which are commonly associated with pollution and toxicity problems. Unlike most organic pollutants, such as organohalides, heavy metals occur naturally in rock-forming and ore minerals and so there is a range of normal background concentrations of these elements in soils, sediments, waters and living organisms. When talking about 'contamination', 'contamination' is a term used when concentrations of substances in an environment give rise to inconsistently high concentrations of the metal relative to the normal background levels; therefore, the presence of the metal is insufficient evidence of pollution, the relative concentration is all important (see Table 1.1, [5]). Examples of critical (trigger) concentrations of heavy metals used in the U.K. and another European country are given in Tables 1.1 and 1.2. The critical values for soils given in Table 1.1 for the U.K. by the Department of the Environment Inter-departmental Committee for the Reclamation of Contaminated Land List of Trigger Concentrations for Contaminants are pragmatic and based mainly on the risk to human health.

Table 1.1: UK Department of the Environment Inter-departmental Committee for the Reclamation of Contaminated Land List of trigger concentrations for environmental metal contaminants (total concentrations except where indicated, UK Department of Environment, 1987).

Contaminant	Proposed usages	Threshold trigger concentration (μg/g)	Background reference [29, 70]
Contaminants which may pose hazards to human health			
Cd	Gardens, allotments	3	0.3
	Parks, playing fields, & open space	15	
Cr	Gardens, allotments	25	90
	Parks, playing fields, & open space	-	
Pb	Gardens, allotments	500	20
	Parks, playing fields, & open space	2000	
Hg	Gardens, allotments	1	0.4
	Parks, playing fields, & open space	20	
Phyotoxic contaminants not normally hazardous to health			
Cu	Any uses where plants grow	130	45
Ni	Any uses where plants grow	70	68
Zn	Any uses where plants grow	300	95

Table 1.2: Guide values and quality standards used in The Netherlands for assessing soil and water contamination by heavy metals (Netherlands Ministry of Housing, Physical Planning and Environment, 1991).

	Soils (μg/g)			
Metals	A	B	C	STV
Cd	1	5	20	0.8
Cr	100	250	800	100
Cu	50	100	500	36
Hg	0.5	2	10	0.3
Ni	50	100	500	35
Pb	50	150	600	85
Zn	200	500	3000	140

Soil value: A = reference value, B = test requirements, C = intervention value; STV = target value for soils. Target values for soils are based on 'standard soil' (10 % organic matter and 25% clay).

Table 1.3: Estimated inputs (in tons) of some metals to the North Sea in 1990

Source	Mercury	Cadmium	Copper	Lead	Zinc
Rivers	25	43	1200	1000	6400
Atmosphere	6.9	74	740	1700	5500
Dredging spoil	19	71	1300	2700	7900
Direct discharges	1.8	17	290	160	1300
Industrial disposal	0.2	0.3	180	220	440
Sewage sludge (ceased by 1998)	0.7	1.2	76	77	160

Table 1.2 shows the critical concentrations used in the Netherlands for contaminated soils. These are: A, the 'normal' reference value; B, the test value to determine the need for further investigations; C, the intervention value above which the soil definitely needs cleaning-up; and STV, the target value for soils which represents the final environmental quality goal for the Netherlands. See also [69] for more information on heavy metal contamination.

According to [23] metal input routes can be classified into three groups: atmospheric inputs, river inputs and other inputs. Most rivers make a major contribution of metals to the sea, the nature of the input depending on the occurrence of metal and ore-bearing deposits in the catchment area. Intense sedimentation in estuaries traps large quantities of metals which become adsorbed on to sediment particles and carried to the bottom. Sediments in industrialized estuaries with major ports contain the legacy of a century or more of waste discharges. Regular dredging of shipping channels in such areas produces large quantities of contaminated dredging spoil, which, except for the most heavily contaminated dredgings, are usually disposed at sea. Much smaller quantities of metals are added to the sea by direct discharges of industrial and other wastes by pipe line, and by disposing sewage sludge and industrial wastes at sea. Although relatively small, these inputs may be locally significant if they are added to sea areas with restricted water circulation. The following is a brief introduction to five specific heavy metals (i.e., mercury, cadmium, copper, nickel, and lead) out of the seven and there importance to the environment [23]. Table 1.3 shows the estimated inputs of some metals to the North Sea[3] in 1990.

Mercury (Hg): Annual global input of mercury to the sea is estimated at 6000-7500 tons, of which 50-75% is the result of human activities, but the industrial use of mercury has been progressively reduced. Mercury is the only contaminant introduced by humans into the sea that has been responsible for

[3]The North Sea is bounded by the Straits of Dover to the south, Denmark to the east, the eastern coast of the UK to the west, and bounded by an invisible line stretching from Shetland to the Norwegian coast to the north. It is intensively used by the surrounding, largely industrialized population of 31 million (plus summer visitors), for shipping, fishing, waste disposal, etc. [23].

human deaths (e.g., 'Minamata disease' in Japan). Natural inputs of mercury to the sea are from weathering of mercury-bearing rocks and degassing of the earths crust, particularly through volcanic activity. As far as is known, human exposure to organic mercury occurs only through the consumption of contaminated fish and sea food. The World Health Organization (WHO) recommended a maximum tolerable consumption of mercury in food of 0.3mg of total mercury per week.

Cadmium (Cd): Annual global input of cadmium to the sea is 8000 tons, of which half is from human sources. Some marine organisms accumulate large concentrations of cadmium, but no environmental effect has been detected. Cadmium was associated with 'itai itai' disease in Japan, but this has not been confirmed elsewhere. Even so, cadmium is included in the 'blacklist' of substances that should not be discharged to sea. The amount of cadmium released to the environment cannot be quantified but are of a variety of diffused sources including sewage sludge.

Copper (Cu): $325000t/year$ of copper enter the sea annually from the erosion of ore-bearing rocks. About 7.5 million tons per year are used in industrial processes. Copper is mostly adsorbed onto particles and most inputs become incorporated in bottom sediments. Copper is the most toxic metal after mercury and silver.

Lead (Pb): Lead contamination in the sea increased dramatically after 1750 (industrial revolution) and especially after 1950 (lead additives to petrol) largely from atmospheric sources. Lead is not particularly toxic to marine organisms and has had no environmental impact. The total world production of lead is about 43 million $t/year$.

Nickel (Ni): Nickel is a heavy metal that is a significant contaminant of sediments in industrialized areas and serious attempts have been made to reduce inputs of nickel to the sea.

Industrial plants have been disposing of waste in Liverpool bay for the past several years at specified licensed sites. Surface sediment samples have been collected from both regions at specified coordinates in the bays, shown in Figures 1.2 and 1.3. The annual data were measured at a specified time, mainly between the 14th and 16th of September, by means of a 0.1 m^2 Day grab. This type of grab has been extensively used for sediment surveys by MAFF and UCNW because of its reliability and ease of operation. This technique permits seabed sampling down to a maximum depth of 15 cm. The fine fraction was analysed for concentration of heavy metals, namely,

- Mercury (Hg)
- Cadmium (Cd)
- Chromium (Cr)
- Copper (Cu)
- Nickel (Ni)
- Lead (Pb)
- Zinc (Zn)

which were all measured in units of $\mu g/g$ (parts per million, ppm) [4].

1.2.2 Aim of Study

In this study, the objective has been, mathematically, to construct and represent the geographical (spatial) distribution of overall metal loading in a marine environmental region. In other words, our aim is to use a mathematical approach, and apply it on the available metal data sets to produce various informative data sets of metal loading. These sets should reflect specific overall distribution of metal concentrations in an aquatic environment.

[4] micrograms per gram of sediment

In [59], McBratney (1992) discusses information in environmental soil management, how the quality and quantity of soil information may be modified by various kinds of uncertainty (stochastic, deterministic and semantic), and how its presentation may be enhanced by the use of information technology. One of these types of uncertainty of soil information that is of interest to us is uncertainty due to vagueness. There are many occasions in soil science especially in soil description when the data represent a concept that is somewhat vague or is qualitative. Fuzzy set or possibility theory deals with this type.

The problem of finding geographical distribution of heavy metals is addressed in Markus and McBratney, 1996 [56]. The authors investigated the occurrence of some metals in urban soil by using Statistical Analysis, Generalized Linear Models and Fuzzy c-means clustering. Fuzzy c-means classified the sampled points into a number of classes according to the level of soil contamination by the metals. Specifically, the aim of the study was to determine the total concentration and spatial distribution of four metals (Pb, Zn, Cu and Cd) in an Australian urban environment. The following is a summary of the three statistical and mathematical analytical approaches used to find the solution.

- *Geostatistical Analysis*: Two types of kriging[5] were used, lognormal and indicator kriging, to generate plots of metal concentrations and probabilities of concentrations that were above environmental limits, respectively.

- *Generalized Linear Models*: These models were incorporated to determine which factors, among the underlying three: soil, geology and distance from the road, influenced the concentration of total metals from the sampled topsoil.

- *Fuzzy c-means Clustering*: A fuzzy c-means analysis was first applied to the original data (i.e. the data of the four chosen metals) to determine the spatial

[5]Kriging is a geostatistical gridding method of spatial interpolation and contouring for irregularly spaced data. For more information see [24, 40]

distribution of each point in relation to another. It was then used to cluster objects of similar variables numerically. For this data, five clusters were formed. Fuzzy c-means was specified for four clusters, but later formed the fifth. A minimum membership grade of 0.5 was selected as a threshold value such that data points with membership greater than 0.5 were visually represented via a map (i.e. these points made up 4 out of the 5 clusters). While points with memberships far less than 0.5 and did not fit any particular class were characterised as an 'extragrade' class, and formed class 5.

Finally, it was concluded that the results of these analysis only quantified, i.e., showed the amount of increasing levels of contaminants in the sampled environment, and confirmed the presence of each metal concentration in this sampled urban environment.

Also, Lehn and Temme (1996) [52] considered the field of research, "handling sites suspected of being contaminated". They recognised that there exists a high demand for formal methods and computer systems that maintain site data and assist in the estimation of hazard. This need for such systems was found to arise as a result of the large number of sites and therefore the large amount of data to be worked on. One of their approaches to this problem, was that they considered applying *fuzzy clustering* to estimate the hazard of sites suspected of being contaminated.

Hence, we find that there is no straightforward solution to the general task at hand. Therefore, using the concept of Fuzzy Set Theory we hope to generate a number of concentration indices (not necessarily similar) to represent the loading distribution in a region. In summary, the tasks of the study are to:

1. Summarize the mathematical method (Fuzzy Aggregation Rules) which will be used to design the loading indices. (Note that, a 'loading' of a site refers to the natural and unnatural concentration of metals found in the sediments of the sampled sites.)

2. Apply the above method on the data sampled from the marine environmental

regions, and calculate the indices.

3. Verify the resulting loading indices using both subjective and objective approaches.

1.3 Previous Research

A number of studies have already been carried out with metal concentrations sampled from Liverpool bay, over the years [3, 14, 16].

A study on metal data sampled from Liverpool bay in 1988 was conducted in the area of mathematical modeling, i.e., [3]. Techniques such as cluster analysis, principal component analysis (PCA) and fuzzy aggregation rules were used to study the distribution of metals within that year. The problem was to find an overall distribution of metal concentrations (or contaminations) given that the metals have different concentration scales and the way of combining the concentrations is not prescribed. Cluster analysis and PCA have been typical choices for this kind of problems [56], but results of both methods are difficult to interpret, unless the data has favorable structure and characteristics. During this study we found that, the difficulty in devising one single loading index comes from the fact that there is no *true* contamination distribution which we should try to match. Finally, fuzzy modeling was employed, and an analysis of the overall contamination of Liverpool bay with the seven metals was carried out using six aggregating operators. As a result we were able to conclude that using different aggregating operators, we can highlight different aspects of spatial distribution of heavy metal loading in Liverpool bay within that year (1988).

In the current study, we continue modeling environmental data sampled from Liverpool bay. With the large amount of environmental data available, further research to construct a mathematical model capable of processing or aggregating all seven metal data sets over a number of years, to produce one informative set, is required. A variety of aggregating operators are researched. Then, loading indices

are produced for each year and compared with respect to the type of information contained by each. The most informative and distinct indices are chosen with the aid of what are called Similarity Measures. The following is an outline of chapters to come. In the next chapter, we preprocess the data for missing and outlying observations. Chapter 3 introduces the concept of fuzzy set theory and research some applications of fuzzy set theory to the field of environmental science. Examples of extending 2-place aggregation operators to n-place ones is given in Chapter 4. Methods to measure similarities or differenes between the information held in the aggregated sets are presented in Chapter 5. Data sampled from Liverpool and Morecambe bay (in 1988) are then used as templates to find the best consistent similarity measure and most informative indices. A temporal change of metal concentrations in Liverpool bay is studied and presented in Chapter 6, over the years, 1986-1992. We conclude our findings in a mathematical and environmental context, in Chapter 7.

The concept of Fuzzy set theory is chosen to mathematically interpret the spatial distribution of overall metal loading in two marine environmental regions, Liverpool bay and Morecambe bay.

Chapter 2

Data Preprocessing

In this chapter we examine the raw data for missing values and outliers, both of which are pertinent characteristics to ecological data of the type considered here.

2.1 Introduction

In the first chapter, we introduced two ecologically studied systems, Liverpool and Morecambe bay, in the U.K. In this chapter, we shall screen the environmental data sampled from both Liverpool and Morecambe bay for any peculiarities. Here we find it important to understand the limitations of the tools used to collect the data from an ecosystem, in order to deal with measurement errors within the data as best as possible. Afterwards, outlier testing is carried out to locate extreme observations within the data. As a result, a finalized and acceptable version of the environmental data is obtained.

It is very unusual for real or observational data to arrive without problems. Most of the time, the process of screening or sifting data can consume considerably more time and effort than the primary analysis of interest. A typical problem in real data are the missing observations. One solution is to discard the data point and all entries associated with it, at which this missing value occurs. But in observational data analysis, scientists who collect the data, are uncomfortable about discarding existing information, possibly due to the unavailability of an alternative sample that

can be used in the place of the missing one. It might be difficult to obtain another sample due to: i) the complexity of the sampling procedure or ii) the specific time of the sampling. In our case, the sampling from the sediment of the bottom of the bay at a certain location (station) cannot be easily repeated (see Chapter 1). Therefore, if discarding data points containing the missing observations is not favored, the only alternative is by way of estimation. Since this solution covers a wide range of methods, the researcher must try to understand the reason behind the occurrence of missing observations before choosing the method of estimation.

It is usually assumed that quantitative data follow a normal distribution. Often, however, observational data do not meet this assumption. Assessing data distribution is also important since it can assist the analyst in identifying and discarding outliers, [43].

2.2 Choice of Base Data: Original metals or relative to Aluminum content?

We start by considering which type of base metal data is more appropriate for our mathematical research. It was pointed out that although heavy metal concentrations were measured in the same unit, the scale range as well as the ecological effect of a metal is specific and different for each metal. For example, Mercury (Hg) has detectable values ranging from 0.02 to 2.09 $\mu g g^{-1}$, while lead (Pb) has values ranging between 70 and 1214 $\mu g g^{-1}$. On the other hand, this large difference in scales between the metals, does not indicate the "harmfulness" or degree of pollution of a metal in Liverpool Bay, (i.e., a small amount of Mercury can be more harmful than a large amount of, say, Chromium).

Also, in our initial research [3], relative concentrations of heavy metals to aluminum content was suggested by the domain expert. This computation is done by dividing the concentrations of each metal at the j^{th} station by the aluminum content at that station. In ocean science, aluminum is called a 'normalizing factor'.

This method of normalization is used to "strip off" the terrestrial effect of Liverpool bay sediment from the sampled data. In other words, if the sediment naturally absorbs a relatively high amount of aluminum, it also absorbs other metals. Thus, increased metal concentrations at that particular station might not be indicative for contamination but may be the expected background concentration. Normalizing using aluminum content would eliminate this uncertainty. In [16], the choice of using data relative to aluminum is used to study the geochemistry of heavy metals in the environment[1] or aid in estimating the degree of trace element enrichment in sediments.

In [3], the normalization of metal concentration with aluminum content did NOT have a significant effect on the final result, compared to that when using the original metal data. Hence, we shall consider the original metal data suitable and sufficient for this mathematical research.

2.3 Missing Observations

One of the common problems in multivariate data analysis, is the presence of missing values. This was the case with the Liverpool bay data used in [3]. Therefore, scanning all metals for missing observations, is an important step (annually sampled data sets in *Appendix (A)*).

In our case, values were registered as missing because they were not detected during trace metal analysis [14, 15], of sediment samples. That is, the instrument used in trace metal analysis can only detect values above a certain minimum level for each metal. Accordingly, concentrations less than the minimum detected level are considered *undetectable* and NOT missing. So, it seemed reasonable to replace the undetectable concentrations of a metal by the minimum concentration of the same metal. Station $P09$ had no record of any concentrations for the 7 metals and was removed from the 1986 data set.

[1] That is, the relationship between where a metal is concentrated and the type of sediment it deposits in.

Table 2.1: Statistical descriptors of original data with missing observations

Liverpool bay 1986	Hg	Cd	Cr	Cu	Ni	Pb	Zn
N	60	60	60	60	60	60	60
Mean	1.10	0.21	22.51	83.79	32.6	161.9	325.92
StDev	0.47	0.15	7.23	229.25	7.02	150.72	134.31
Q1	0.79	0.1	18.28	45.23	28	101.25	247
Median	1.04	0.19	22.5	55	31.35	120.5	309.5
Q3	1.4	0.28	25.15	64.8	35	175.5	356.25
Minimum	0.3	0.05	0.05	1.31	22	27.5	126
Maximum	2.45	0.79	48.3	1826	59	1105	952
Skewness	0.68	1.47	0.68	7.69	1.54	4.73	2.69
Kurtosis	0.27	3.03	3.4	59.43	3.31	26.98	9.83
1987							
N	57	57	57	57	57	57	57
Mean	1.16	3.7	91.78	79.06	42.17	233.49	386.16
StDev	0.41	10.02	95.68	30.4	5.57	191.42	158.85
Q1	0.9	0.7	65.6	62.55	38.05	157	297.5
Median	1.1	1.1	76.4	73.3	41.1	186	351
Q3	1.4	2.1	93.85	84.7	44.45	224	405.5
Minimum	0.4	0	41.4	43.6	33.7	87	222
Maximum	2.1	61.8	788.8	206.1	58.6	1196	1103
Skewness	0.51	4.82	7.14	2.72	1.1	3.79	2.59
Kurtosis	-0.36	24.34	52.83	8.99	0.81	15.12	8.06

Continued, Table 2.1: Statistical descriptors of original data with missing observations

Liverpool bay 1988	Hg	Cd	Cr	Cu	Ni	Pb	Zn
N	70	70	70	70	70	70	70
Mean	0.54	0.65	65.36	70.7	40.69	234.2	280.39
StDev	0.49	0.47	13.91	48.25	9.23	224.55	126.53
Q1	0.16	0.36	54	42.5	34	103.5	195
Median	0.36	0.51	65	51	39	135.5	246
Q3	0.78	0.76	74.25	73.5	45	260.5	318
Minimum	0.02	0.11	38	23	25	70	135
Maximum	2.09	2.46	96	225	68	1214	904
Skewness	1.16	2.11	0.37	1.64	1.2	2.47	2.44
Kurtosis	0.62	5.62	-0.4	1.58	1.7	6.58	8.28
1989							
N	61	61	61	61	61	61	61
Mean	0.47	0.52	67.58	77.32	27.22	146.48	246.72
StDev	0.18	0.56	17.26	48.68	4.63	126.92	90.35
Q1	0.34	0.24	61.95	44.8	24.8	73.5	180.6
Median	0.45	0.31	69.3	59.4	26.6	96.1	218.1
Q3	0.54	0.66	75.55	95.85	29.35	144.35	295.15
Minimum	0.1	0.09	0.2	23.3	14.1	45.7	137.1
Maximum	1.19	2.99	98.4	264	44.8	624.3	531.1
Skewness	1.37	3	-1.35	1.68	0.78	2.32	1.33
Kurtosis	3.59	10.05	3.87	3.1	3.46	4.98	1.58

Continued, Table 2.1: Statistical descriptors of original data with missing observations

Liverpool bay 1990	Hg	Cd	Cr	Cu	Ni	Pb	Zn
N	26	26	26	26	26	26	26
Mean	0.44	0.23	29.57	24.83	22.08	92.01	122.88
StDev	0.31	0.16	17.77	14.54	5.7	76.77	56.46
Q1	0.21	0.11	19.38	15.18	18.85	54	73.68
Median	0.43	0.19	23.8	20.55	22.05	74.45	109.65
Q3	0.68	0.33	33	29.25	25.78	92.65	176.7
Minimum	0.02	0.05	8	5.5	7.3	40	52.9
Maximum	1.08	0.6	76.6	67.4	34.2	413.1	231.1
Skewness	0.46	0.99	1.59	1.6	-0.19	3.44	0.53
Kurtosis	-0.65	0.14	2.21	2.68	0.84	13.01	-1.04
1991							
N	40	40	40	40	40	40	40
Mean	0.64	0.06	59.1	92.08	35.73	96.08	139.83
StDev	0.63	.05	18.5	380.05	10.86	89.52	101.87
Q1	0.34	0.03	47.33	13.08	30.3	46.95	85.05
Median	0.46	0.05	52.7	18.35	33.45	58.45	104.45
Q3	0.7	0.07	65.15	23.58	37	93.83	151.73
Minimum	0.19	0.01	38.5	9.7	25	37.1	46.9
Maximum	4.06	0.22	129	2397.6	78	415.6	624.6
Skewness	4.35	1.86	2.1	6.04	2.73	2.34	3.25
Kurtosis	22.43	3.1	5.2	37.28	8.56	4.83	13.11

Continued, Table 2.1: Statistical descriptors of original data with missing observations

Liverpool bay 1992	Hg	Cd	Cr	Cu	Ni	Pb	Zn
N	40	40	40	40	40	40	40
Mean	0.64	0.06	2.37	82.14	35.73	96.08	139.83
StDev	0.63	0.05	2.81	318.4	10.86	89.52	101.87
Q1	0.34	0.03	1.3	13.08	30.3	46.95	85.05
Median	0.46	0.05	1.6	18.35	33.45	58.45	104.45
Q3	0.7	0.07	2.3	23.58	37	93.83	151.73
Minimum	0.19	0.01	0.5	9.7	25	37.1	46.9
Maximum	4.06	0.22	17.4	2000	78	415.6	624.6
Skewness	4.35	1.86	4.36	5.93	2.73	2.34	3.25
Kurtosis	22.43	3.1	21.74	36.18	8.56	4.83	13.11
Morecambe bay 1988							
N	201	201	201	201	201	201	201
Mean	0.11	0.2	28.58	19.14	10.63	66.48	71.33
StDev.	0.07	0.42	12.65	18.08	4.55	52.34	33.05
Q1	0.04	0.09	18.3	11.80	7.74	45	48.7
Median	0.09	0.14	28.2	14.9	10.3	56.6	69.6
Q3	0.17	0.19	37.2	20.75	12.85	71.95	89.8
Minimum	0	0.02	6.63	2.19	2.43	0.2	0.56
Maximum	0.34	5.69	98.80	170	54.5	505	261
Skewness	0.47	11.38	1.07	5.03	4.64	4.83	1.29
Kurtosis	-0.74	146.11	3.54	34.23	42.36	31.77	4.92

Table 2.1 summarizes the data sets with the aid of some statistical descriptors. As mentioned in Chapter 1, the heavy metal concentrations were measured in the same units, $\mu g/g$ of sediment, keeping in mind that the scale range for each metal is specific and different for most metals. This difference in the magnitude of concentrations is chemically established between the metals and can be seen clearly in all sampled

Table 2.2: Anderson Darling normality test of data with missing observations

Liverpool bay		Hg	Cd	Cr	Cu	Ni	Pb	Zn
1986	P-Value	0.117	0	0	0	0	0	0
	A-Squared	0.592	1.769	1.578	18.918	1.8	8.281	3.821
1987	P-Value	0.021	0	0	0	0	0	0
	A-Squared	0.896	14.79	12.879	4.365	1.794	9.689	4.618
1988	P-Value	0	0	0.285	0	0	0	0
	A-Squared	3.227	3.639	0.439	7.542	1.654	7.738	4.157
1989	P-Value	0.002	0	0	0	0.015	0	0
	A-Squared	1.335	6.404	1.556	3.158	0.957	7.375	2.175
1990	P-Value	0.509	0.017	0	0.002	0.889	0	0.038
	A-Squared	0.323	0.918	1.752	1.307	0.19	3.915	0.775
1991	P-Value	0	0	0	0	0	0	0
	A-Squared	4.953	3.105	2.555	13.005	3.507	6.14	4.087
1992	P-Value	0	0	0	0	0	0	0
	A-Squared	4.953	3.105	6.923	12.757	3.507	6.14	4.087
Morecambe bay		Hg	Cd	Cr	Cu	Ni	Pb	Zn
1988	P-Value	0	0	0	0	0	0	0.001
	A-Squared	4.93	43.94	1.59	21.03	5.02	21.2	1.41

years. Also clear is the difference between the size of annually sampled data. Finally, the Anderson Darling test is used to check the assumption of normality. A p-value > 0.05, illustrated in Table 2.2. We found that most variables did not have a normal distribution, as usually assumed for observational data. In the next section, we search for outliers.

2.4 Outlier Detection

An observation is an "outlier", if it appears to deviate markedly from other members of the sample in which it occurs. Outliers are usually caused by imprecision in the data collection. An outlying observation may be merely an extreme manifestation of the random variability inherent in the data. If this is the case, the values should be retained and processed in the same manner as the other observations in the sample. On the other hand, an outlying observation may be the result of gross deviation from prescribed experimental procedure, or an error in calculating or recording the numerical value, i.e., human error, or the actual physical limitation of field or laboratory equipment [35, 37]. Although an outlier may not be immediately apparent on examination of the data, its presence will affect the accuracy of a study. Therefore, as in our case, it may be desirable to investigate the reason behind this aberrant value. Also, a statistical test may always be used to lend support to a judgment that a physical reason does exist for an outlier.

There are a number of criteria for testing outliers [34, 37, 38]. It should be pointed out that almost all criteria for detecting outliers are based on an assumed underlying normal distribution of the data, e.g., Dixon's test (for small data samples $n < 25$) and Grubbs test ($n > 25$). When the data are not approximately normally distributed, it is stated that the probabilities associated with these tests will be different. So, what if the sample fails to approximate to normality after the analyst exhausts all possible transformation of the data to a normal distribution? In this case, Chebyshevs' Inequality can be used as a procedure to check for the presence of suspected outliers in non-normally distributed samples.

2.4.1 Grubbs' Test

The following procedure is a test which is used to detect outlying observations in approximately normalized samples, introduced by Grubbs' [37, 38]. This test is considered to be a modified 't' test. It enables the researcher to compute the statistics for the largest and the smallest values, within the data samples.

In this test, the doubtful observation is included in the calculation of a numerical value of the sample criterion (or statistic). The statistical value is then compared with a critical value, based on the theory of random sampling, to determine whether the doubtful observation is to be retained or rejected. The critical value is that value of the sample criterion, which would be exceeded by chance with a specified small probability. This is on the assumption that all the observations did indeed constitute a random sample from a common system of causes. This significance level can be thought of as the risk of mistakenly rejecting a good observation. Therefore, if there exists a real change in the value of an observation that arises from non-random causes (human error, loss of calibration instruments, change of measuring instrument, or even change of time measurements) then the observed (or calculated) value would exceed the "critical value" based on random sampling theory. Tables of critical values are available for several different significance levels, for example, 5% and 1%. For statistical tests of outlying observations, it is generally recommended that a low significance level, such as 1%, be used and that significance levels greater than 5% should not be common practice.

Criteria For Single Samples:

The following is a summary of Grubbs criteria. Let the sample of n observations be denoted in order of increasing magnitude by $x_1 \leq x_2 \leq x_3 \leq \cdots \leq x_n$. Then apply the following steps.

1. Select the level of significance.

2. Calculate the observed criteria. For the doubtful value x_n or x_1 , i.e., the

largest and smallest value respectively, compute

$$T_n = \frac{(x_n - \bar{x})}{s}, \qquad T_1 = \frac{(\bar{x} - x_1)}{s}$$

with mean and standard deviation $\bar{x} = \frac{\sum_n^{i=1} x_i}{n}$ $s = (\frac{\sum_n^{i=1}(x_1 - \bar{x})^2}{n-1})^{1/2}$, respectively. The critical values of 'T' for testing the largest or smallest values at $\alpha = 1\%, 2.5\%$ and 5%, i.e., one-sided significance levels, are given in *Appendix (B).*

3. If the observed criterion, T_n or T_1, at the chosen significance level α is equal to or exceeds the critical value, $T_k \geq T(\alpha, n)$, for $k = 1$ or n, then the doubtful value x_n (or x_1) is an outlier according to this criterion.

4. Grubbs test can also be used to determine whether or not the $2nd$ smallest, $2nd$ largest or any other value is an outlying observation. The only difference is that each time an outlier has been detected and rejected, the observations must be re-numbered and used to compute a new mean and standard deviation before proceeding with the above test criterion.

Grubbs [37] pointed out that selecting a significance level α, sometimes depends on whether the researcher believes that outliers can or cannot occur simultaneously on both sides of a sample. For instance, suppose we are interested in outliers occurring on *either* side, but do not believe that outliers can occur on both sides, simultaneously. This is because, we believe that at some time during the experiment something possibly happened to cause an extraneous variation on the high side or on the low side, but that it was very unlikely that two or more such events could have occurred. That is, one being an extraneous variation on the high side *and* the other an extraneous variation on the low side. If in this case the researcher uses the $\alpha = 0.05$ point from the table in *Appendix (B)* as the critical value, the true significance level would be twice 0.05, or 0.10. So, if we wish a significance level of 0.05 and not 0.10, we must in this case use as a critical value the 0.025 point.

2.4.2 Chebyshev Inequality

Sometimes, even with the help of transformation functions, the data samples may not approximate a normal distribution. In this case, Grubbs test is not applicable. Therefore, we turned to a method that did not rely on the assumed normality of the data sample, the Chebyshev Inequality. The inequality is valid for all data distributions [42]. It states the following:

If a random variable X has a mean μ and variance σ^2, then for every $\frac{\epsilon}{\sigma} \geq 1$,

$$P(\mid X - \mu \mid \geq \epsilon) \leq \frac{\sigma^2}{\epsilon^2} \tag{2.1}$$

In words, Chebyshev's inequality states that the probability that X differs from its mean by at least ϵ, is less than or equal to $\frac{\sigma^2}{\epsilon^2}$. The inequality (2.1) can then be used to determine an interval, $I = [\mu - \epsilon, \mu + \epsilon]$, such that the probability that a random observation falls outside I is at most $\frac{\sigma^2}{\epsilon^2}$. Selecting a level of significance $\alpha = 0.05$ or 0.01, the researcher is able to compute ϵ from $\frac{\sigma^2}{\epsilon^2} = \alpha \Rightarrow \epsilon = \frac{\sigma}{\sqrt{\alpha}}$.
Outliers in this case are determined as the values outside the interval I.

Example (2.4.2): Let a sample X with any distribution have $\mu = 25$ and variance, $\sigma^2 = 16$. Then, $P(\mid X - 25 \mid \geq \epsilon) \leq \frac{16}{\epsilon^2}$.
To test that an observation $x = 100$ differs from a mean of 25 by ϵ is at most $\alpha = 0.01$, we compute, $\epsilon = \frac{\sigma}{\sqrt{\alpha}} = 40$.
Then, for any data set with $\mu = 25$ and $\sigma = 4$, at least a fraction $1 - \alpha$ of the data are within 4 standard deviations on either side of the mean, i.e., in the interval $[\mu - \frac{\sigma}{\sqrt{\alpha}}, \mu - \frac{\sigma}{\sqrt{\alpha}}] = [-15, 65]$.
In other words, $1 - \alpha = 0.99$ or 99% of the data can be expected to lie within ten standard deviations on either side of μ. But, for a random observation $X = 100$, we can say that the probability that it differs from a mean of 25 by 4 standard deviations is *greater* than 0.01. Hence, $X = 100$ is an outlier.

Finally, with observational data it is sometimes helpful to enlist the aid of a domain expert when conducting any outlier testing.

2.4.3 Outlier Testing: Results

Transformation of data samples that did not approximate to a normal distribution was carried out on all observations sampled from Liverpool bay (1986-1992) and Morecambe bay (1988). This was done to modify the scale upon which the data were measured, so that the assumption of normality was made valid and a search for outliers was done, using Grubbs test. In some cases, transformation of the data did not validate the assumption of normality, and in this case we relied on Chebyshevs inequality.

The logarithmic transformation, $F(X) = \log X$, in addition to functions from a family of power transformations on X, were chosen. The latter was of the form

$$F(X) = X^{\lambda} \tag{2.2}$$

where the parameter $\lambda \in \Re$. The value of λ could be adjusted so that $F(X)$ was as close as possible to an approximate normal distribution, i.e., P-value > 0.05. At first, typical power functions for $\lambda = -2, -1, -0.5, 0.5, 1, 2$ and $\log X$ were tried. Tuning of λ values in equation (2.2) was done to find the best transformation with the highest P-value, by manually increasing or decreasing λ by 0.1. After each transformation (for each value of λ), each metal sample was tested again for normality for all years.

Outlier testing was then conducted on all metals collected in Liverpool and Morecambe bay. Testing of suspected outliers of the largest and smallest observations was done. Metal samples that were successfully transformed to an approximately normal distribution were tested using Grubbs test, whereas samples that failed to satisfy the normality assumption were tested using Chebyshevs inequality. In all, only three data samples registered outliers, i.e., Liverpool bay in 1986 and 1987, and Morecambe bay in 1988. Outliers were only found for the largest observations. Table 2.3 summarizes the outlying observations.

Stations with detected outliers were removed from the respective annually sampled data sets. Descriptive statistics were calculated for the three new data samples in *Appendix (B)*. Further outlier testing of the 2nd largest observations of normally

Table 2.3: Outliers detected in the two environmental regions using Grubbs Test for normal samples and Chebyshevs Inequality for non-normal samples.

Sampling Data	Normality Y/N	Largest observation	Sampling station	New sample size
Liverpool bay				
1986				58
Cadmium	N	1826	M10	
Lead	N	1105	M09	
Zinc	N	952	M09	
1987				54
Cadmium	Y	61.8	K08	
Chromium	N	788.8	N09	
Lead	N	1196	M09	
Morecambe bay 1988				198
Zinc	Y	381	485	
Cadmium	N	5.69	33	
Chromium	N	98.8	485	
Copper	N	170	485	
Nickel	N	54.5	485	
Lead	N	505	363	

distributed metals, that registered outliers, were tested in the new data samples. Similar steps previously used to test outliers of the first smallest or first largest observation using Grubbs criterion were followed for the normalized samples. No further outliers were detected. Correlation coefficients between the metals were calculated for each finalized data set, *Appendix (B)*.

2.5 Conclusion

Data samples from Liverpool bay and Morecambe bay were processed for missing and outlying observations. Annually sampled metal data sets from Liverpool bay in 1986 and 1988 were the only years that showed missing values, with 1986 containing the largest number of missing observations. Based on scientific expertise, missing observations were substituted by the minimum sampled concentration of the same metal instead of discarding the data point.

Testing of outliers was done using two approaches. The outlier tests were based on whether the metal sets were or were not approximately normally distributed, i.e., the Grubbs' test and Chebyshevs' inequality, respectively. Only samples of 1986 and 1987 from Liverpool bay, and 1988 from Morecambe bay registered the presence of outliers. As a result of this finding, the data points containing the outliers were discarded.

Preprocessing of metal data for missing observations and suspected outliers was carried out. The finalized version of annually sampled environmental data, listed in *Appendix (B)*, shall be used to study the spatial distribution of metal concentrations in Liverpool bay, throughout the thesis.

Chapter 3

Using Fuzzy Set Theory in Environmental Sciences

In this chapter we introduce the basics of fuzzy set theory and details several applications related to field of environmental sciences. Also, we attempt to construct a reference (model) set of contamination of Liverpool bay.

3.1 An Introduction to Fuzzy Set Theory

The concept of a fuzzy set can be directly attributed to L.A. Zadeh, from his seminal work in 1965 [79]. Zadeh's purpose for introducing the fuzzy set was to provide a concept which maybe of use with classes (or sets) of objects encountered in the real physical world. These classes, more often than not, are characterized by imprecision, which for various reasons cannot have or do not have precisely defined attributes of membership (i.e., boundaries). For example, the set of plants clearly include roses, tulips, vegetables, etc. as its members, and clearly excludes such objects as rocks, animals, gases etc. However, such objects as bacteria, plankton, etc. have an ambiguous status with respect to the set of plants. Similarly with heavy metals, the property of 'metal contamination' includes all conditions from natural occurring levels to pollution. These inexactly defined classes are the basis of fuzzy sets. Therefore, *fuzzy set* is a class of objects with a continuum of grades of membership.

Ordinary or crisp sets allow only for binary membership (i.e., true or false); an object is a member or is not a member of any given set. Fuzzy sets, however, consider the possibility of a partial membership. Therefore, fuzzy sets are seen as a generalization of crisp sets to situations where the class boundaries cannot be defined.

The following section is an introduction to the basic theory of fuzzy sets. For more information on fuzzy set theory refer to the following texts [27, 44, 47, 49, 79].

3.1.1 Definitions

Fuzzy sets

Let X be a universe of discourse (i.e., a universal set X that covers a definite range of objects), with a generic element of X denoted by x. Thus $X = \{x\}$.

Let a crisp set A be defined with respect to X, with the aid of a *characteristic function*, $\mu_A(x)$. This function describes the membership in the set by declaring which elements x of X are members of the set A and which are not. The set A is defined by μ_A as follows:

$$\mu_A(x) = \begin{cases} 1 & \text{for } x \in A \\ 0 & \text{for } x \notin A \end{cases} \tag{3.1}$$

In other words, the characteristic function associated with A is a mapping, that formally can be expressed by

$$\mu_A : X \longrightarrow \{0, 1\}.$$

Example 3.1.1 : The characteristic function

$$\mu_A(x) = \begin{cases} 1 & \text{for } 0 \leq x < 1.35 \\ 0 & \text{otherwise} \end{cases}$$

describes the set of all non-negative real numbers smaller than 1.35. The point of discontinuity at 1.35 can be seen to be natural, if the characteristic function is interpreted as the set of body-heights of children who are shorter than 1.35 meters.

The adequacy of characteristic functions with codomain $\{0, 1\}$ has to be questioned if, for instance, body heights are considered for which a person should be called '*tall*'. The word *tall* can have different meanings depending on the context in which it is used, e.g., for a child or an adult? Then, if we wanted to represent the set of *tall* adults, the use of a fuzzy set in this situation would free us from the restriction of having to categorize each person as being or not being a member of this set. Of course there are some body heights which will always be classified as *tall* (e.g., 1.8 m) or *not tall* (e.g., 1.3 m) but for others (e.g., 1.45 m) a definite classification is hard to find. This method would therefore allow us to make more subtle distinctions and represent more closely the types of concepts which humans use, such as *old, young, short, fat,* and so on.

One method to model gradual transition is to use other values of membership in addition to 0 (does certainly not belong to it) and 1 (does certainly belong to it). A mathematically simple way to introduce a gradual membership consists in taking the values of membership from the compact interval $[0, 1]$. Therefore, if our universal set was the set of real numbers, concepts such as *small, large, close to 5,* and so on, would be more naturally represented as a fuzzy set than as a crisp set.

Therefore, a fuzzy set can be seen as a generalization of the idea of a crisp (non-fuzzy) set, by extending the range of the characteristic function from the binary pair

$\{0, 1\}$ to the unit interval, I=[0, 1]. This can be achieved by a function called the *membership function*, which assigns values to the elements of X within this specified range. Each such value, $\mu_A(x)$, for $x \in X$ is called a "degree of membership" or "membership grade" of x in A.

Definition 1 (Fuzzy Set). *: For a universal set X, a **fuzzy set** A of X is associated with a membership function:*

$$\mu_A : X \longrightarrow [0, 1]. \tag{3.2}$$

$\mathcal{P}(X)$ denotes the class of all fuzzy sets on X.

One of the first questions asked concerning fuzzy models, is the relationship of fuzziness to probability. Are fuzzy sets just a clever disguise for statistical models? In one word, the answer is NO. In fuzzy sets, the term 'possibility' should not be equated with the statistical concept of 'probability'. Here, possibility refers to the value of the membership function (which is used to construct the fuzzy sets) associated with a given value of a attribute x and is not derived from a probability distribution. Also, these two types of models possess different kinds of information: Fuzzy memberships represent similarities of objects to imprecisely defined properties, while probabilities convey information about relative frequencies (e.g., the relative frequency, r/n, of an event A occurring r out of a total of n repeated experiments) [9].

Membership Functions

Any fuzzy set A of X can be described by directly assigning a degree of membership $\mu_A(x)$ to each element $x \in X$. This is practically feasible only if the universal set consists of a finite number of elements. If the number of elements in X is very large or a continuum is used for X (e.g., to measure temperature or velocity), then $\mu_A(x)$ is best represented with the help of an appropriate parameterized function, also known as a membership function. This would allow the user to adjust the parameters within the function according to the given problem. Also, the assignment

of the membership function of a fuzzy set is subjective in nature and, in general, should reflect the context in which the problem is viewed [44, 49, 47, 50].

If $X = \Re$, then in most cases linguistic expressions like 'tall', 'about 10', and 'approximately between reference values a and b' may be encountered. These expressions may be interpreted using a suitable class of membership functions $\mu : X \longrightarrow [0, 1]$. One function that can present an interpretation of 'tall' is the *monotonic non-decreasing* function

$$\mu(x) = \begin{cases} 0, & \text{if } x \leq a \\ \frac{x-a}{b-a}, & \text{if } a \leq x \leq b \\ 1, & \text{if } x \geq b \end{cases} \tag{3.3}$$

where $a < b$. This is also known as an asymmetric left variant type membership function.

Other interpretations are piece-wise *linear* functions, whose parameters are the coordinates of the defining points. An example of this is the normalized version of the data sets in X, [76]

$$\mu(x) = \begin{cases} \frac{x}{b}, & \text{if } a \leq x \leq b \\ 0, & \text{if } x < a \\ 1, & \text{otherwise} \end{cases} \tag{3.4}$$

where $a = \min\{x\}$ and $b = \max\{x\}$.

To interpret linguistic expressions like 'about 10', we may simply adopt symmetrical *triangular* functions like

$$\mu(x) = \begin{cases} \frac{x-a}{b-a}, & \text{if } x \in (a, b], \\ \frac{c-x}{c-b}, & \text{if } x \in (b, c], \\ 0, & \text{otherwise}, \end{cases} \tag{3.5}$$

as well as *Guassian* curves like

$$\mu(x) = e^{-a(x-m)^2} \tag{3.6}$$

where $a > 0$, $m \in \Re$. Or the trigonometric based cosine function

$$\mu(x) = \begin{cases} \frac{1+\cos(a\pi(x-m))}{2} & \text{when } x \in [m - \frac{1}{a}, m + \frac{1}{a}] \\ 0 & \text{otherwise} \end{cases} \tag{3.7}$$

Again, where $a > 0$, $m \in \Re$. Some membership functions are specific, in that they can only be used to describe certain classes of objects. These were called '*non-admissible functions*' [44, 49]. An example is the class of *Exponential* functions like

$$\mu(x) = \begin{cases} 1 - e^{(-a(x-b))}, & \text{if } x \geq b \\ 0, & \text{if } x < b \end{cases} \tag{3.8}$$

where $a > 0$ and $b \in \Re$. Kandel, [44], characterized such a function as a monotonically increasing function that does not satisfy the condition $0 \leq \mu(x) \leq 1$ for all $x \in X$ (but only approximates to 1).

In the general formulas of (3.6) and (3.7), m denotes the real number for which the membership grade is required to be one, and a is a parameter that determines the rate at which, for each x, the function decreases with the increasing difference $|m - x|$ [47].

Similarly, the expression 'approximately between a reference value b and a reference value c' is most simply characterized by the *trapezoidal* function

$$\mu(x) = \begin{cases} \frac{x-a}{b-a}, & \text{if } a \leq x < b \\ 1, & \text{if } b \leq x \leq c \\ \frac{x-d}{c-d}, & \text{if } c < x \leq d \\ 0, & \text{if } x < a \text{ or } x > d, \end{cases} \tag{3.9}$$

where $a < b < c < d$ and a, b, c, $d \in \Re$.

Therefore, with the availability of various membership functions, fuzzy sets representing the same concepts may vary considerably. As an example consider the following.

Example 3.1.1: Consider three fuzzy sets whose membership functions are given by (3.5), (3.6) and (3.7), respectively. These sets can be used to express the 'class of real numbers that are close to 2'. In these functions, let $a = 1$, $b = 2$, $c = 3$ and $m = 2$. In spite of their differences, the three fuzzy sets are similar in the sense that the following properties hold for each A_i ($i \in \mathbb{N}_3$)

(i) $\mu_{A_i}(2) = 1$ and $\mu_{A_i}(x) < 1$ for all $x \neq 2$

(ii) A_i is symmetric with respect to $x = 2$, that is $\mu_{A_i}(2 + x) = \mu_{A_i}(2 - x)$, $\forall x \in \Re$

(iii) $\mu_{A_i}(x)$ decreases monotonically from 1 to 0

The three membership functions are also similar in that numbers outside the interval $[1, 3]$ are excluded from the associated fuzzy sets. This is because their membership grades are either equal to 0 or negligible.
These properties are also necessary in order to represent the given concept of, say, '*tall*'. This similarity does not reflect the concept itself, but rather the context in which the concept of '*tall*' is used within the context of adults or children [47].

Whether a particular shape is suitable or not can be determined only in the context of a particular application. According to Klir and Yuan [47], however, many applications were found not to be that overly sensitive to variation in shape. In such cases, it was suggested that, the use of a simple shape is more convenient, such as the triangular shape of μ_{A_i}. Practically, except for some vague semantic guidelines (i.e., concepts that can only be expressed linguistically, such as in Example 3.1.1), there are no restrictions in designing a membership function.

3.1.2 Notations and concepts

In this section we shall introduce some basic notations and concepts used through out the text. First, Table 3.1 presents some common mathematical symbols and a glossary of some special fuzzy sets.

Table 3.1: Some mathematical and fuzzy set notations

Mathematical symbols	
$x = \{x_1, x_2, \cdots, x_n\}$	The set of features
$S = \{s_1, s_2, \cdots, s_m\}$	the set of objects
X	The data set matrix comprising of m (rows) by n (columns), such that $X \subset \Re^n$
n	The dimensionality of the feature space (which is also the number of variables of x)
m	The number of objects of s
$x_i(s_j)$	The value of the i^{th} variable for the j^{th} data point
Fuzzy set symbols	
$U = \{u_1, u_2, \cdots, u_m\}$	Discrete finite universal set (universe of discourse)
$\mathcal{P}(U)$	Set of all fuzzy subsets of U
$\mu_A(u_i)$	Degree of membership of $u_i \in U$ in the fuzzy set A
ϕ	Empty set
M	0.5 fuzzy set, where all $\mu_A(u) = 0.5$
$LI(u_i)$	Loading index value of $u_i \in U$
I	Unit fuzzy set, where all $\mu_A(u) = 1$
Singleton fuzzy set, A	A is said to be a singleton fuzzy set if $\exists k$ such that $\mu_A(u_k) \neq 0$.

Basic concepts of fuzzy sets

Here, we shall introduce some basic concepts of fuzzy sets. Let A be a fuzzy set on U, with membership function $\mu_A : U \longrightarrow [0, 1]$.

- The α-**cut** of a fuzzy set A is a crisp set A^α. This set contains all elements of the universal set, whose membership grades in A are greater than or equal to a specified value, $\alpha \in [0, 1]$. In other words,

$$A^\alpha = \{u| \quad \mu_A(u) \geq \alpha\}. \tag{3.10}$$

  Then the new set is a crisp one with the following membership grades,

$$\mu_{A^\alpha}(u) = \begin{cases} 1 & \text{if } u \in A^\alpha \\ 0 & \text{otherwise} \end{cases} \tag{3.11}$$

  A variation of the α-cut is the **strong** α-cut [44]. It is defined on U and as a crisp set,

$$A^{\alpha+} = \{u| \quad \mu_A(u) > \alpha\}. \tag{3.12}$$

- A fuzzy set A of U is called **normal** if there exists at least one element $u \in U$ such that $\mu_A(u) = 1$, otherwise it is called **subnormal** (i.e., $\mu_A(u) < 1$).

- The **core** of A is a crisp subset of U which consists of all elements with membership grades equal to 1.

$$Core(A) = \{u| \quad \mu_A(u) = 1 \text{ and } u \in U\}. \tag{3.13}$$

  The core can be thought of as the most representative elements of A.

- Given A, a fuzzy set of U, the **support** of A is a crisp set of U whose elements all have nonzero membership grades in A.

$$Supp(A) = \{u| \quad \mu_A(u) > 0 \text{ and } u \in U\}. \tag{3.14}$$

It is obvious that the support of A is equivalent to the strong α-cut of A when $\alpha = 0$, i.e., $A^{0+} = \{u| \ \ \mu_A(u) > 0\}$. Also, the 1-cut of A, denoted $A^1 = \{u| \ \ \mu_A(u) \geq 1\} = \{u| \ \ \mu_A(u) = 1\}$, is the same as the core of A.

- The **height** of a fuzzy set A is the largest membership grade obtained by any element, denoted as:

$$height(A) = \sup_{u \in U}[\mu_A(u)] \tag{3.15}$$

which becomes

$$height(A) = \max_{u \in U}[\mu_A(u)] \tag{3.16}$$

for a finite U. Therefore a normal fuzzy set is defined to have height equal to 1.

- The **cardinality** of a fuzzy set A on a finite U is

$$|A| = \sum_{i=1}^{n} \mu_A(u_i), \quad u_i \in U \tag{3.17}$$

while the **relative cardinality** of A is

$$\|A\| = \frac{|A|}{|U|} = \frac{1}{n} \sum_{i=1}^{n} \mu_A(u_i), \quad u_i \in U \tag{3.18}$$

- The **complement** of a fuzzy set A on U ($\mu_{\bar{A}} : U \longrightarrow [0,1]$) is a fuzzy set $\bar{A}$ on U, defined by a function $h : [0,1] \longrightarrow [0,1]$ as

$$\mu_{\bar{A}} = h(\mu_A), \quad \forall u \in U.$$

The function h is defined using the following set of axioms [28, 50]

(i) h is a function of one argument in $[0,1]$, taking values in $[0,1]$ (i.e., $\mu_{\bar{A}}(u)$ depends only on $\mu_A(u)$, $u \in U$).

(ii) $h(0) = 1$ and $h(1) = 0$;

(iii) h is continuous and strictly monotonically decreasing;

(iv) h is involutive, i.e., $\quad h(h(a)) = a, \quad a \in [0,1]$;

(v) $a + b = 1, \quad a, b \in [0,1] \iff h(a) + h(b) = 1$

These five axioms specify a unique function h as

$$h(a) = 1 - a, \quad \text{i.e., } \mu_{\bar{A}} = 1 - \mu_A. \tag{3.19}$$

Equation (3.19) is known as the **standard complement**.

- Let A and B be two fuzzy sets on U. Then A is said to be **contained** in B (or equivalently, A is a *subset* of B, or A is *smaller than or equal to* B) if and only if $\mu_A(u) \leq \mu_B(u)$, i.e.,

$$A \subseteq B \iff \mu_A(u) \leq \mu_B(u), \forall u \in U.$$

- Two fuzzy sets A and B are *equal*, $A = B$, if and only if $\mu_A(u) = \mu_B(u)$ for all $u \in U$.

Example 3.1.2: Let U be a list of possible holiday destinations with distances by air from London in miles, e.g., U = {(Cairo,2280), (Athens,1501), (Kuwait,3254), (Paris,215), (Casablanca,1293)}. Let the fuzzy set A correspond to "distance of air travel at most 1000 miles from London". From this context, we expect μ_A to be a decreasing function, which can be expressed using the function

$$\mu(u) = \begin{cases} \frac{1}{1+[\frac{1}{0.0099}(u-1000)]^2} & \text{when } u \in [0, 1000] \\ 0 & \text{otherwise} \end{cases}$$

Then, A can be defined as : A = {(Cairo,0.3), (Athens,0.8), (Kuwait,0.1), (Paris,1), (Casablanca,0.9)}. Applying some of the concepts mentioned above, we can see that the fuzzy set A has $height(A) = 1.0$, core$(A) = \{Paris\}$, $supp(A) = U$, and $A^{0.5}$ = { Athens, Paris, Casablanca }.

3.1.3 Basic operations on fuzzy sets

Operations on fuzzy sets are considered to be an extension of the classical set theoretic operations from crisp (ordinary) set theory. Two examples of classical operations are the union operation (i.e., $A \cup B = \{u|\ u \in A \text{ or } u \in B\}$) and the intersection operation (i.e., $A \cap B = \{u|\ u \in A \text{ and } u \in B\}$), defined for two crisp sets A and B. We use the same symbols in fuzzy set theory. In the following, intersection and union, are introduced in the framework of fuzzy sets. Let A and B be two fuzzy sets of some crisp set $U = \{u_1, u_2, \cdots, u_n\}$. The **intersection** of A and B, is a fuzzy set C for all $u \in U$, denoted as $C = A \cap B$, whose membership function is defined by

$$\mu_{A \cap B}(u) = \min[\mu_A(u), \mu_B(u)] = \mu_A(u) \wedge \mu_B(u) \tag{3.20}$$

Where 'min' or standard intersection denotes the minimum operator and is commonly symbolized by '$\wedge$'.

The **union** (or standard union) of A and B is a fuzzy set C, denoted $C = A \cup B$, whose membership function is defined by

$$\mu_{A \cup B}(u) = \max[\mu_A(u), \mu_B(u)] = \mu_A(u) \vee \mu_B(u) \tag{3.21}$$

Where 'max' denotes the maximum operator, symbolized by '$\vee$'.
These pair of operations min and max have favorable properties like the distributive laws

$$A \cap (B \cup C) = (A \cap B) \cup (A \cap C) \tag{3.22}$$

and

$$A \cup (B \cap C) = (A \cup B) \cap (A \cup C). \tag{3.23}$$

Also, the DeMorgan laws hold

$$\overline{A \cup B} = \bar{A} \cap \bar{B} \tag{3.24}$$

and

$$\overline{A \cap B} = \bar{A} \cup \bar{B} \tag{3.25}$$

Convenient arithmetic representation for the *minimum* and *maximum* operators are

$$\min(a, b) = \frac{a + b - |a - b|}{2}, \tag{3.26}$$

$$\max(a, b) = \frac{a + b + |a - b|}{2}. \tag{3.27}$$

Where a and b are real numbers and $|a - b|$ denotes the absolute value between a and b .

More operations on fuzzy sets will be presented in Chapter 4. But first, we discuss some applications of fuzzy set theory in the field of environmental science.

3.2 Environmental applications

Application of fuzzy mathematical methods in various fields has been discussed by many authors. Some of these examples are, in soil science [12, 13, 26, 58, 81], ecosystem and environmental management [11, 7, 55, 76] and transportation planning [46], just to name a few. In the next section we give a summarized survey of the application of fuzzy methods in some of these studies.

3.2.1 Soil fertility assessment

Application of fuzzy mathematical methods in soil sciences has been researched by many authors. Burrough (1989) [12], summarizes the reasoning behind using fuzzy methods in soil science very well. The author states that users of soil or environmental information have a clear notion (or central concept) of what they need, but are often unsure about just where the boundaries of this central concept should be drawn. An example of a vaguely formulated query is 'Where are all area's of marine sediment *significantly saturated* with disposed sewage?'. Such vaguely formulated

questions are then translated using the basic units of information available, i.e., collected data or expert knowledge.

In this case, fuzzy methods were seen appropriate whenever the user needs to deal with ambiguity or vagueness in mathematically or conceptually modeled data of empirical phenomena (i.e., data that rely solely on observation and experiments).

In [12] soil profile data (e.g., soil depth, chemical status, etc.) was analyzed using the standard Boolean model and a fuzzy set based model. In the Boolean model, a crisp membership function

$$\begin{aligned} \mu_A(x) &= 0 \quad \text{for } x < c \\ \mu_A(x) &= 1 \quad \text{for } x \geq c \end{aligned} \tag{3.28}$$

is used to describe the attributes $x \in A$, where c defines the exact boundary condition of A. Another approach, adopted in [12] is the Semantic Import model (SI). It uses a priori fuzzy membership function with which attributes can be assigned a degree of membership. The SI model was useful in situations where users have a good qualitative idea of how to group data by selecting the boundaries for the class intervals. A fuzzy memebership function suitable for the SI model is the symmetric function

$$\mu_A(x) = \frac{1}{1 + a(x-c)^2} \quad \text{for } x \in [0, P], \;\; P \in \Re^+ \tag{3.29}$$

The parameter a is the *dispersion index*, and c is the value of the property x at the central concept (where $\mu_A(c) = 1$). The parameter c is named the *ideal centre* or *standard index* [12]. For a chosen c, and defined lower and upper *cross-over* points b_1 and b_2 respectively, the value a is calculated such that $\mu_A(b_1) = 0.5 = \mu_A(b_2)$.

Case studies were used as examples for the application of the SI model, to deal with soil related queries in two geographical areas. Soil properties measured at various soil profiles were defined via symmetric (3.29) or asymmetric left (right) membership functions,

$$\begin{aligned} \mu_A(x) &= 1 \qquad\qquad\qquad\quad \text{for } x \geq c \\ \mu_A(x) &= \{1 + a(x-c)^2\}^{-1} \quad \text{for } x < c \end{aligned} \tag{3.30}$$

Table 3.2: Parameters of membership functions for Türen data

Soil property	Type of function	Lower cross-over value	Central value	Upper cross-over value
DPP	A	15	30	30
DMT	A	80	100	100
S1	S	20	40	60
C1	S	15	25	35
OM1	A	1.0	1.5	1.5
S2	S	20	40	60
C2	S	15	25	35
OM2	A	0.5	1.0	1.0
S3	S	20	40	60
C3	S	15	25	35
OM3	A	0.5	1.0	1.0

Key: DPP, depth of plough pan (cm); DMT, depth to mottling (cm); S1, C1, OM1, percent sand, clay and organic matter content of layer 1 (0-20 cm); other layers are 2, 30-40 cm; 3, 70-80 cm deep.
A: asymmetric function; S: symmetric function.

depending on a predefined concept by the user.

In [12], examples of case studies that illustrate the application of fuzzy set methods were summarized. In one case study, quantitative data of 11 soil properties were collected on a farm in Türen, Venezuela. The soil of the farm was surveyed on a 75 $\times$ 75 m regular grid over an area of 825$\times$ 375 m. The properties were gathered by: (i) sampling 69 profiles (points) at three different depths, 0-20, 30-40, and 70-80 cm, for sand, clay and organic matter content (9 properties), (ii) measuring the depth to plough pan (which was known to limit root growth), and (iii) measuring the depth to mottles (which is used to estimate drainage conditions). Table 3.2 summarizes the 11 soil properties. Membership functions (3.29) and (3.30) were used to reflect the general soil survey experience in the area. In the first example, the user wanted to answer the following queries:

(1) Where is there a reasonable possibility of finding areas of the field with sand somewhere in the soil profile?

(2) Where is there a reasonable possibility of finding areas of the field where the soil profile is sandy throughout?

For this example, only data related to the sand content of the 0-20 and 70-80 cm layers were used. That is, those fuzzy sets constructed using soil properties S1 (percent of sand content in layer 1 (0-20 cm)) and S3 (percent of sand content in layer 3 (70-80 cm)), respectively. To answer question (1), degrees of the membership functions, for both soil properties S1 and S3, were compared at each site using the maximum operation (Equation (3.21)). For question (2) the minimum degree of membership, Equation (3.20), was used. The resulting fuzzy sets of maximum and minimum degrees of membership were mapped using contour plots. In conclusion, the resulting plots showed that:
(1) there are large parts in the soil profile in which the possibility of sand occurring somewhere exceeds 0.6, (2) whereas the possibility of finding parts with completely sandy profiles, is much more limited.

To show how a Boolean approach can lack in performance compared to a fuzzy methodology, another example was given. Again, the Türen data was used. The user considers the question: 'Where on the farm are the best soil conditions for growing maize?' which was reformulated as 'where are the areas of well-drained, medium-textured, organic matter-rich soil that do not have shallow plough pans?'. The soil data for all eleven properties were used to answer this question. The Boolean methodology comprised first of constructing a set of 11 Boolean maps. The 11 Boolean maps were defined using the function

$$\begin{aligned} \mu_A(x) &= 1 \quad \text{for } b_1 \leq x \leq b_2 \\ \mu_A(x) &= 0 \quad \text{Otherwise} \end{aligned} \tag{3.31}$$

Those points x falling within the class boundaries (the lower and upper cross-over values) were deemed to be "suitable", while all points x falling outside these lim-

its were deemed "not suitable". Therefore, the 50% cross-over values (b_1 and b_2) were used to establish exact class limits, and classify each site with respect to each property as being suitable ($\mu_A(x) = 1$) or not ($\mu_A(x) = 0$). The maps are then entered into separate overlays in a geographic information system (GIS). The set of eleven Boolean maps are compared with each other, and all sites for which the crisp degree of membership 'true' is returned, were seen to have met the desired specifications. This was done using the Boolean intersection. The end result showed that the field was not suitable. Because experience had shown the field is suitable for growing maize and the soil profiles required do occur on it, it was concluded that the Boolean approach was unsatisfactory.

Burrough concluded that the use of strict Boolean approach with simple true/false logic in combination with an exact (observational) data model is often inappropriate for soil survey and land evaluation because of the: (i) continuous nature of soil variation, (ii) uncertainties associated with describing the phenomenon or in the measurements made on it, and (iii) inexactness in formulating the queries. Fuzzy methods, e.g., semantic import model, allow users to define flexible class membership functions that match practical experience. The results of operations with fuzzy sets yielded quantitative degrees of aggregated membership functions that can be mapped. Also, the fuzzy based maps were able to show how closely sites match up to requirements. A down side to the fuzzy approach is that the choice of membership functions, class centers and cross-over values relies mostly on expert knowledge and the queries posed. In all, a fuzzy approach appeared to be more suited for exploring a database and providing more detail about the gradual evaluation of sites or objects in terms of the questions posed, than the exact Boolean approach.

The general symmetrical membership function (3.2) was also used to assess soil fertility in [13, 26, 41]. In all three studies, a comparison between classical and fuzzy procedures to answer queries on soil fertility in Canada and the Philippines, was carried out. The authors similarly remarked that:

- Given the continuous nature of the variation in soil properties, many envi-

ronmental problems cannot realistically be modeled using the exact Boolean approach.

- A crisp membership function divides the objects into only two membership classes, 0 (unsuitable) and 1 (suitable). As a result, of this much information is lost, such that objects with attribute values close to the exact boundary conditions are rejected.

- The user must realize that associated with a fuzzy approach is the problem of how to define the parameters of the continuous membership function. It is important that parameters are chosen so that the resulting logical models will better describe the problem at hand.

McBratney et al. [58] also give a brief encounter on most of these studies. In soil science, fuzzy set theory is principally used for classification. It is used to reduce a complex system, represented by some sets of data, into explicitly defined classes. Although there exist other classification approaches, such as cluster analysis, the fuzzy set approach, e.g., semantic import model, can deal with uncertainty specifically due to imprecise boundaries between categories. The class pre-specification is based either on expert judgement or conventionally imposed definitions. [58]

3.2.2 Inland evaluation

Fuzzy set theory is also used to evaluate whether land is suitable or unsuitable for a particular purpose.

An application of fuzzy set theory to the identification of non-point sources of land pollution is presented in [76]. The case study focused on land within seven sub-watersheds (objects) located within the Kewaunee river watershed in Wisconson, USA. A watershed is also known as a catchment area. That is, that area of land in which rainfall collects (or is drained into a stream) to form the supply of river [22]. The objective was to identify priority watersheds. That is, those watersheds with the most serious pollution problems and to which scarce resources have been

allocated for diminishing the problem (abatement).

To analyze the pollution problem in the Kewaunee river watershed, a data matrix of seven sub-watersheds (rows) sampled with respect to seven criteria (columns) was compiled. Here the columns $k = 1, 2, \cdots, 7$ represent the seven criteria which emphasize agricultural aspects within the sub-watersheds, e.g., erosion of agricultural land and manure spreading. The rows $i = 1, 2, \cdots, 7$, represent the set of sub-watersheds sampled within a 139 mile^2 of the Kewaunee river watershed. To compare the watersheds equally, a function similar to that of (3.4) was used. Entries x_{ik} in each column k were mapped to the unit interval, $Y : X \longrightarrow [0, 1]$ by dividing x_{ik} to the largest entry in its column. This produced seven sets whose entries were real numbers between 0 and 1. From here on we shall refer to sub-watersheds as watersheds.

To identify priority watersheds, watersheds were classified depending on the relationship between each pair. Two fuzzy classification models were used. One model ranks watersheds based on pair-wise comparison (Model I), while another identifies similarity relationships among the watersheds (Model II). Model I used the fuzzy membership function

$$D_k(i,j) = \begin{cases} 1 & \text{, if } y_{ik} - y_{jk} > 0 \\ 0 & \text{, if } y_{ik} - y_{jk} < 0 \\ 0.5 & \text{, if } y_{ik} - y_{jk} = 0 \end{cases} , k = 1, 2, \cdots, 7$$

for a pair of watersheds i and j, while Model II used the fuzzy membership function,

$$r_{ij} = 1 - c|\sum_{k=1}^{n=7} d(y_{ik}, y_{jk})|.$$

Where d is $d(y_{ik}, y_{jk}) = y_{ik} - y_{jk}$, and c a constant chosen such that $0 \leq r_{ij} \leq 1 \forall i, j$. Model I was used to compute a fuzzy dominance relationship between the watersheds. For more description of each model see [76].

In the end, three sub-watersheds were identified as priority ones. In both models, the results conformed with the best judgement of personnel in the Wisconsin

Department of Natural Resources who are familiar with the Kewaunee watershed. In conclusion, the author found that

- The fuzzy set models could be applied to a range of environmental management problems, where objects are to be compared on the basis of several properties.
- It is not necessary for the units used to measure the criteria in fuzzy set modeling to be the same, or for the information to be in quantitative form.

An application of fuzzy set theory in environmental science is discussed in [11]. The study is about habitat quality determination and whether land parcels or land segments, selected for examination in Kentucky, are unsuitable for mining. Therefore, the task of the Kentucky Department of Natural Resources and Environmental Protection (DNREP) was to identify a subset E that consists of all parcels of land which are unsuitable for mining. Because value judgements made to identify such parcels are complex, these parcels or subsets were considered fuzzy. So, if M was defined as the subset of parcels which are suitable for mining, then its complement $\bar{M}$ was the subset of parcels which were unsuitable.

Eleven quality variables, $X = \{x_j\}$, $j = 1, \cdots, 11$, were used to assess suitability membership of parcels in M. Some variables, such as endangered plants, nature preserves and wild rivers, take either 1 or 0 as membership values depending on the existence or non-existence of these items in the parcel. On the other hand, other variables such as recreation value may take any membership value between 0 and 1 based on the quality of the parcels as judged by other state agencies. Both crisp and fuzzy membership functions were used to determine the degrees of membership of suitable parcels for mining in the set M with respect to a quality variable x_j. Symmetric and asymmetric fuzzy membership functions were used.

Since $\bar{M}$ is the complement of M, its degrees of membership are such that 0 refers to the parcel being suitable and 1 totally unsuitable for mining, for the set of eleven quality variables x_j, $j = 1, \cdots, 11$, at that parcel. In addition, the membership or importance of a quality variable in the set $\bar{M}$ was taken into account. This was done

by assigning weights $w_j \in [0,1]$ to each property x_j. Finally, to determine if a set M is unsuitable for mining given the vector of quality variables $(x_1, x_2, \cdots, x_{11})$, two fuzzy operations were used to compute the land unsuitability indices, $\mu_{\bar{M}}(X)$: the weighted average

$$\mu_{wa}(x_1, x_2, x_3, \cdots, x_{11}) = w_1(x_1 + w_2 x_2 + \cdots + w_{11} x_{11}),$$

where $\sum_j w_j = 1$, and the maximum operation

$$\mu_{\max}(x_1, x_2, \cdots, x_{11}) = \max(x_1, x_2, \cdots, x_{11}).$$

Finally, a strong α-level fuzzy set of those parcels which had membership indices $\mu_{\bar{M}}(X) > 0.95$ were selected as land totally unsuitable for mining in Kentucky. The same approach was also applied as an example to the classification of ecosystems (i.e., wetland classification).

Bosserman and Ragade (1982) [11] concluded that a fuzzy description of an object is able to incorporate large number of variables that most adequately characterize the object. Also, it was found that observers and their judgments are essential in defining and classifying ecosystem phenomena (i.e., choosing the membership functions and defining their parameters). Finally, methods based on fuzzy set theory were found to provide a bridge by which subjective human judgment can be made compatible with exact scientific methods.

A landform segmentation model (LSM) for partitioning agricultural landscapes into terrain element classes (output) is introduced in [55]. These elements are chosen to display significant differences with respect to soil properties, which are needed for precision farming. In this paper, the author wished to produce a generic method for the classification of landform elements such that the chosen method can utilize and incorporate expert knowledge and judgement. He found that classification procedures based on statistical analysis and ordination of terrain variables (input) for a particular site result in classifications that are optimal only for a given site. That is, the results were specific to each unique site and can not be easily generalized. Therefore, a continuous fuzzy approach was chosen, since it permits experts

to identify desired conceptual landform elements and to define each element using imprecise semantics. For example, the terrain element class of *level crest* has been suggested and described using fuzzy landform attributes.

Raw digital elevation data was collected from two sites in Alberta, Canada, then interpolated into regular grid cells. From the interpolated data, ten terrain variables were computed and used as input variables. Three of the variables were chosen to describe the local shape and orientation of a grid cell related to the movement of water in the landscape. An example is the 'slope gradient' variable. Six variables that represent measures of relative slope position formed another group. A final derivative called the 'wetness index' was chosen because of the importance of moisture availability for crop growth in the moisture limited agricultural landscapes of western Canada. Table 3.3 shows the first group of derivative relating to landform shape, i.e., slope gradient, profile curvature and plan curvature. A detailed description of all ten terrain variables can be found in [55].

The aim of the study was to define 15 terrain element classes, predefined by the expert, using a fuzzy approach and the input data of ten terrain variables. Application of the procedure is summarized in the following steps.

Step 1. Fuzzy membership functions were first used to define 20 fuzzy landform attributes, using the input data of nine out of the ten terrain variables. The fuzzy membership models were based on Burrough et al. [13] semantic import model

$$\mu_A(x) = \frac{1}{[1 + ((x - c)/d)^2]} \times 100, \tag{3.32}$$

where x is the value of a terrain variable at each grid cell. Symmetric, left asymmetric and right asymmetric fuzzy membership functions were used. For each fuzzy landform attribute expert judgement and information from literature (where applicable) were used to select appropriate values for c and d, expressing a fuzzy concept. The parameters were then substituted in (3.32) to compute the degree of membership $\mu(x)$ of each terrain variable value x in its

Table 3.3: Examples of some terrain variables used in [55] for landform identification

Abbreviation of terrain derivative	Name of terrain derivative	Description of terrain derivative
SLOPE	Slope gradient	Slope gradient
PROF	Profile curvature	Rate of change of slope in the down slope direction
PLAN	Plan curvature	Rate of change of slope in the across slope direction

Table 3.4: Heuristic rule base for converting the terrain variables from Table 3.3 into fuzzy landform attributes

No.	Input terrain derivative	Output fuzzy landform attribute	Description of fuzzy landform attribute	Model	Standard index (c)	Dispersion index (d)
1	PROF	CONVEX-D	Relatively convex in profile (down)	Left asymmetric	10.0	5.0
2	PROF	CONCAVE-D	Relatively concave in profile (down)	Right asymmetric	-10.0	5.0
3	PROF	PLANAR-D	Relatively planar in profile (down)	Symmetric	0.0	5.0
4	PLAN	CONVEX-A	Relatively convex in plan (across)	Left asymmetric	10.0	5.0
5	PLAN	CONCAVE-A	Relatively concave in plan (across)	Right asymmetric	-10.0	5.0
6	PLAN	PLANAR-A	Relatively planar in plan (across)	Symmetric	0.0	5.0
7	SLOPE	NEAR-LEVEL	Nearly level slope gradient	Right asymmetric	1.0	2.0
8	SLOPE	REL-STEEP	Relatively steep slope gradient	Left asymmetric	5.0	2.0

c and d are parameters defining the dispersion and cross over point for each terrain derivative. Both parameters are defined as in Equation (3.30).

corresponding fuzzy landform attribute. As an example, Table 3.4 shows the resulting eight fuzzy landform attributes calculated using the terrain variables from Table 3.3. The heuristic rule-base for converting the terrain variables into fuzzy landform attributes, the parameters used and type of SI model used are given in the paper [55]. For example, the fuzzy landform attribute that describes the degree to which a site (or grid cell) is considered to be nearly level in slope gradient, NEAR-LEVEL, was calculated using the input terrain variable SLOPE. The right asymmetric fuzzy membership function,

$$\mu_{NEAR-LEVEL}(SLOPE(x)) = \frac{1}{[1 + ((SLOPE(x) - 1.0)/2.0)^2]} \times 100, \tag{3.33}$$

Step 2. The next step was to convert the 20 fuzzy landform attributes into fuzzy degrees of membership which express the possibility that a given cell or site belong to each of $n = 15$ defined terrain element classes. For this, an operation based on the 2-place weighted sum was used, where the combined weights summed to 1. The weighted sum operator was used to compute each of the 15 defined terrain element classes, $B_1, B_2, \cdots, B_{15}$, resulting in 15 different aggregated values, one for each of the 15 different terrain element classes, for every grid cell. Step 1. and Step 2. were applied for each grid cell.

Step 3. Finally, to assign each grid cell to a single terrain element class, the maximum operator was used to see which of the 15 classes had the maximum degree of membership.

The proposed fuzzy logic based methodology (i.e, landform segmentation methodology)

- can be applied to a wide variety of agricultural landscapes and generalized according to the magnitude and scale of the landscape and data.
- The fuzzy procedure supported explicit linguistic expressions of imprecise semantics (e.g., the slope is steep) required to define an abstract set of soil

landform attributes.

In [66], classification of environmental impacts using fuzzy sets is presented as an example. The example considers the impacts of effluent discharges from a factory. Two categories of impacts, *acceptable* and *not-acceptable*, and two types of effluents, *nutrients* and *toxins*, were considered for simplicity. Normally each discharge would be evaluated separately and then regulated, based on the result. But this approach was not always seen reasonable. The difference between a given factory A that discharges 99% of the allowable level of nutrients and B that discharges 101% of this level is negligible (i.e., 1% above the allowable level of discharge) and probably within the range of measurement error. However, the former would meet the discharge criteria and the latter would not. If factory A also discharges 99% of the allowable level of toxins while B discharges almost *none*, this would not affect the outcome. On the other hand, factory B could legitimately argue that it pollutes less than factory A. Therefore, instead of evaluating each discharge individually as either acceptable or not, fractional values for the acceptability of each discharge could be assigned using fuzzy set theory. Then, to obtain an overall acceptability level, these partial memberships are combined using a scoring rule.

The first step was to assign an acceptability level to each level of pollution discharge using a plausible membership function. The 'level of acceptability' was seen as a continuous decreasing function of nutrient (or toxin) loading, so that a small increase in nutrient discharges leads to a small decrease in acceptability. Once the partial memberships μ_N and μ_T are calculated for the nutrients and toxins respectively, the next step is to combine them to define the *total membership*, μ. Most environmental standards are based on the non-compensatory combination rule,

$$\mu = \min(\mu_N, \mu_T)$$

the standard fuzzy intersection. However this approach to classifying environmental impacts is perceived as very conservative. That is, it considers only the most unacceptable indicators, no matter how many favorable indicators there may be to

counter it. So, from the view point of Silvert (1997) [66], the combination rule is that it must be *compensatory*. This means that a good score for one variable (high membership in the fuzzy set 'acceptable') can partly compensate for a poor score (low membership) from another variable. Hence, combination rules, other than the standard intersection and union operations, were considered for the combination of the partial membership of acceptable discharges. These will be discussed further in Chapter 4.

Further applications of fuzzy set theory to land and environmental impact evaluation can be found in [30, 68].

3.2.3 Evaluation of a marine environment

Fuzzy set theory is also viewed as a powerful tool for classifying marine environmental conditions and for describing the occurrence of natural changes in an environment. It is seen as an approach that has the ability to integrate different kinds of observations in a way that permits a good balance between favorable and unfavorable observations, and between incommensurable effects such as social impacts.

Application of a fuzzy set procedure to evaluate benthic impacts under fish farms is given as an example in [67]. Conditions of a seabed under fish farms can be surveyed by divers. Observations may include visual records of the abundance and diversity of fauna and flora (i.e., animal and plant life, respectively; fauna and flora = benthic biota), as well as geochemical cores obtained with hand-held samplers. It is not always practical to deal with 'scientific' quantitative data, especially when a large number of farms are to be monitored and also, in some instances, if special equipment is required. Other data might be required, such as a strong sulphide smell to the core, and are considered virtually impossible to quantify.

In 1998, a pilot project was carried out to explore the use of fuzzy logic for developing indices of benthic conditions under a fish farm in Eilat, Isreal. The farm had been studied by divers for several years. Observations of eight different benthic variables from 100 dive logs under fish pens were used.

Using these observations, four fuzzy sets were defined representing nil, moderate, severe and extreme impacts. The partial fuzzy memberships were obtained by a procedure which first assigns membership values, called 'association rules', to each of the eight observations. These observations were: the extent of bacterial mats, thickness of bacterial mats, colour of bacterial mats, quantity of seagrass, quantity of epi-macrofauna, degree of bioturbation by macrofauna, degree of bioturbation by fish, and visibility. The assignment of observations were mainly qualitative, i.e., made by divers without use of measuring instruments. Each observation was also assigned a weight reflecting its importance in the benthic assessment process. For example, seagrass coverage was 'abscent', 'few', or 'normal'. The presence of seagrass is generally considered to be a strong indicator of a healthy seabed. So if the divers identified the seagrass cover as 'normal', the partial membership for nil, moderate, severe, and extreme impacts were assigned as

$\mu_{NIL} = 0.8$, $\mu_{MOD} = 0.2$, $\mu_{SEV} = \mu_{XTR} = 0$,

a method known as 'association rules'. To visualize the results, a graphical representation of the partial membership in the four fuzzy sets over time was produced. In the resulting graph, it was seen that a lot of useful information was available, but was difficult to interpret. For this reason the four fuzzy sets were combined to produce a single comprehensive score which would represent an overall measure of environmental quality. The weighted impact score, defined as

$$SCORE = 0\mu_{NIL} + 1\mu_{MOD} + 2\mu_{SEV} + 4\mu_{XTR},$$

for data collected over the period of study, from 1991 until 1994, was used.

As a result of this project, Silvert (2000) [67] found that in addition to facilitating a simple and practical sampling scheme, this procedure gave the researcher access to an historical database that might had to be discarded if they were only prepared to accept rigorously quantitative measurements.

Another application of fuzzy sets is introduced by Urbanski (1999) [71], for the evaluation of an environment in coastal waters. The lack of a well suited data model for coastal water areas was viewed as a problem in the development of successful

coastal water applications. The reason for this is the spatial and temporal variability of many parameters used to describe coastal waters like temperature, salinity, amount of nutrient or wave height.

The study focused on locating places in the Gulf of Gdansk (Poland) vulnerable to algae blooms, which are known to constitute a highly toxic threat to sea life as well as human beings. First this was done by classifying the data sets, using a fuzzy membership function. The raw data consisted of concentrations of three variables: nitrogen forms (NO_3+NO_2+NH_4), phosphorus (PO_4) and temperature of the water measured at each station. Then, using these measurements, probability of reaching values equal to or greater then a threshold (i.e., for nitrogen (x_1) 3 $\mu mol\ dcm^{-3}$, for phosphorus (x_2) 1 $\mu mol\ dcm^{-3}$, for temperature (x_3) 18^oC) for each station was calculated. The probabilities were then reclassified into 3 classes according to the shape of the histogram (e.g., small, medium, and extreme vulnerability to algal blooms). A sigmoidal function based on the trigonometric cosine

$$\mu_A(x) = 1 - \cos^2\left(\frac{x - p_{min}}{(p_{max} - p_{min})(\pi/2)}\right)$$

such that

$$\mu = 0 \quad \text{for } x \leq p_{min}$$

$$\mu = 1 \quad \text{for } x \geq p_{max}$$

was used to define the partial memberships in each class. Values of p_{min} were selected based on the values for nitrogen and phosphorus content, and temperature, by searching for the local minimum. Values of p_{max} were defined based on the assumption that 15% of the studied area is extremely vulnerable ($\mu = 1$). Therefore, the marked value for which 15% of the data had higher values was defined as p_{max}, for each parameter. The membership function defined as above was considered relative and qualitative, because it allowed the outline of the gulf areas of higher and lower vulnerability without facilitating any quantitative analysis. Calculation of the *index of vulnerability* using the defined oceanography parameters $\{A_1, A_2, A_3\}$ was carried out next. The combination of information (fuzzy sets) was used to create land

evaluation maps through fuzzy set operations, based on the same technique used in [12].

3.3 Conclusion

In this Chapter, formulation of different membership functions and the combination of information through simple fuzzy operations is defined. A survey of fuzzy set applications in some fields of environmental sciences is given. A symmetric and asymmetric fuzzy membership function and judgment assignment of membership values were repeatedly used in environmental applications. As for the combination of information via fuzzy operations, most applications concentrated on the standard intersection, standard union and the weighted average operations. For more information on the theory behind fuzzy sets, see [33].

The use of a fuzzy set approach rather than a Boolean approach was preferred as an application tool in environmental science.

Chapter 4

Fuzzy aggregation and loading indices

In the previous chapter we found that common combination rules, such as the standard fuzzy intersection and the simple average, were used in many environmental applications. Here we consider more complex combination rules that may be used for the formulation of overall heavy metal indices in a marine environment.

In this chapter, a general view of combination rules that can be used for the aggregation of environmental information is presented. A selection of aggregating operations will be used to generate "*loading indices*" in a marine environment. The chapter is divided as follows: Section 1 introduces 2-place aggregating operations and examples of existing n-place aggregation operators. Methods of generalizing associative aggregation operators are presented in Section 2. In Section 3, aggregation rules that can take into account the importance of the fuzzy sets being combined are summarized. Finally, in Section 4, n-place aggregation operations are applied used to construct loading indices of the two marine environmental regions.

4.1 Aggregation operations (AO)

Aggregation operations combine a set of fuzzy subsets to produce one fuzzy set. Dubois and Prade highlighted as one of the most attractive features of fuzzy set theory its provision of a mathematical setting for the integration of individual attributes, represented by membership functions [28]. At the application level, many authors found that fuzzy set theoretic operations have proved useful in many different fields, an example of which is the field of multi-attribute evaluation. In return, this type of application gave the necessary motivation to search for classes of operations beyond the straightforward extensions of classical set theoretic operations [28]. Applications of fuzzy set methods and its use in multicriteris evaluation, using various aggregation operators can be found in [36].

Fuzzy intersections and unions are alternatives of the set theoretic operations for crisp sets. Being a richer model, fuzzy sets can be combined using other formulas, which together with the set theoretic operations are called **fuzzy aggregation connectives**.

Next, we shall introduce alternative operators to that of the standard intersection operation and standard union operation for aggregating or combining two fuzzy sets.

4.1.1 Fuzzy intersection and fuzzy union operations

Instead of minimum and maximum operators, many other operations can be used on two fuzzy sets, A and B, defined on a universal set U with a common element $u \in U$. For a function $I : [0,1] \times [0,1] \longrightarrow [0,1]$ to be acceptable as an operator for intersection, I has to satisfy some axioms. These are stated below and lead to the concept of **t-norms**.

Definition 2 (T-norm operators). *Let I be a binary operation such that,*

$$I : [0,1] \times [0,1] \longrightarrow [0,1].$$

I is said to be a t-norm *operator if the following conditions are met for all $a, b, c, d \in [0,1]$:*

(i) $I(a,b) = I(b,a)$ *(Commutativity)*

(ii) $I(a, I(b,c)) = I(I(a,b), c)$ *(Associativity)*

(iii) $I(a,b) \geq I(c,d)$ *if* $a \geq c$ *and* $b \geq d$ *(Monotonicity)*

(iv) $I(a,1) = a$ *(One-identity)*

It can be easily verified that I *reduces to the crisp intersection if* $a, b, c, d \in \{0,1\}$ *There are two more alternative conditions [32, 47]:*

(v.a) $I(a,a) = a$ *(Idempotence property)*

(v.b) $I(a,a) < a$ *(Archimedean property)*

The union type operators on two fuzzy sets are implemented by **t-conorms**. These are also two-place operations defined as follows.

Definition 3 (T-conorm operators). *Let* U *be a binary operation on the unit interval*

$$U : [0,1] \times [0,1] \longrightarrow [0,1]$$

such that for all $a, b, c, d \in [0,1]$

(i) $U(a,b) = U(b,a)$ *(Commutativity)*

(ii) $U(a, U(b,c)) = U(U(a,b), c)$ *(Associativity)*

(iii) $U(a,b) \geq U(c,d)$ *if* $a \geq c$ *and* $b \geq d$ *(Monotonicity)*

(iv) $U(a,0) = a$ *(Zero-identity)*

(v.a) $U(a,a) = a$ *(Idempotency property)*

(v.b) $U(a,a) > a$ *(Archimedian property)*

The minimum and maximum operators are examples of intersection and union, respectively. They are considered to be "the standard" type of fuzzy operations. This is because they perform as the corresponding operations for crisp sets when the range of membership grades is $\{0, 1\}$. The reason for the special attention they receive in the literature is twofold. First, they are simple and intuitive. As [49] states: 'from a practical point of view, the pair (min and max) are comfortable to work with arithmetically as well as graphically'. Second, the minimum operator is the largest t-norm amongst those satisfying properties 1 to 4, and the maximum operator is the smallest t-conorm among those satisfying the respective 4 properties. In other words, the 'min' operator is viewed as the weakest fuzzy intersection, where as the 'max' operator is viewed as the strongest fuzzy union.

The min and max operations are the only pair of distributive and idempotent t-norms and t-conorms, respectively. Therefore, if one wants to preserve the equalities

$$A \cap A = A \quad \text{and} \quad A \cup A = A$$

for fuzzy sets A, one turns to this pair of operators. But in some applications fuzzy sets do affect each other when united or intersected. In such cases other operators (e.g., parameterized operators) are often used instead of min and max to represent these operations in different contexts.

Examples of t-norm operators

- **Algebraic Product**: $I(a, b) = a \cdot b$
- **Bounded Difference**: $I(a, b) = \max(0, a + b - 1)$
- **Hamacher Product**: $I(a, b) = \frac{a \cdot b}{(a+b)-(a \cdot b)}$
- **Drastic Intersection**: $I_D(a, b) = \begin{cases} a & \text{when b=1} \\ b & \text{when a=1} \\ 0 & \text{otherwise} \end{cases}$

Notice that, $I_D(a,b) \leq \max(0, a+b-1) \leq a \cdot b \leq \min(a,b)$. [47]

Examples of parametric two place t-norms are

- **Dubois and Prade (1980)**: $I_\alpha(a,b) = \frac{a \cdot b}{\max(a,b,\alpha)}$, for $\alpha \in [0,1]$.
  This operator ranges from the $\min(a,b)$ for $\alpha = 0$ to the product operator for $\alpha = 1$. It also can be written in the following form:

$$I_\alpha(a,b) = \begin{cases} \frac{a \cdot b}{\alpha} & \text{for } a,b \in [0,\alpha] \\ \min(a,b) & \text{elsewhere} \end{cases}$$

- **Hamacher Product family**: $\frac{a \cdot b}{r+(1-r)(a+b-a \cdot b)}, \quad r \leq 0$
  This operator ranges form the product operator for $r = 1$, to drastic intersection as $r \to \infty$.

Examples of t-conorms

The following are examples of t-conorm operators, defined on two fuzzy sets, A and B on $[0,1]$, where $a \in A$ and $b \in B$.

- **Algebraic (or Probabilistic) Sum**: $U(a,b) = (a+b) - (a \cdot b)$
- **Bounded Sum**: $U(a,b) = \min(1, a+b)$
- **Hamacher Sum**: $U(a,b) = \frac{(a+b)-2(a \cdot b)}{1-(a \cdot b)}$
- **Drastic Union**: $U_D(a,b) = \begin{cases} a & \text{when b=0} \\ b & \text{when a=0} \\ 1 & \text{otherwise} \end{cases}$

Notice that, $\max(a,b) \leq (a+b) - (a \cdot b) \leq \min(1, a+b) \leq U_D(a,b)$.

Examples of parametric two placed t-conorms are:

- **Dubois and Prade**: $U_\alpha(a,b) = \frac{(a+b)-(a \cdot b)-\min(a,b,\alpha)}{max(1-a,1-b,\alpha)}, \quad$ for $\alpha \in (0,1)$.
  This operator ranges from the max operator for $\alpha = 0$ to the probabilistic sum when $\alpha = 1$.

- **Sugeno's Operation**: $U(a,b) = \min(1, a+b+\lambda a \cdot b), \qquad \lambda > -1,$
  ranges from the bounded sum for $\lambda = 0$ to drastic union as $\lambda \to \infty$.

- **Hamacher Sum family**: $\frac{a \cdot b + (r-2)a \cdot b}{r+(r-1)a \cdot b}, \quad r > 0,$
  ranges from the probabilistic sum for $r = 1$ to $U_{max}(a,b)$ as $r \to \infty$.

4.1.2 Alternative aggregation operators of two fuzzy sets

We introduce three examples of fuzzy aggregating operations. They are, the Mean operators, the Symmetrical sum and Symmetrical difference operators.

Mean or Averaging Operations

Mean operations are used to generate fuzzy sets that lie between the 'min' and 'max' operators.

Definition 4 (Mean operators). *Let A and B be fuzzy sets of U. Then a mean operation is defined as a mapping*

$$\mathrm{m} : [0,1] \times [0,1] \longrightarrow [0,1].$$

given that the following conditions are satisfied for $a, b \in [0,1]$,

(i) m *is commutative:* $\mathrm{m}(a,b) = \mathrm{m}(b,a)$

(ii) m *is increasing with respect to both arguments and continuous.*

(iii) $\min(a,b) \leq \mathrm{m}(a,b) \leq \max(a,b)$ *such that* $\mathrm{m} \notin \{\min, \max\}$.

Examples of such operators are:

- **Arithmetic Mean**: $\mathrm{m}(a,b) = \frac{a+b}{2}$
- **Harmonic Mean**: $\mathrm{m}(a,b) = \frac{2a \cdot b}{a+b}$
- **Geometric Mean**: $\mathrm{m}(a,b) = \sqrt{a \cdot b}$

- **Generalised Mean**: $\mathrm{m}_\alpha(a,b) = \left(\frac{a^\alpha + b^\alpha}{2}\right)^{\frac{1}{\alpha}}, \quad \alpha \in R$
  which is also the general formula that produces the arithmetic mean when $\alpha = 1$, and the 'Quadratic' mean, when $\alpha = 2$. [10]

Although these operations are strictly increasing, they are not associative. The only associative mean operators that are also increasing are those known as the family of **median** operations:

- $med_\alpha(a,b) = \begin{cases} \max(a,b) & \text{if } a,b \in [0,\alpha] \\ \min(a,b) & \text{if } a,b \in [\alpha,1] \\ \alpha & \text{otherwise} \end{cases}$

Symmetrical Sum Operators

In some cases, a pair of sets to be combined may have comparable features (e.g., the set of "good" objects vs. the set of "bad" objects), such that symmetry exists between their two complementary sets. In such a case, appropriate set operations should be defined in a way that it does not matter whether we deal with a set or its complement [65]. Such operations, are known as Symmetric sums. [10, 50, 65]

Definition 5 (Symmetric sums). *Symmetric sums are operations defined by a rule of combination* $\sigma : [0,1] \times [0,1] \longrightarrow [0,1]$,
such that

(i) $\sigma(0,0) = 0$, $\sigma(1,1) = 1$ *(Boundary conditions)*

(ii) $\sigma(a,b) = \sigma(b,a)$ *(Commutative)*

(iii) σ *is continuous and increasing with respect to both arguments*

(iv) σ *is auto dual. That is, with respect to the complement to 1, we have:*
$1 - \sigma(a,b) = \sigma(1-a, 1-b)$,
i.e., σ *is independent of whether we deal with sets or their complements.*

The general form of a symmetric sum can be given by

$$\sigma(a,b) = \frac{g(a,b)}{g(a,b) + g(1-a,1-b)} \tag{4.1}$$

such that the generating function g is an increasing real mapping which is positive, continuous and $g(0,0) = 0$. The following are examples of symmetric sums

- $med_{\frac{1}{2}}(a,b) = \begin{cases} \max(a,b) & \text{if } a,b \in [0,\frac{1}{2}] \\ \min(a,b) & \text{if } a,b \in [\frac{1}{2},1] \\ \frac{1}{2} & \text{otherwise} \end{cases}$

which is considered to be the only symmetric sum which is associative and also a mean operator.

- $\sigma(a,b) = \frac{a \cdot b}{1-a-b+2a \cdot b}$, for $g(a,b) = a \cdot b$, where $a,b \in (0,1)$ (Associative)
- $\sigma(a,b) = \frac{a+b-a \cdot b}{1+a+b-2a \cdot b}$, for $g(a,b) = a + b - a \cdot b$, (NOT associative)

Examples of symmetric sum that make use of the 'min' and 'max' operators as the generating functions are,

- $\sigma(a,b) = \frac{\min(a,b)}{1-|a-b|}$ for $g(a,b) = \min(a,b)$
- $\sigma(a,b) = \frac{\max(a,b)}{1-|a-b|}$ for $g(a,b) = \max(a,b)$

which are also mean operators.

Symmetrical Difference Operators

Other interesting operators that combine two fuzzy sets, are referred to as *symmetrical difference* operators [44].

Definition 6 (Symmetric difference). *Let $A \Delta B$, where Δ denotes the symmetrical difference between fuzzy sets. Symmetrical differences can be generated by a mapping*

$$\mathrm{d} : [0,1] \times [0,1] \longrightarrow [0,1]$$

such that

(1) $\mathrm{d}(0,0) = \mathrm{d}(1,1) = 0$

(2) $\mathrm{d}(0,1) = \mathrm{d}(1,0) = 1$

(3) $\mathrm{d}(a,b) = \mathrm{d}(b,a)$

(4) $\forall a,\ b \in [0,1], \quad \mathrm{d}(a,b) = \mathrm{d}(1-a, 1-b).$

A general form of symmetrical difference operators is

$$\mathrm{d}(a,b) = f(g(a,b), g(1-a, 1-b))$$

where the generating functions

(i) f and g are any continuous mappings from $[0,1]^2$ and $[0,1]$.

(ii) f is commutative

(iii) $f(g(0,0), g(1,1)) = 0$ and $f(g(0,1), g(1,0)) = 1$

Examples of symmetrical difference operations are [44]

- $\mathrm{d}(a,b) = \max(\min(1-a, b), \min(a, 1-b))$
  where $g(a,b) = \min(1-a, b)$ and $f(a,b) = \max(a,b)$.
  This is consistent with the usual definition of $A\Delta B = (\bar{A} \cap B) \cup (A \cap \bar{B})$ translating $\cap$ and $\cup$ into min and max. Here, Δ is associative.

- $\mathrm{d}(a,b) = |a-b|$
  where $g(a,b) = 1 - a + b$ and $f(a,b) = \frac{|a-b|}{2}$. This symmetrical difference operation is consistent with $A\Delta B = (\bar{A} \cap B) \cup (A \cap \bar{B})$ translating $\cap$ and $\cup$ into $A \cap B = \max(0, a+b-1)$ and $A \cup B = \min(1, a+b)$. Here, Δ is NOT associative.

4.1.3 Aggregation Operators of More than Two Fuzzy Sets

More often there are more than two fuzzy sets to be considered for aggregation. Therefore, aggregating operations on fuzzy sets are ones by which several fuzzy sets are combined in a desirable way, to produce a meaningful expression in terms of a single fuzzy set. In order for a function $\mathcal{A}$ to qualify as an intuitively meaningful aggregation operator of n-arguments, it must satisfy at least three conditions.

Definition 7 (n-place aggregation connective). *An n-place aggregation connective is defined by the mapping*

$$\mathcal{A} : [0,1]^n \longrightarrow [0,1].$$

(1) $\mathcal{A}(0,\cdots,0) = 0$ *and* $\mathcal{A}(1,\cdots,1) = 1$ ***(Boundary conditions)***

(2) $\mathcal{A}(a_1,\cdots,a_n) = \mathcal{A}(a_{i_1}, a_{i_2}\cdots,a_{i_n})$, *for any permutation* $i_1, i_2, \cdots, i_n$ *of* $1,\cdots,n$. *In other words, the aggregation is indifferent to the ordering of the arguments,* a_i. ***(Commutativity)***

(3) *For any pair* $(a_1,\cdots,a_n)$ *and* $(b_1,\cdots,b_n)$ *of n-arguments, such that* a_i, $b_i \in [0,1]$ *for all* $i \in \mathbb{N}_n$*:*

$$a_k \geq b_k \forall i = 1,\cdots,n \Longrightarrow \mathcal{A}(a_1,\cdots,a_n) \geq \mathcal{A}(b_1,\cdots,b_n).$$

That is, $\mathcal{A}$ is ***monotonic*** *increasing in all arguments.*

Next, we shall present a summary of a variety of aggregation operators, grouped as follows: (i) generalized t-norms (ii) generalized t-conorms, (iii) mean type aggregations. [28, 32, 47, 8, 10]

Although fuzzy intersection and union operators do not cover all operations by which n fuzzy sets can be aggregated, they do cover all aggregating operations that are associative. The benefit of this property is that it will allow us to extend the definition of fuzzy intersection (union) aggregations involving only two sets to any number of sets [32, 47, 50].

Fuzzy Intersection and Union Aggregations

An aggregation $\mathcal{A}$ is said to be an intersection or union type operation, if one of the following additional conditions, to that of definition (7), is met:

(4.a) $\mathcal{A}(a_1, \cdots, a_n) \leq \min(a_1, \cdots, a_n)$,

This is characterized as a *conjunctive* or severe behaviour [10, 28, 50].

(4.b) $\mathcal{A}(a_1, \cdots, a_p) \geq \max(a_1, \cdots, a_n)$,

This is characterized as a *disjunctive* or indulgent behavior.

Defining an intersection or union operation on n arguments from one acting on 2 arguments, is possible as long as the operation to be extended is associative. Examples of straightforward extended aggregations to the case of $n > 2$ are the

- Minimum :

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = \min(a_1, a_2, \cdots, a_n)$$

- Product :

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = a_1 \cdot \cdots \cdot a_n$$

- Maximum :

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = \max(a_1, a_2, \cdots, a_n)$$

Mean aggregation Operators

The generalized aggregation operation selected for the analysis of ecological impacts in [66] (e.g., impacts of factory discharges) was *compensatory*. The idea is that a good score for one attribute (high membership in the fuzzy set) can partly compensate for a poor score (low membership). From Silvert's (1997) point of view, the importance of using a compensatory combination rule is that it provides an objective method for dealing with the reality that ecological impacts are inevitably balanced

against each other, and against social and economic factors in the decision making process. Mean aggregation operations are such functions characterized as having a *compromise* or cautious behavior. That is, results generated always lie between the *maximum* and *minimum* aggregation operations, i.e.,

$$\min(a_1, \cdots, a_n) \leq \mathcal{A}(a_1, \cdots, a_n) \leq \max(a_1, \cdots, a_n).$$

Definition 8. *An operator $\mathcal{A}$ is called a* mean aggregation of n arguments *if it satisfies the following conditions:*

(i) *The aggregation is indifferent to the ordering of the arguments.* ***(Commutativity)***

(ii) $\mathcal{A}(a_1, \cdots, a_n) \leq \mathcal{A}(b_1, \cdots, b_n)$ *if* $a_i \leq b_i$ *for all* i . ***(Monotonicity)***

(iii) $\mathcal{A}(a, a, \cdots, a) = a$, *for* $a \in [0, 1]$ ***(Idempotency)***

Therefore, mean operations are the only aggregation operations that lie between the standard intersection and standard union aggregation operations, i.e., (4.1.3), and that are idempotent [28, 32, 47].

The **Generalized mean** is a class of aggregating operations that cover the entire interval between the *minimum* and *maximum* operations,

$$\mathcal{A} = \left(\frac{a_1^\alpha + \cdots + a_n^\alpha}{n}\right)^{\frac{1}{\alpha}} = \left(\frac{\sum_{i=1}^n a_i^\alpha}{n}\right)^{\frac{1}{\alpha}} \tag{4.2}$$

The following aggregating operations are examples of how the general formula reduces to other mean operations for various values of $\alpha \in \Re$.

- **Arithmetic Mean**:

$$\mathcal{A}_\alpha = \frac{a_1 + \cdots + a_n}{n} \quad \text{for} \quad \alpha = 1 \tag{4.3}$$

- **Harmonic Mean**:

$$\mathcal{A}_\alpha = \frac{n}{\frac{1}{a_1} + \cdots + \frac{1}{a_n}} \quad \text{for} \quad \alpha = -1 \tag{4.4}$$

- **Geometric Mean**:

$$\mathcal{A}_\alpha = \left(a_1 \cdot \cdots \cdot a_n\right)^{1/n} \quad \text{for} \quad \alpha \to 0 \tag{4.5}$$

The generalized mean approaches the

- *maximum* aggregating operator as $\alpha \to \infty$ and
- *minimum* aggregating operator as $\alpha \to -\infty$.

Parameterized operations

This group of generalized n-place aggregating operators are sometimes preferred to, say, formulating a new operator each time a different problem is faced [25, 66, 67]. The following are such operations.

- Beta-Gamma combination rule

$$\mathcal{A}(a_1, \cdots, a_n) = \left(\prod_{i=1}^{n} a_i\right)^{\beta} \cdot \left(1 - \prod_{i=1}^{n}(1 - a_i)\right)^{\gamma} \quad , \beta, \gamma \in [0, 1] \tag{4.6}$$

The beta-gamma rule ranges from the product ($\beta = 1, \gamma = 0$), to the algebraic sum ($\beta = 0, \gamma = 1$). It also includes the special cases of the geometric mean ($\beta = \frac{1}{n}, \gamma = 0$) and zimmermanns γ-family ($\beta = 1 - \gamma$),

$$\mathcal{A}(a_1, \cdots, a_n) = \left(\prod_{i=1}^{n} a_i\right)^{1-\gamma} \cdot \left(1 - \prod_{i=1}^{n}(1 - a_i)\right)^{\gamma} \quad , 0 \leq \gamma \leq 1. \tag{4.7}$$

which ranges from the product ($\gamma = 0$) to the algebraic sum ($\gamma = 1$). These parameters are known as 'grades of compensation'.

- Symmetric sum

$$\begin{aligned} \mathcal{A}(a_1, \cdots, a_n) &= \frac{a}{1-a} \\ &= \left\{\left(\frac{a_1}{1-a_1}\right)^{w_1} \cdot \left(\frac{a_2}{1-a_2}\right)^{w_2} \cdot \left(\frac{a_3}{1-a_3}\right)^{w_3} \cdots \right\}^{\frac{1}{w_1+w_2+w_3+\cdots}} \end{aligned} \tag{4.8}$$

such that $\sum_{i=1}^{n} w_i = 1$. The value $\frac{a}{1-a}$ is defined as the weighted geometric mean of the ratios for the membership, $\frac{a_i}{(1-a_i)}$. This type of operator considers both fuzzy sets and their complements in the calculation.

4.2 Generalizing 2-Place aggregation operators

We present generalization of 2-place aggregations to n-place ones. First, recall the associativity law, one of the properties satisfied by 2-place intersection and union aggregations An aggregation

$$\mathcal{A} : [0,1] \times [0,1] \longrightarrow [0,1]$$

is said to be associative, if for all $a, b, c \in [0,1]$

$$\mathcal{A}(\mathcal{A}(a,b),c) = \mathcal{A}(a,\mathcal{A}(b,c)) \tag{4.9}$$

The importance of this property is that, it ensures that we can take the aggregation of any number of sets in any order of pair-wise grouping desired, i.e., extend an aggregation to more than $n = 2$ sets. As for the property of commutativity, it ensures that fuzzy aggregation is symmetric, that is, indifferent to the order in which the sets are combined. Then using this basic property,

a 2-place aggregation operator can be extended to an **n-place aggregation operator**

$$\mathcal{A}(a_1, a_2, ..., a_n) = \mathcal{A}(a_{i_1}, \mathcal{A}(a_{i_2}, ..., a_{i_n})) \tag{4.10}$$

where $a_{i_1}, a_{i_2}, \cdots, a_{i_n}$ is any permutation of $a_1, a_2, ..., a_n$.

To illustrate this in simple terms, we use the basic definition of a 2-place associative aggregations (4.9). Then the aggregation of $n = 3$ fuzzy sets should not depend on the order in which the elements, are combined, i.e.,

$$\mathcal{A}(a_1, a_2, a_3) = \mathcal{A}(\mathcal{A}(a_1, a_2), a_3) = \mathcal{A}(a_1, \mathcal{A}(a_2, a_3)) = \mathcal{A}(\mathcal{A}(a_1, a_3), a_2)$$

In general, the associativity law makes certain that, when constructing our models of $n > 2$ sets, the resulting aggregated sets produced by a specific operator will not differ or depend on the ordering of fuzzy sets to be aggregated.

4.2.1 Methods of generalizing aggregation operators

Due to the variety of aggregating operators presented in the literature [10, 28, 32, 47], it is understandable that difficulties may be encountered when attempting to design a general n-place aggregation for respective 2-place operators. Because of this, we experimented with two possible approaches. Here is a summary of both approaches.

A. This approach relies on using the definition of associativity. This is done by successively adding elements for $n = 3, 4, \cdots$,etc., to design a 3-place, 4-place, $\cdots$,etc. aggregating operator, and gradually derive a general pattern for an n-place aggregation.

B. This approach relies on: (i) aggregating each pair of fuzzy sets, of a fuzzy model [1], to obtain the first group of aggregated sets; e.g., for three fuzzy sets A, B, C, aggregate each pair of sets, resulting in $\mathcal{A}(A, B) = Z$ and C is left since n is odd, (ii) then aggregate each pair from the first group in (i) to obtain a second group of aggregated sets, e.g., $\mathcal{A}(Z, C) = Y$, ... and so on; (iii) finally, the nth aggregated set is obtained. Since here we are dealing with associative operators (as well as commutative), the order in which pairs of fuzzy sets are aggregated will not alter the final result.

Note that because this approach is time consuming, it was thought of with models consisting of a small number of sets to be aggregated (e.g., $2 < n \leq 10$).

Both approaches should give the same pattern regardless of whether the first or second approach is used.

A summary of proposed steps is given below for the first approach, approach **A**.
Step1: Choose a 2-place aggregation operator and check whether the operator is associative and obtain the 3-place aggregation operator.

[1] In this study, the model consists of the process of deriving a problem-specific membership function with which objects can be assigned a membership grade, to evaluate the loading indices

Step2: Design an n-place general formula for your chosen aggregation.

Step3: Prove the n-place aggregation general formula by the method of Mathematical induction.

Definition 9 (Mathematical Induction Method). *Let $P(n)$ be a statement concerning a positive integer 'n'. Then using mathematical induction, we prove that this statement is true for every integer 'n' greater or equal to some lowest integer 'n_0'.The following steps are required by the proof:*

(1) *Prove that $P(n_0)$ is true.*

(2) *Prove that if $P(k)$ is true, where $k \geq n_0$, then it is also true for the next larger integer, $P(k+1)$.*

Then the mathematical induction principle guarantees that $P(n)$ is true for all $n \in Z^+$. [2]

The following are extensions carried out on some operators.

4.2.2 Examples of generalized operators

Simple operators: Minimum, Maximum and the Algebraic product

One straightforward extension is that of the minimum aggregation, $\mathcal{A}(a,b) = \min(a,b)$, $\forall a, b \in [0,1]$, which is an intersection type operator. To design a general pattern, we first derive a 3-place operator.

1. Assume, without any loss of generality, that $a_1 < a_2 < a_3$, then

$$\mathcal{A}_{\min}(a_1,a_2,a_3) = \mathcal{A}_{\min}(\mathcal{A}_{\min}(a_1,a_2),a_3) = \mathcal{A}_{\min}(a_1,\mathcal{A}_{\min}(a_2,a_3)) = a_1$$

2. Similarly for $n = 4, \quad a_1 < a_2 < a_3 < a_4$,

$$\mathcal{A}_{\min}(a_1,\cdots,a_4) = \mathcal{A}_{\min}(\mathcal{A}_{\min}(a_1,a_2,a_3),a_4) = \mathcal{A}_{\min}(a_1,\mathcal{A}_{\min}(a_2,a_3,a_4)) = a_1$$

3. Following this design for $n > 4$, it is obvious that the final pattern of an n-place minimum aggregating operator will be as follows,

$$\begin{aligned}\mathcal{A}_{\min}(a_1, \cdots, a_n) &= \mathcal{A}_{\min}(\mathcal{A}_{\min}(a_1, \cdots, a_{n-1}), a_n) \\ &= \mathcal{A}_{\min}(a_1, \mathcal{A}_{\min}(a_2, \cdots, a_n)) \\ &= \min(a_1, \cdots, a_n) \end{aligned} \tag{4.11}$$

The next step is to prove (4.11) using the principle of mathematical induction. Therefore, carrying out the proof steps, we have

(i) For $n = n_0 = 2$, let $a_{i_1} < a_{i_2}$ be a permutation of $a_1, a_2 \in [0, 1]$. Then
$\mathcal{A}_{\min}(a_1, a_2) = \min(a_{i_1}, a_{i_2}) = a_{i_1}$ is true.

(ii) Let (4.11) be true for some integer $n > n_0$ such that for any permutation $a_{i_1}, a_{i_2}, \cdots, a_{i_n}$ of $a_1, a_2, \cdots, a_n$, we have $a_{i_1} < a_{i_2} < \cdots < a_{i_n}$.
Then for $(n + 1)$

$$\begin{aligned}\mathcal{A}_{\min}(\mathcal{A}_{\min}(a_1, \cdots, a_n), a_{n+1}) &= \mathcal{A}_{\min}(\min(a_{i_1}, \cdots, a_{i_n}), a_{n+1}) \\ &= \min(a_{i_1}, a_{i_{(n+1)}}) = a_{i_1}\end{aligned}$$

where $a_{i_1}, a_{i_{(n+1)}}$ is a permutation of a_1, a_{n+1} given that $a_{i_1} < a_{i_{(n+1)}}$. Hence, the minimum n-place operator is true for every integer n.

Other operators which are as easily extendable are the product (4.12) and the maximum (4.13) operations. Similarly, both operators can be proven using the same steps followed as in the case of deriving the minimum operator.

$$\mathcal{A}_{max}(a_1, \cdots, a_n) = \max(a_i, \cdots, a_n) \tag{4.12}$$

$$\mathcal{A}_{PR}(a_1, \cdots, a_n) = a_1 \cdot a_2 \cdot \cdots \cdot a_n \tag{4.13}$$

Hamacher Product

The extension procedure can also be applied to the Hamacher product. The following proposition and its corollary introduce the idea that will lead to the main result of this section.

Proposition 1. *The extended aggregation operator based on the Hamacher Product is*

$$\mathcal{A}(a_1, a_2, ..., a_n) = \frac{\prod_{i=1}^{n} a_i}{\sum_{i=1}^{n} \prod_{j=1, j\neq i}^{n} a_j - (n-1) \prod_{i=1}^{n} a_i} \tag{4.14}$$

Proof. 1. Starting with the 2-place hamacher product and the associativity law, we have

$$\mathcal{A}(\mathcal{A}(a_1, a_2), a_3) = \mathcal{A}(a_1, \mathcal{A}(a_2, a_3)) \tag{4.15}$$

$$\text{Hence,} \quad \mathcal{A}(a_1, a_2, a_3) = \frac{a_1 \cdot a_2 \cdot a_3}{a_1 \cdot a_2 + a_1 \cdot a_3 + a_2 \cdot a_3 - 2a_1 \cdot a_2 \cdot a_3} \tag{4.16}$$

2. The same is done for $n = 4$ with the end result

$$\mathcal{A}(\mathcal{A}(a_1, \mathcal{A}(a_2, a_3)), a_4) = \mathcal{A}(a_1, \mathcal{A}(a_2, \mathcal{A}(a_3, a_4))) \tag{4.17}$$

$\mathcal{A}(a_1, a_2, a_3, a_4) =$

$$\frac{a_1 \cdot a_2 \cdot a_3 \cdot a_4}{a_1 \cdot a_2 \cdot a_3 + a_1 \cdot a_2 \cdot a_4 + a_1 \cdot a_3 \cdot a_4 + a_2 \cdot a_3 \cdot a_4 - 3a_1 \cdot a_2 \cdot a_3 \cdot a_4} \tag{4.18}$$

3. This is continued for $n \geq 2$, until we can identify a pattern to design the general formula. Therefore, observing the denominator of equations (4.16) and (4.18), i.e.,

   for $n = 3$, $\quad a_1 \cdot a_2 + a_1 \cdot a_3 + a_2 \cdot a_3 - 2a_1 \cdot a_2 \cdot a_3$ and

   for $n = 4$, $\quad a_1 \cdot a_2 \cdot a_3 + a_1 \cdot a_2 \cdot a_4 + a_1 \cdot a_3 \cdot a_4 + a_2 \cdot a_3 \cdot a_4 - 3a_1 \cdot a_2 \cdot a_3 \cdot a_4$

   we can see they indicate a clear pattern. On this basis, we can attempt to construct the n-place Hamacher product as

$$\mathcal{A}(a_1, a_2, ..., a_n) = \frac{\prod_{i=1}^{n} a_i}{\sum_{i=1}^{n} \prod_{j=1, j\neq i}^{n} a_j - (n-1) \prod_{i=1}^{n} a_i} \tag{4.19}$$

   or equivalently,

$$\mathcal{A}(a_1, a_2, ..., a_n) = \frac{\prod_{i=1}^{n} a_i}{\sum_{i=1}^{n} a_1 \cdot a_2 \cdots \hat{a}_i \cdots a_n - (n-1) \prod_{i=1}^{n} a_i}. \tag{4.20}$$

   Where, $\hat{a}_i$ denotes the i^{th} element left out from the product of all elements, of the i^{th} summed up parameter.

4. Proof by induction: The formula (4.19) is correct for $n = 2, n = 3$ and $n = 4$ by design. Next, assume that (4.19) is true for some n. Then, for $(n+1)$, we have to prove that the $(n+1)$-place formula has the same representation, i.e.,

$$\mathcal{A}(a_1, a_2, ..., a_n, a_{n+1}) = \frac{\prod_{i=1}^{n+1} a_i}{\sum_{i=1}^{n+1} \prod_{j=1, i\neq j}^{n+1} a_j - (n) \prod_{i=1}^{n+1} a_i} \tag{4.21}$$

From associativity,

$$\text{take } \mathcal{A}(a_1, ..., a_n, a_{n+1}) = \mathcal{A}(\mathcal{A}(a_1, ..., a_n), a_{n+1}).$$

Then, $\mathcal{A}(\mathcal{A}(a_1, ..., a_n), a_{n+1})$

$$= \frac{\frac{\prod_{i=1}^{n} a_i}{\sum_{i=1}^{n} \prod_{j=1, j\neq i}^{n} a_j - (n-1) \prod_{i=1}^{n} a_i} \cdot a_{n+1}}{\frac{\prod_{i=1}^{n} a_i}{\sum_{i=1}^{n} \prod_{j=1, j\neq i}^{n} a_j - (n-1) \prod_{i=1}^{n} a_i} + a_{n+1} - \frac{\prod_{i=1}^{n} a_i}{\sum_{i=1}^{n} \prod_{j=1, j\neq i}^{n} a_j - (n-1) \prod_{i=1}^{n} a_i} \cdot a_{n+1}}$$

$$= \frac{(\prod_{i=1}^{n} a_i) \cdot a_{n+1}}{\prod_{i=1}^{n} a_i + a_{n+1}[\sum_{i=1}^{n} \prod_{j=1, j\neq i}^{n} a_j - (n-1) \prod_{i=1}^{n} a_i] - (\prod_{i=1}^{n} a_i) \cdot a_{n+1}}$$

$$= \frac{\prod_{i=1}^{n+1} a_i}{\underbrace{a_{n+1}(\sum_{i=1}^{n} \prod_{j=1, j\neq i}^{n} a_j)}_{(1)} + \underbrace{\prod_{i=1}^{n} a_i}_{(2)} - (n-1)(\prod_{i=1}^{n} a_i) a_{n+1} - \prod_{i=1}^{n+1} a_i} \tag{4.22}$$

Breaking down expression (1) leads us to

$$a_{n+1}(\sum_{i=1}^{n} \prod_{j=1, i\neq j}^{n} a_j) = a_{n+1}[(\hat{a}_1 \cdot a_2 \cdot \cdots \cdot a_n) + (a_1 \cdot \hat{a}_2 \cdot \cdots \cdot a_n) + ... + (a_1 \cdot a_2 \cdot \cdots \cdot \hat{a}_n)]$$

$$= (\hat{a}_1 \cdot a_2 \cdot \cdots \cdot a_n \cdot a_{n+1}) + (a_1 \cdot \hat{a}_2 \cdot \cdots \cdot a_n \cdot a_{n+1}) + ... + (a_1 \cdot a_2 \cdot \cdots \cdot \hat{a}_n \cdot a_{n+1})$$

Considering the above expression together with (2), which is the product $a_1 \cdot a_2 \cdot \cdots \cdot a_n \cdot \hat{a}_{n+1}$, we obtain

(1)+(2) $= \sum_{i=1}^{n+1} \prod_{j=1, j\neq i}^{n+1} a_j$

Then,

$$\mathcal{A}(a_1, a_2, ..., a_n, a_{n+1}) = \frac{\prod_{i=1}^{n+1} a_i}{\sum_{i=1}^{n+1} \prod_{j=1, i\neq j}^{n+1} a_j - (n) \prod_{i=1}^{n+1} a_i} \tag{4.23}$$

Hence, the n-place Hamacher product, defined for an element vector $[a] = (a_1, a_2, ..., a_n)$, holds for all n.

□

Bounded Difference

Due to the variety in aggregating operators present, different methods to design and derive n-place formulas (Step 2 of the extension procedure) are sometimes needed. As will be shown, this applies when trying to extend 2-place operators that consist of two mathematical expressions. An example of such is the Bounded difference aggregation,

$$\mathcal{A}(a,b) = \max(0, a+b-1) \tag{4.24}$$

Here, the bounded aggregation has two different solutions depending on the conditions satisfied by its elements a and b to be aggregated.

case 1: For $a+b \leq 1$, we have $\mathcal{A}(a,b) = 0$

case 2: For $a+b > 1$, we have $\mathcal{A}(a,b) = a+b-1$

Therefore, there exist two cases to deal with when extending such aggregations.

The steps of extension to follow are the same. As before, we start with the chosen operator ($n=2$) by adding an element to the associative equation (4.9), i.e.,

$$\mathcal{A}(a_1,a_2,a_3) = \begin{cases} 0 & \text{, if } \sum_{i=1}^{3} a_i \leq 2 \\ \sum_{i=1}^{3} a_i - 2 & \text{, if } \sum_{i=1}^{3} a_i > 2 \end{cases} \tag{4.25}$$

A diagram can be used to illustrate the extension of both cases (see Figure 4.1). Finally, by design, an n-place aggregation is reached, then proved by induction. This can be illustrated using the bounded difference aggregation.

Proposition 2. *The extended aggregation operator based on the Bounded Difference is*

$$\mathcal{A}(a_1,a_2,\cdots,a_{n-1},a_n) = \begin{cases} 0 & \textit{if } \sum_{i=1}^{n} a_i \leq n-1 \\ \sum_{i=1}^{n} a_i - (n-1) & \textit{if } \sum_{i=1}^{n} a_i > n-1 \end{cases} \tag{4.26}$$

Equivalently,

$$\mathcal{A}(a_1,a_2,\cdots,a_{n-1},a_n) = \max\{0, \sum_{i=1}^{n} a_i - (n-1)\} \tag{4.27}$$

Figure 4.1: A diagram showing the left hand case extension of an intersection operator based on the bounded difference aggregation. A similar solution is reached for the right hand case.

Proof. Use Equation (4.32), the Bounded difference intersection. The equation can be rewritten as

$$\mathcal{A}(a_1, a_2) = \begin{cases} 0 & \text{, if } a_1 + a_2 \leq 1 \quad \text{(Case 1)} \\ a_1 + a_2 - 1 & \text{, if } a_1 + a_2 > 1 \quad \text{(Case 2)} \end{cases}$$

To start the extension we first construct a 3-place aggregation using the associativity property.

1. **For** $n = 3$:

   Since the Bounded Difference is associative,

   $$\mathcal{A}(\mathcal{A}(a_1, a_2), a_3) = \mathcal{A}(a_1, \mathcal{A}(a_2, a_3))$$

   and

   $$\mathcal{A}(a_1, a_2, a_3) = \begin{cases} 0 & \text{, if } \sum_{i=1}^{3} a_i \leq 2 \\ \sum_{i=1}^{3} a_i - 2 & \text{, if } \sum_{i=1}^{3} a_i > 2 \end{cases} \tag{4.28}$$

2. **For** $n = 4$,

   $$\mathcal{A}(a_1, a_2, a_3, a_4) = \begin{cases} 0 & \text{, if } \sum_{i=1}^{4} a_i \leq 3 \\ \sum_{i=1}^{4} a_i - 3 & \text{, if } \sum_{i=1}^{4} a_i > 3 \end{cases} \tag{4.29}$$

3. ... and so on. Hence, for $n \geq 2$ there exist two cases

   $$\mathcal{A}(a_1, a_2, \cdots, a_n) = \begin{cases} 0 & \text{if} \sum_{i=1}^{n} a_i \leq n - 1 \\ \sum_{i=1}^{n} a_i - (n-1) & \text{if} \sum_{i=1}^{n} a_i > n - 1 \end{cases} \tag{4.30}$$

4. Proof by induction:

   Assume that $\sum_{i=1}^{n+1} a_i \leq n$, then

   $$\begin{aligned} \mathcal{A}(a_1, a_2, \cdots, a_n, a_{n+1}) &= \mathcal{A}(\mathcal{A}(a_1, a_2, \cdots, a_{n-1}, a_n), a_{n+1}) \\ &= \mathcal{A}(0, a_{n+1}) = \max(0, 0 + a_{n+1} - 1) \end{aligned}$$

But since, $a_{n+1} \in [0,1]$ then

$$\mathcal{A}(a_1, a_2, \cdots, a_n, a_{n+1}) = 0, \qquad \text{for } \sum_{i=1}^{n+1} a_i \leq n$$

Alternatively, when $\sum_{i=1}^{n+1} a_i > n$

$$\begin{aligned} \mathcal{A}(a_1, a_2, \cdots, a_n, a_{n+1}) &= \mathcal{A}(\mathcal{A}(a_1, a_2, \cdots, a_{n-1}, a_n), a_{n+1}) \\ &= \left[\sum_{i=1}^{n} a_i - (n-1)\right] + a_{n+1} - 1 \\ &= a_1 + a_2 + ... + a_n + a_{n+1} - (n-1) - 1 \\ &= \sum_{i=1}^{n+1} a_i - n \end{aligned} \tag{4.31}$$

Hence, the n-place bounded difference extension is true for all n □

Bounded Sum

The same approach used to extend the Bounded difference, i.e., approach A., can also be used to extend the Bounded Sum,

$$\mathcal{A}(a_1, a_2) = \min(1, a_1 + a_2) \tag{4.32}$$

a union type aggregating operator.

Proposition 3. *The extended aggregation operator based on the Bounded Sum is,*

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = \begin{cases} 1 & \text{if} \sum_{i=1}^{n} a_i \geq 1 \\ \sum_{i=1}^{n} a_i & \text{if} \sum_{i=1}^{n} a_i < 1 \end{cases} \tag{4.33}$$

Equivalently,

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = \min(1, \sum_{i=1}^{n} a_i) \tag{4.34}$$

This is illustrated in Figure 4.2.

Proof. The proof is similar to that followed for the bounded difference.

Figure 4.2: A diagram showing the left hand case extension of a union operator based on the bounded sum aggregation. A similar solution is reached for the right hand case.

1. **For** $n = 3$ the bounded sum is

$$\mathcal{A}(a_1, a_2, a_3) = \begin{cases} 1 & , \text{if } \sum_{i=1}^{3} a_i \geq 1 \\ \sum_{i=1}^{3} a_i & , \text{if } \sum_{i=1}^{3} a_i < 1 \end{cases} \tag{4.35}$$

2. **For** $n = 4$

$$\mathcal{A}(a_1, a_2, a_3, a_4) = \begin{cases} 1 & , \text{if } \sum_{i=1}^{4} a_i \geq 1 \\ \sum_{i=1}^{4} a_i & , \text{if } \sum_{i=1}^{4} a_i < 1 \end{cases} \tag{4.36}$$

3. $\cdots$ and so on. Then, for $n \geq 2$ there exists two cases

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = \begin{cases} 1 & \text{if} \sum_{i=1}^{n} a_i \geq 1 \\ \sum_{i=1}^{n} a_i & \text{if} \sum_{i=1}^{n} a_i < 1 \end{cases} \tag{4.37}$$

4. Proof by induction: Assume that $\sum_{i=1}^{n} a_i \geq 1$ then

$$\begin{aligned} \mathcal{A}(a_1, a_2, \cdots, a_n, a_{n+1}) &= \mathcal{A}(\mathcal{A}(a_1, a_2, \cdots, a_{n-1}, a_n), a_{n+1}) \\ &= \mathcal{A}(1, a_{n+1}) = \min(1, 1 + a_{n+1}) \end{aligned}$$

But since, $a_{n+1} \in [0, 1]$ then

$$\mathcal{A}(a_1, a_2, \cdots, a_n, a_{n+1}) = 1, \quad \text{for } \sum_{i=1}^{n+1} a_i \geq 1$$

Alternatively, when $\sum_{i=1}^{n+1} a_i < 1$

$$\begin{aligned} \mathcal{A}(a_1, a_2, \cdots, a_n, a_{n+1}) &= \mathcal{A}(\mathcal{A}(a_1, a_2, \cdots, a_{n-1}, a_n), a_{n+1}) \\ &= \left[\sum_{i=1}^{n} a_i\right] + a_{n+1} \\ &= \sum_{i=1}^{n+1} a_i \end{aligned} \tag{4.38}$$

Similarly, assume that $\sum_{i=1}^{n} a_i < 1$ then

$$\begin{aligned} \mathcal{A}(a_1, a_2, \cdots, a_n, a_{n+1}) &= \mathcal{A}(\mathcal{A}(a_1, a_2, \cdots, a_{n-1}, a_n), a_{n+1}) \\ &= \mathcal{A}(\sum_{i=1}^{n} a_i, a_{n+1}) \\ &= \min(1, \sum_{i=1}^{n} a_i + a_{n+1}) \\ &= \min(1, \sum_{i=1}^{n+1} a_i) \end{aligned}$$

But $a_i \in [0,1]$ for all $i = 1, \cdots, n+1$. Hence

$$\mathcal{A}(a_1, a_2, \cdots, a_{n+1}) = \begin{cases} 1 & \text{if} \sum_{i=1}^{n+1} a_i \geq 1 \\ \sum_{i=1}^{n+1} a_i & \text{if} \sum_{i=1}^{n+1} a_i < 1 \end{cases} \tag{4.39}$$

□

Algebraic Sum

The algebraic sum is another union type aggregating operator. Its 2-place formula is

$$\mathcal{A}(a_1, a_2) = a_1 + a_2 - a_1 \cdot a_2 \tag{4.40}$$

Proposition 4. *The extended union aggregation based on the Algebraic Sum is*

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = \sum_{i=1}^{n} (-1)^{i+1} \underbrace{\sum_{j_1=1}^{n-i+1} \sum_{j_2=j_1+1}^{n-i+2} \cdots \sum_{j_i=j_{i-1}+1}^{n} a_{j_1} \cdot a_{j_2} \cdots a_{j_i}}_{(1)} \tag{4.41}$$

for all $n \geq 2$. To simplify, denote expression (1) as S_i. Then Equation (4.41) becomes

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = \sum_{i=1}^{n} (-1)^{i+1} S_i \tag{4.42}$$

Before proceeding to the proof consider the following lemma.

Lemma 1. *Let $a_1, a_2, \cdots, a_n$ be elements in [0,1]. Let*

$$S_i = \sum_{j_1=1}^{n-i+1} \sum_{j_2=j_1+1}^{n-i+2} \cdots \sum_{j_i=j_{i-1}+1}^{n} a_{j_1} \cdot a_{j_2} \cdots a_{j_i}. \tag{4.43}$$

such that $a_{j_1} \cdot a_{j_2} \cdots a_{j_i}$ is the product of i elements, where $i = 1, \cdots, n$. Then the addition of an element, a_{n+1} to S_i, still preserves the formula for $(i+1)$, i.e.,

$$S_i \cdot a_{n+1} + S_{i+1} = S'_{i+1} \tag{4.44}$$

or

$$\begin{aligned} S'_{i+1} &= [a_1a_2\cdots a_i + a_1a_2\cdots a_{i+1} + \cdots + a_{(n-i+1)}a_{(n-i+2)}\cdots] \cdot a_{n+1} \\ &\quad + a_1a_2\cdots a_{i+1} + a_1a_2\cdots a_{i+2} + \cdots + a_{(n-i+1)}a_{(n-i+2)}\cdots \end{aligned} \tag{4.45}$$

This is for all $i = 1, \cdots, n-1$ *where,*

$$S_1 = a_1 + a_2 + \cdots + a_{n+1} \quad \textit{and} \tag{4.46}$$

$$S_{n+1} = a_1 \cdot a_2 \cdots a_{n+1} \tag{4.47}$$

Proof. Consider $S_i \cdot a_{n+1}$, such that

$$S_i \cdot a_{n+1} = a_1a_2\cdots a_i \cdot a_{n+1} + a_1a_2\cdots a_{i+1} \cdot a_{n+1} + \cdots + a_{(n-i+1)}a_{(n-i+2)}\cdots a_{n+1}$$

To find S'_{i+1}, we need the product of all elements taken $i+1$ at a time. The expression $S_i \cdot a_{n+1}$ contains all of these products which also contain the element a_{n+1} in them. Therefore, the only missing products are those that contain all elements taken $i+1$ at a time, from the elements $\{a_1, a_2, \cdots, a_n\}$, i.e.,
$a_1a_2\cdots a_{i+1} + a_1a_2\cdots a_{i+2} + \cdots + a_{(n-i+1)}a_{(n-i+2)}\cdots$.
But the summation of these is S_{i+1}. Therefore,

$$S'_{i+1} = S_i \cdot a_{n+1} + S_{i+1}$$

□

Example (4.2.2): For $n = 2$, Equation(4.41) is solved as follows

$i = 1$:

$$S_1 = (-1)^2 \sum_{j_1=1}^{2} a_{j_1} = a_1 + a_2$$

$i = 2$:

$$S_2 = (-1)^3 \sum_{j_1=1}^{1} \sum_{j_2=2}^{2} a_{j_1} \cdot a_{j_2} = -a_1 \cdot a_2$$

Hence, combining both expressions, we obtain Equation (4.40). Similarly, for $n = 3$.

$i = 1$:

$$S_1 = (-1)^2 \sum_{j_1=1}^{3} a_{j_1} = a_1 + a_2 + a_3$$

$i = 2$:

$$S_2 = (-1)^3 \sum_{j_1=1}^{2} \sum_{j_2=2}^{3} a_{j_1} \cdot a_{j_2} = (-1)^3 (a_1 \cdot a_2 + a_1 \cdot a_3 + a_2 \cdot a_3)$$

$i = 3$:

$$S_3 = (-1)^4 \sum_{j_1=1}^{1} \sum_{j_2=2}^{2} \sum_{j_3=3}^{3} a_{j_1} \cdot a_{j_2} \cdot a_{j_3} = (-1)^4 a_1 \cdot a_2 \cdot a_3$$

Then combining all three expressions we obtain the 3-place algebraic sum

$$\mathcal{A}(a_1, a_2, a_3) = a_1 + a_2 + a_3 - [a_1 \cdot a_2 + a_1 \cdot a_3 + a_2 \cdot a_3] + a_1 \cdot a_2 \cdot a_3 \quad (4.48)$$

Proof. (of Proposition (4)) Let Equation (4.40) be the 2-place algebraic sum union aggregation operator. Assume that this operator is true for some integer n, Equation

(4.42), then for $(n+1)$

$$\mathcal{A}(a_1, a_2, \cdots, a_n, a_{n+1}) = \underbrace{\sum_{i=1}^{n}(-1)^{i+1}S_i}_{1} + a_{n+1} - \sum_{i=1}^{n}(-1)^{i+1}S_i \cdot a_{n+1}$$

From (1), take out the term for $i = 1$, and combine to a_{n+1} to get $S_1^{'}$, Lemma (4.44). Then we have

$$= S_1 + a_{n+1} + \sum_{i=2}^{n}(-1)^{i+1}S_i - a_{n+1} \cdot \sum_{i=1}^{n}(-1)^{i+1}S_i$$

$$= S_1^{'} - \sum_{i=2}^{n}(-1)^{i}S_i - a_{n+1} \cdot \sum_{i=1}^{n}(-1)^{i+1}S_i$$

Let $j = i + 1 \rightarrow i = j - 1$. When $i = 1 \rightarrow j = 2$; and when $i = n \rightarrow j = n + 1$. Then, take out the term $S_{n+1}^{'} = a_{n+1} \cdot S_n = a_1 \cdot a_2 \cdots a_n \cdot a_{n+1}$, Lemma (4.44).

$$= S_1^{'} - \sum_{i=2}^{n}(-1)^{i}S_i - a_{n+1} \cdot \sum_{j=2}^{n+1}(-1)^{j}S_{j-1}$$

$$= S_1^{'} - \sum_{i=2}^{n}(-1)^{i}S_i - a_{n+1} \cdot \sum_{j=2}^{n}(-1)^{j}S_{j-1} - (-1)^{n+2}S_n \cdot a_{n+1}$$

Without any loss of generality, denote j by i,

$$= S_1^{'} - \sum_{i=2}^{n}(-1)^{i}S_i - a_{n+1} \cdot \sum_{i=2}^{n}(-1)^{i}S_{i-1} - (-1)^{n+2}S_{n+1}^{'}$$

$$= (-1)^2 S_1^{'} - \sum_{i=2}^{n}(-1)^{i}\left[S_i + a_{n+1} \cdot S_{i-1}\right] - (-1)^{n+2}S_{n+1}^{'}$$

But, based on the lemma, $S_i^{'} = S_i + a_{n+1} \cdot S_{i-1}$. Therefore,

$$= (-1)^{1+1}S_1^{'} + \sum_{i=2}^{n}(-1)^{i+1}S_i^{'} + (-1)^{n+2}S_{n+1}^{'}$$

$$= \sum_{i=1}^{n+1}(-1)^{i+1}S_i^{'} \qquad (4.49)$$

□

The generalized form of the algebraic sum also can be presented as

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = 1 - \prod_{i=1}^{n}(1 - a_i)$$

obtained from the family of γ-operators [25, 48].

Hamacher Sum

The 2-place hamacher sum union aggregation is

$$\mathcal{A}(a_1, a_2) = \frac{a_1 + a_2 - 2a_1 \cdot a_2}{1 - a_1 \cdot a_2} \tag{4.50}$$

Proposition 5. *The extended aggregation based on the Hamacher Sum is*

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = \frac{\sum_{i=1}^{n}(-1)^{i+1}(i) \cdot S_i}{1 - \sum_{i=2}^{n}(-1)^{i}(i-1) \cdot S_i} \tag{4.51}$$

Proof. The proof of Equation (4.51) consists of two parts: proof of the numerator, and proof of the denominator. Given the 2-place Hamacher sum, Equation (4.50), assume that the formula is true for some integer n, Equation (4.51). Then for $(n+1)$ we have

$$\mathcal{A}(a_1, a_2, \cdots, a_n, a_{n+1}) = \frac{\frac{\sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i}{1-\sum_{i=2}^{n}(-1)^{i}(i-1)\cdot S_i} + a_{n+1} - 2 \cdot \frac{\sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i}{1-\sum_{i=2}^{n}(-1)^{i}(i-1)\cdot S_i} \cdot a_{n+1}}{1 - \frac{\sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i}{1-\sum_{i=2}^{n}(-1)^{i}(i-1)\cdot S_i} \cdot a_{n+1}}$$

Simplifying the formula, we obtain

$$\begin{aligned} Numerator &= \sum_{i=1}^{n}(-1)^{i+1}(i) \cdot S_i + a_{n+1} - a_{n+1} \cdot \sum_{i=2}^{n}(-1)^{i}(i-1) \cdot S_i \\ &\quad - 2\left(\sum_{i=1}^{n}(-1)^{i+1}(i) \cdot S_i\right) \cdot a_{n+1} \qquad (4.52) \\ Denominator &= 1 - \sum_{i=2}^{n}(-1)^{i}(i-1) \cdot S_i - \left(\sum_{i=1}^{n}(-1)^{i+1}(i) \cdot S_i\right) a_{n+1} \qquad (4.53) \end{aligned}$$

We start with the proof of the numerator. We want to prove that

$$Numerator = \sum_{i=1}^{n+1}(-1)^{i+1}(i) \cdot S_i'. \tag{4.54}$$

Consider the expression (4.52),

$$\begin{aligned}
Numerator &= \sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i + a_{n+1} - a_{n+1}\cdot\sum_{i=2}^{n}(-1)^{i}(i-1)\cdot S_i \\
&\quad - 2\cdot a_{n+1}\left(\sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i\right) \\
&= \sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i + a_{n+1} - a_{n+1}\cdot\sum_{i=1}^{n}(-1)^{i}(i-1)\cdot S_i - \\
&\quad 2\cdot a_{n+1}\sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i \\
&= \sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i + a_{n+1} - a_{n+1}\sum_{i=1}^{n}(-1)^{i}(i)\cdot S_i \\
&\quad + a_{n+1}\sum_{i=1}^{n}(-1)^{i}\cdot S_i - 2\cdot a_{n+1}\sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i \\
&= \underbrace{\sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i}_{(1)} + a_{n+1} + a_{n+1}\underbrace{\sum_{i=1}^{n}(-1)^{i}(i+1)\cdot S_i}_{(2)}
\end{aligned}$$

From (1), take out the term for $i=1$, then combine with a_{n+1} to obtain S_1'. Also, in the second summation (2), substitute $j=i+1$, then $i=j-1$. When $i=1\rightarrow j=2$; $i=n\rightarrow j=n+1$.

$$\therefore Numerator = S_1' + \sum_{i=2}^{n}(-1)^{i+1}(i)\cdot S_i + a_{n+1}\sum_{j=2}^{n+1}(-1)^{j-1}(j)\cdot S_{j-1}$$

equivalently,

$$= S_1' + \sum_{i=2}^{n}(-1)^{i+1}(i)\cdot S_i + a_{n+1}\underbrace{\sum_{j=2}^{n+1}(-1)^{j+1}(j)\cdot S_{j-1}}_{(3)}$$

From (3), take out the term for $j = n+1$. This term is $(-1)^{n+2}(n+1) \cdot S_n \cdot a_{n+1}$.

$$\begin{aligned} Numerator &= S_1' + \sum_{i=2}^{n}(-1)^{i+1}(i) \cdot S_i + a_{n+1}\sum_{j=2}^{n}(-1)^{j+1}(j) \cdot S_{j-1} \\ &\quad + (-1)^{n+2}(n+1) \cdot S_n a_{n+1} \\ &= (-1)^2(1) \cdot S_1' + \sum_{i=2}^{n}(-1)^{i+1}(i) \cdot (S_i + a_{n+1} \cdot S_{i-1}) \\ &\quad + (-1)^{n+2}(n+1)S_{n+1}' \\ &= (-1)^2(1) \cdot S_1' + \sum_{i=2}^{n}(-1)^{i+1}(i) \cdot S_i' + (-1)^{n+2}(n+1)S_{n+1}' \end{aligned}$$

Hence,

$$Numerator = \sum_{i=1}^{n+1}(-1)^{i+1}(i) \cdot S_i'$$

Next, we want to prove the denominator

$$Denominator = 1 - \sum_{i=2}^{n}(-1)^i(i-1) \cdot S_i \tag{4.55}$$

We begin with Equation (4.53)

$$Denominator = 1 - \sum_{i=2}^{n}(-1)^i(i-1) \cdot S_i - \underbrace{\left(\sum_{i=1}^{n}(-1)^{i+1}(i) \cdot S_i\right)}_{1} a_{n+1}$$

Substitute for i in (1), $j = i+1$. When $i = 1 \rightarrow j = 2$; $i = n \rightarrow j = n+1$.

$$= 1 - \sum_{i=2}^{n}(-1)^i(i-1) \cdot S_i - a_{n+1}\underbrace{\sum_{j=2}^{n+1}(-1)^j(j-1) \cdot S_{j-1}}_{2} \tag{4.56}$$

From (2), take out the term for $j = n+1$ to get $S_{n+1}' = S_n \cdot a_{n+1} = a_1 \cdot a_2 \cdots a_{n+1}$. Then, without any loss of generality, substitute j for i.

$$\begin{aligned} &= 1 - \sum_{i=2}^{n}(-1)^i(i-1) \cdot S_i - a_{n+1}\sum_{j=2}^{n}(-1)^j(j-1) \cdot S_{j-1} \\ &\quad - (-1)^{n+1}(n) \cdot S_{n+1}' \\ &= 1 - \sum_{i=2}^{n}(-1)^i(i-1)\left(S_i + S_{i-1} \cdot a_{n+1}\right) - (-1)^{n+1}(n) \cdot S_{n+1}' \\ &= 1 - \sum_{i=2}^{n}(-1)^i(i-1)S_i' - (-1)^{n+1}(n) \cdot S_{n+1}' \end{aligned} \tag{4.57}$$

Hence,

$$Denominator \quad = \quad 1 - \sum_{i=2}^{n+1} (-1)^i (i-1) S_i^{'}$$

Therefore, the hamacher sum

$$\mathcal{A}(a_1, a_2, \cdots, a_n, a_{n+1}) \quad = \quad \frac{\sum_{i=1}^{n+1} (-1)^{i+1} (i) \cdot S_i^{'}}{1 - \sum_{i=2}^{n+1} (-1)^i (i-1) S_i^{'}} \tag{4.58}$$

is true for $n+1$. Hence, it is true for n. □

In the next section, we introduce examples of operators for the n-place aggregation of weighted arguments.

4.3 Using Weights in Fuzzy Aggregation

4.3.1 Weighted Fuzzy Intersections and Unions

With the aid of conjunctive and disjunctive type aggregations, Filev and Yager [32] talked about a subclass of these aggregations called *Weighted Intersections and Unions*. This term refers to the intersection and union type aggregations when the fuzzy sets A_i have weights associated with them.

Given a group of fuzzy sets, $A_1, A_2, \cdots, A_n$ of U, let each set be associated with a weight $w_i \in [0,1]$, $i = 1, \cdots, n$. Each weight, w_i, corresponds to the importance of the fuzzy set A_i, such that the larger w_i is, the more important the respective fuzzy set in the aggregation is. In the following we shall define weighted intersections and unions as a weighted aggregation, $\mathcal{A}$, resulting in a fuzzy set R

$$R = \mathcal{A}(f\{a_1, w_1\}, \cdots, f\{a_n, w_n\}).$$

Before applying $\mathcal{A}$, we must transform the original fuzzy sets A_i using their associated weights. So, let f be a *transformation function* used on each set, resulting in a modified fuzzy set b_i, i.e.,

$$b_i = f\{a_i, w_i\}$$

Then the aggregated operation $\mathcal{A}$ is calculated as

$$R = \mathcal{A}(b_1, \cdots, b_n).$$

The form of the transformation function f will depend primarily on the operation $\mathcal{A}$, whether it is an intersection or union type aggregation. The following is a general class of transformations for intersection and unions respectively, both suggested by [32].

1. **Transformation functions for intersection type aggregations**

   Let $\bar{w}_i = 1 - w_i$. Then

   - $b_i = \bar{w}_i \vee a_i$

- $b_i = \bar{w}_i + w_i a_i$
- $b_i = (1 + a_i - w_i) \wedge 1$
- $b_i = [a_i]^{w_i}$

2. **Transformation functions for union type aggregations**

- $b_i = w_i \wedge a_i$
- $b_i = w_i \cdot a_i$
- $b_i = (a_i + w_i - 1) \vee 0$
- $b_i = 1 - [1 - a_i]^{w_i}$

Examples of such weighted aggregations are the weighted sum and weighted maximum,

$$\mathcal{A}(A_1, \cdots, A_n) = \sum_{i=1}^{n} w_i \cdot a_i \tag{4.59}$$

$$\mathcal{A}(A_1, \cdots, A_n) = \max(w_1 a_1, w_2 a_2, \cdots, w_n a_n) \tag{4.60}$$

respectively.

4.3.2 OWA

There exists a family of mean-like operators known as the ordered weighted averaging operators. The abbreviation OWA is usually used in the literature to refer to these operations [32, 47, 51, 78]. The following definitions introduce the basic concepts associated with OWA operators.

Let the vector $(a_{i_1}, a_{i_2}, \cdots, a_{i_n})$ be a permutation of the vector $(a_1, \cdots, a_n)$ in which the elements are ordered, i.e., $a_{i_1} \geq a_{i_2} \geq \cdots \geq a_{i_n}$. Also, let $\mathbf{w} = (w_1, \cdots, w_n)$ be a weighting vector, such that

1. $w_k \in [0, 1]$ for all $k = 1, \cdots n$ and
2. $\sum_{k=1}^{n} w_k = 1$.

Definition 10 (Ordered weighted averaging operators). *An OWA operator, '$\mathcal{A}$', of n arguments is a mapping:*

$$\mathcal{A} : [0,1]^n \times [0,1] \longrightarrow [0,1]$$

such that

$$\begin{aligned} \mathcal{A}(a_1, \cdots, a_n) &= w_1 a_{i_1} + \cdots + w_n a_{i_n} \\ &= \sum_{k=1}^{n} w_k \cdot a_{i_k} \end{aligned}$$

OWA operators hold the properties of monotonicity, commutativity and idempotency [78]. Notice that an argument a_k is not associated with a particular weight w_k, but gets a weight according to its place in the ordered vector a. The following example will help to illustrate this concept.

Example (4.3.2): Let $w = (0.3, 0.1, 0.2, 0.4)$, and $a = (0.6, 0.9, 0.2, 0.7)$.
Then for $(a_{i_1}, a_{i_2}, \cdots, a_{i_n})$ a permutation of $(a_1, \cdots, a_n)$, the reordered vector is $(a_{1_2}, a_{2_4}, a_{3_1}, a_{4_3}) = (0.9, 0.7, 0.6, 0.2)$,
then
$\mathcal{A}(0.6, 0.9, 0.2, 0.7) = 0.3 \cdot (0.9) + 0.1 \cdot (0.7) + 0.2 \cdot (0.6) + 0.4 \cdot (0.2) = 0.54$

An important aspect of OWA operators, is that they can represent various aggregation operators. The following are examples of OWA special cases.

1. Let $w^{\cdot} = (1, 0, 0, \cdots, 0)$, then $\mathcal{A}_{w^{\cdot}}(a_1, \cdots, a_n) = \max(a_1, \cdots, a_n)$
2. Let $w_{\cdot} = (0, 0, 0, \cdots, 1)$, then $\mathcal{A}_{w_{\cdot}}(a_1, \cdots, a_n) = \min(a_1, \cdots, a_n)$
3. Let $w = (1/n, \cdots, 1/n)$, then $\mathcal{A}_w(a_1, \cdots, a_n) = \frac{1}{n} \sum_{k=1}^{n} a_k$
4. Let $w = (0, \frac{1}{n-2}, \frac{1}{n-2}, \cdots, \frac{1}{n-2}, 0)$, then
   $\mathcal{A}_w(a_1, \cdots, a_n) = \frac{1}{n-2}[\sum_{k=1}^{n} a_k - (\min(a_1, \cdots, a_n) + \max(a_1, \cdots, a_n))]$
   (Competition Jury).

5. Let w_{med}, be defined as follows,

$$\text{for } n \text{ odd} = \begin{cases} w_{\frac{n+1}{2}} = 1 \\ w_k = 0 \qquad \text{for all other } k \end{cases}$$

$$\text{for } n \text{ even} = \begin{cases} w_{\frac{n}{2}} = w_{\frac{n}{2}+1} = 0.5 \\ w_k = 0 \qquad\qquad\quad \text{for all other } k \end{cases}$$

Then the resulting $\mathcal{A}_{w_{med}} = (a_1, \cdots, a_n)$ is called the 'Median' aggregation [32].

In general, for any OWA operator, '$\mathcal{A}$'

$$\mathcal{A}_{w_*}(a_1, \cdots, a_n) \leq \mathcal{A}_w(a_1, \cdots, a_n) \leq \mathcal{A}_{w^*}(a_1, \cdots, a_n)$$

$$or \quad \min(a_1, \cdots, a_n) \leq \mathcal{A}_w(a_1, \cdots, a_n) \leq \max(a_1, \cdots, a_n)$$

4.3.3 Fuzzy Integrals as Aggregation Operators

In [3, 51], fuzzy aggregation operators were used to define overall loading indices, which indicate the degree of overall metal concentration at a given site. This was done without any consideration to the level of importance of each metal, with respect to its ecological effect. Therefore, a future prospective was suggested in that these levels can be used to design an *Index of metal importance*, by weighting the fuzzy metal sets and then applying an appropriate fuzzy aggregation.

Consider a group of environmental monitoring research scientists who are uncertain about if some metals (or contaminants) are harmful or not to the environment. The uncertainty here is related to the lack of distinct boundaries.

To add to this, the effect of a combination of metals is difficult to assess or predict. Therefore, here it is assumed that a perfect level of contamination reached by a metal (i.e., harmful or not) would point to full membership in one and only one of these sets. However, since monitoring of metal levels can depend on other

factors, such as the chemical interaction between two or more metals, considering the convex combination (weighted sum aggregation) of metals

may not always be perfect, and some uncertainty may exist. In order to represent this type of uncertainty, we could assign a value to each possible (nested) crisp subset of metals to which each metal (element) may belong. This value would indicate the degree of evidence or certainty of the metals importance or membership in the set. This type of uncertainty is known as a *fuzzy measure.*

Fuzzy Measures

This method differs from the assignment of grades of membership in fuzzy sets. In the latter case, a value $\mu_A(u)$ is assigned to each object (station) u of the universal set U, signifying its degree of membership in a particular set A with unsharp boundaries. The fuzzy measure, on the other hand, assigns a value to each crisp subset of the universal set of elements (metals), signifying the "importance" of each subset of metals.

Definition 11 (Fuzzy Measure). *: Given a universal set* $M = \{m_1, m_2, \cdots, m_n\}$ *of elements and a nonempty family* $\mathcal{P}(M)$ *of subsets of* M*, a set function* g*,*

$$g : \mathcal{P}(M) \longrightarrow [0, 1]$$

is a mapping from crisp subsets of M *into the unit interval, satisfying the following properties:*

(1) $g(\phi) = 0, \quad g(M) = 1$ *(Boundary requirements).*

(2) $\forall A, B \in \mathcal{P}(M)$*, if* $A \subseteq B$ *then,* $g(A) \leq g(B)$ *(Monotonicity).*

Then g *is called a fuzzy measure on* M*.*

Property (1) states that regardless of our evidence of membership (of an element), the element in question definitely does not belong to the empty set and definitely does belong to the universal set, $\mathcal{P}(M)$. The monotonicity requirement states that,

when we know with some degree of certainty that the element m_i belongs to a set A, then our degree of certainty that it belongs to a larger set B containing the former set, can be greater or equal, but not smaller [47].

Next, we shall give some examples of the function g. As given in Definition (11), these measures assume only the property of monotonicity and thus are seen as a generalization of Probability measures [27]. This generalization is obtained by replacing the additivity by the monotonicity property. The Probabilistic measure, λ-fuzzy measure, Dirac measure and U-decomposable measures are particular cases of fuzzy measures that are given next.

- **Probabilistic Measure**:

  Consider the additivity property of probabilities for disjoint sets, i.e., if two sets A and B are mutually exclusive

  , then $A \cup B$ denotes the set "either A or B occurs". Then, a probability measure is a fuzzy measure iff

  (1) For all sets A, $g(A) \in [0,1]$ and $g(M) = 1$

  (2) If $\forall\ A, B \in \mathcal{P}(M)$ such that $A \cap B = \phi$, then

  $$g(A \cup B) = g(A) + g(B) \quad \text{(Additivity Property)} \tag{4.61}$$

- **λ-Fuzzy Measure**:

  Relaxing the additivity property and replacing it with the monotonicity one, then for any A, $C \in \mathcal{P}(M)$, crisp subsets of M, if $A \subseteq C$, $\exists B$, such that $C = A \cup B$ and $A \cap B = \phi$ [27], then we have

  $$g_\lambda(A \cup B) = g(A) + g(B) + \lambda g(A) g(B) \tag{4.62}$$

  for $\lambda > -1$, g is called a λ-fuzzy measure. For, $\lambda = 0$, g is the probabilistic measure.

  Another special case is when $\lambda = -1$. In this case, $\forall\ A \subseteq M$, $\forall\ B \subseteq M$, g is

known as a plausibility measure i.e.,

$$g(A \cup B) = g(A) + g(B) - g(A \cap B) \tag{4.63}$$

A plausibility measure satisfies the following axioms:

(1) For all sets A, $g(\phi) = 0$; $g(M) = 1$.

(2) $\forall\ A, B \subseteq M$,

$$g(A \cup B) \leq g(A) + g(B) - g(A \cap B)$$

[27]. But for $g(A \cap B) = g(A) \cdot g(B)$, Equation (4.63) becomes

$$g(A \cup B) = g(A) + g(B) - g(A) \cdot g(B) \tag{4.64}$$

- **T-conorm based fuzzy measures**:

  For any two disjoint subsets A and B of M, we define

  $$g(A \cup B) = U(g(A), g(B)) \tag{4.65}$$

  where U is a t-conorm (union type operation), then g is a fuzzy measure (since t-conorms are monotonic by definition). These type of measures are called U-decomposable fuzzy measures. It follows, from the associativity property of t-conorms, for any A, a crisp subset of M, that

  $$g(A) = U_{m_i \in A}\ \big(g\{m_i\}\big) \tag{4.66}$$

  where $g(A)$ is uniquely determined by the collection $g\{m_i\}$. Here, U is the n-place extension of the t-conorm in Equation (4.65). To calculate $g(A)$ by Equation (4.66) it is enough to know the values for the individual elements of M, i.e., $g\{m_i\}$. These values will be discussed further. An example of a t-conorm based measure is:

  $$g(A) = \max_{m_i \in A}\ \big(g\{m_i\}\big)$$

  Similarly, formulas of fuzzy measures can be derived using t-norm operators [32].

The Concept of Fuzzy Integral

Using the notion of fuzzy measures, Sugeno developed the concept of fuzzy integral [62]. The operation of Sugeno fuzzy integral is based on a fuzzy measure, $g(A_i)$, which in turn relies on the identification of the fuzzy densities, $g\{m_i\}$ for all $i = 1 \cdots n$, (i.e., λ-fuzzy measure).

Before calculating g_λ, the analyst must determine the values of the measures corresponding to individual elements of M, which reflect the importance of each element within a research environment. These values, $g\{m_1\}, \cdots, g\{m_n\}$ known as *fuzzy densities*, will be denoted as $g^1, \cdots, g^n$, respectively, where $g^i = g\{m_i\} \in [0, 1]$. The i^{th} fuzzy density, g^i, is interpreted as the degree of importance of the element m_i towards the final evaluation. These densities can be (i) subjectively assigned by an expert, or (ii) can be derived from training data, as done in [62, 21]. The subjective assignment approach is sometimes the only method to assess the worth of non-numeric sources of information (such as intelligence reports) [45].

To calculate the λ-fuzzy measures (4.62) after determining the fuzzy densities, we must first obtain the value of λ by solving

$$\lambda + 1 = \prod_{i=1}^{n} (1 + \lambda g^i), \quad \lambda \neq 0. \tag{4.67}$$

The required λ is the unique real root greater than -1.

Let $A = \{m_{i_1}, \cdots, m_{i_L}\}$ be a subset of M, such that $\{i_1, \cdots, i_L\} \subset \{1, \cdots, n\}$. Then a sequence of nested subsets $A_1, \cdots, A_L$, are obtained by subsequently adding the elements one at a time. Let the fuzzy densities $g(\{m_{i_1}\})$ and $g(\{m_{i_2}\})$ (i.e., g^{i_1} and g^{i_2}) represent the assigned weights of importance in a fuzzy measure, for elements m_{i_1} and m_{i_2}, respectively. Also, let $g(\{m_{i_1}\} \cup \{m_{i_2}\})$ be the measure when the two elements m_{i_1} and m_{i_2} are combined, i.e., $g(A_2) = g(\{m_{i_1}\} \cup \{m_{i_2}\})$. Because m_{i_1} and m_{i_2} are interrelated, $g(\{m_{i_1}\} \cup \{m_{i_2}\})$ does not necessarily equal $g\{m_{i_1}\} + g\{m_{i_2}\}$. It is however, clear that $g(\{m_{i_1}\} \cup \{m_{i_2}\})$ should be greater or equal than $g\{m_{i_1}\}$ and $g\{m_{i_2}\}$, i.e.,

$$g(\{m_{i_1}\} \cup \{m_{i_2}\}) \geq \max\{g\{m_{i_1}\}, g\{m_{i_2}\}\}$$

In this case, $g(A \cup B)$ can be calculated using the Sugeno λ-fuzzy measure (4.62). The measures $g(A)$ are then calculated recursively as follows:

$g(A_1) = g^{i_1}$

and

$g(A_k) = g^{i_k} + g(A_{k-1}) + \lambda g^{i_k} g(A_{k-1}) \quad$ for $1 < k \leq n$

such that

$g(A) = g(A_n)$

---

where λ is obtained by solving equation (4.67), using the fuzzy densities predetermined by the researcher, g^i.

Now, let H be a fuzzy set on M with grades of membership, $H = (\mu_H(m_1), \cdots, \mu_H(m_n))$. Here we are looking for one representative value of the membership grades to which the concept, H, is satisfied by all elements m_i's. We want this aggregate value to show how all elements of M agree with the characteristic H, at the same time taking into account the importance of each element m_i, $\forall i = 1 \cdots n$. For simplicity, we shall denote $\mu_H(m_i)$ as a_i.

Using the notion of fuzzy measures, Sugeno developed the concept of the fuzzy integral [21]. This is a nonlinear function that is defined with respect to a fuzzy measure, especially the λ-fuzzy measure. Therefore, using the concept of fuzzy integrals, we can arrive at our respective representative value.

Definition 12 (Sugeno Fuzzy Integral). *: Let M be a finite set, and H be a fuzzy subset of M. defined by a membership function, $\mu_H : M \longrightarrow [0,1]$ The fuzzy integral over M, of the function μ_H with respect to a fuzzy measure g, is defined by*

$$\mathcal{A}_g^{FI}(a_1, \cdots, a_n) = \sup_{\alpha \in [0,1]} \{t(\alpha, g(H_\alpha))\} \tag{4.68}$$

where H_α is the α-level set (α-cut) of the fuzzy set H, $H_\alpha = \{m : \mu_H(m) \leq \alpha\}$ and t is a t-norm (intersection type operator).

Since M is finite, H has at most n different α-level sets, ranging from $H_0 = M$ to $H_{height(H)}$ containing only the elements for which the membership function of H, μ_H, reaches its maximum. In the original formula, the t-norm was the minimum operator [21, 50, 32, 45]

$$\mathcal{A}_g^{FI}(a_1, \cdots, a_n) = \sup\ [\min(\alpha, g(H_\alpha))]. \tag{4.69}$$

The value obtained from (4.69), which compares the objective evidence and the subjective importance (the fuzzy densities) in terms of the minimum operator, is interpreted as the grade of agreement between real possibilities, $\mu_H(m)$, and the expectations, g. In other words, it can be interpreted as the 'highest pessimistic' grade of agreement between the evidence and the expectation.

In Keller (1994) [45], a generalization of the definition of fuzzy integral involved replacing the minimum operator with more general aggregating operators, t-norms and t-conorms. It was noted that in order to replace the minimum with another t-norm or maximum with another t-conorm, the new operators must satisfy the distributive law. Examples of such t-norms that are mutually distributive with respect to the maximum are the minimum, product, bold union, and the drastic product. To calculate the fuzzy integral, given a finite set M and a membership function μ_H,

1. Rearrange the elements of M such that their corresponding grades of membership are in descending order $\quad a_{i_1} \geq a_{i_2} \geq \cdots \geq a_{i_n}$,
   and consequently the set of fuzzy densities, $g^i\ \forall\ i = 1, \cdots, n$.

2. Let the sequence of nested subsets be denoted by $A_1 = \{m_{i_1}\}, A_2 = \{m_{i_1}, m_{i_2}\}, \cdots,$ $A_n = M$. Thus, each $A_k \subseteq M$ is the a_{i_k}-cut of M, where $a_{i_k} > a_{i_{k+1}}$.

3. Then, the fuzzy integral (4.68), with respect to a fuzzy measure, g over M, becomes

$$\mathcal{A}_g^{FI}(a_1, \cdots, a_n) = \max_{k=1}^{n}[\min(a_{i_k}, g(A_k)] \tag{4.70}$$

   where (4.70) is simpler to compute than (4.68).

Example 4.3.3 : Using a simple illustration, with $n = 4$, such that $A_n = M = \{u_1, u_2, u_3, u_4\}$, we have,

$$\mathcal{A}_g^{FI}(0.6, 0.1, 0.3, 0.9) = \max[(\min(0.9, g(\{u_4\})), (\min(0.6, g(\{u_1, u_4\})),$$
$$(\min(0.3, g(\{u_1, u_3, u_4\})), (\min(0.1, g(\{u_1, u_2, u_3, u_4\}))]$$

Another type of fuzzy integral, which uses the concept of fuzzy measures, is known as the *Choquet fuzzy integral.* The formula for the choquet integral is

$$\mathcal{A}_g^{FI}(a_1, \cdots, a_n) = a_{i_n} + \sum_{k=2}^{n} (a_{i_{k-1}} - a_{i_k}).g(A_{k-1}) \tag{4.71}$$

Some information on the application of the Choquet fuzzy integral, as an aggregation operator, can be found in [20, 62]. More information on the concept of fuzzy measures and fuzzy integrals and their application can be found in [74].

4.4 Fuzzy Modelling of Metal Loading in Liverpool bay and Morecambe bay

Previously we introduced the theory behind constructing a basic fuzzy model for information fusion. In this chapter we construct such a model to represent a marine environment. The model uses the heavy metal content, sampled from the sediment and derives what we call metal loading indices. These indices represent various spatial distributions of heavy metal loading in the marine environment.

4.4.1 An Introduction: Spatial data and multi-variate analysis

First consider the word 'spatial', and the connection between a fuzzy environmental model, on the one hand, and 'spatial data analysis' used mostly by geographical information systems (GIS), on the other hand. Questions that relate to multi-variate analysis of attributes in a geographical space are classified as being either aspatial (i.e., referring to geometrical issues such as area size or shape), or spatial (i.e., referring to locational properties such as the relationship between the objects with respect to their location: spatial relationship) [39]. Spatial data is a collection of points located in a geographical space, and attached to it a set of one or more attribute values. In [39], spatial analysis (SA) is defined as a collection of techniques for analysing geographical events, whereas [6] defines SA as '*a general ability to manipulate spatial data into different forms and extract additional meaning as a result*'.

Bailey (1994) [6] stated that it is important to make a distinction between spatial summarization of data and spatial analysis of data (be it statistical or mathematical) in GIS. The former refers to basic functions for the selective retrieval of spatial data within defined areas of interest and the computation, tabulation or mapping of various basic summary statistics of that information. The latter is more concerned with the investigation of patterns in spatial data, in particular, seeking possible relationships between such patterns and other attributes within the study region,

and with the modelling of such relationships for the purpose of understanding or prediction. Finally, it is widely acknowledged that existing GIS offer a powerful array of techniques for spatial summarization which are in many cases, a prerequisite to spatial analysis (SA) [6].

Three main categories of SA are identified, [39]. These are statistical spatial data analysis (SDA), map based analysis and mathematical modelling. Many applications concentrate on SDA techniques [6, 39] because of the widespread application of these techniques (e.g., descriptive statistics, graphical representation, multiple regression) compared to 'customized' techniques which were not yet developed to the stage where they were widely used.

Haining (1994) [39] mentioned that GIS require robust operations to summarize data for purposes of identifying data properties and pattern detection, which should also be relatively easy to carry out and implement. A grouping of these operations was given as:

[**A**] Operations that depend on accessing the location and/or attribute values of the cases.

[**B**] Operations that depend on identifying spatial relationships between the cases.

[**C**] Operations that involve interaction between type [A] and [B] operations.

4.4.2 Detailed objectives and problem-specific difficulties

Having specified the problem (Chapter 1), the data (Chapter 2), and the underlying theory (Chapter 3), we can now detail the specific objectives of the first part of the Research Assignment: Designing loading indices.

The aim is to develop a practical procedure to evaluate overall **spatial distribution of metal concentrations and contamination**, using a sample of metal concentrations from sediments in Liverpool bay and Morecambe bay. Therefore, we seek to:

- Develop a model that can be applied to a wide range of measurement scales of the different metals.

- Verify that the model is applicable to different marine environments.

The main difficulty in this study is that we lack prior knowledge about the expected pattern of metal distribution in a marine environment. A similar problem was faced by the authors of [81]. Thus *a priori* information would enable us to measure the performance of a technique, for modelling metal distribution with respect to the concept of contamination. Unfortunately, this is not the case for our research problem. The only available information about possible distributions came from the domain expert. So, our conclusions will be based mainly on the subjective satisfaction of the domain expert with the visual output we produce.

The use of statistical techniques has been considered in the analysis of heavy metals [56] and soil information [12]. On the one hand, such methods were found to be at most times user friendly, i.e., well understood by the user [6]. On the other hand, results of some of these methods might defy interpretation, as we suggest in [51].

Based on our collection and analysis of quantitative information, there are two aims within our research that we share with that of SA. The first is the careful description of environmental data and patterns in a geographical space. The second is the exploration of the pattern of events, and the association between them in space in order to gain a better understanding of the process that might be responsible for the distribution of these events.

One part of our objective, to find a pattern for the flow of contaminants in Liverpool bay, can be viewed as a spatial type analysis. For example, one possible question is: are large/small values of attribute A spatially close to large/small values of attribute B across the set of locations? Subsequently, we may ask how data properties vary across the map or between one part of the map and another. A visual representation will then aid us to find if there exist spatial trends in the value of the attributes over the region. Therefore, operations involved in the fuzzy

modelling of spatial data of a marine environment, can be grouped into the first two operations identified for GIS, i.e., operation [A] and [B]. In our case, operations of type [A] are: identification of properties of attributes (descriptive statistics), missing case/attribute value estimation, and design of fuzzy membership functions. Operations of type [B] are: aggregation operations for constructing the loading indices. A statement made by [60] highlights the importance of using innovative and unconventional techniques in SDA:
'*techniques are wanted that are able to hunt out what might be considered to be localized pattern in geographically referenced data but without being told either 'where' to look or 'what' to look for, or 'when' to look*'. This encouraged us to look beyond the classical statistical techniques and turn to non-conventional methods.

Considering the detailed objectives, the difficulties we are facing and the conclusions of the survey in Chapter 3, a mathematical analysis of the metal data sets using fuzzy set theory was chosen. From the review in 3.2, it was found that the fuzzy set approach has not been applied to analyzing metal distribution in a marine environment. Referring to the above quote from [60], we believe that the chosen approach will lead to "discovering" interesting phenomena in data, and consequently in the respective geographical region. We expect to find contamination patterns (distributions) in Liverpool bay and Morecambe bay, without previous knowledge on "where" to look and "what" to look for. Thus the current research can be considered as a pilot study, in which different concepts of metal spatial distribution are constructed and explored. Admittedly, this study is largely ad-hoc, and might have a practical significance in the field of environmental monitoring of heavy metal distribution. Nevertheless, we believe that the general methodology of data analysis in a marine environment will be useful in other environmental studies and other geographical regions.

4.4.3 A methodology for analysis of heavy metal distributions in a marine environment

In Chapter 2, the finalized data and its summary statistic is given for the two marine environments: Liverpool bay and Morecambe bay (in 1988). This data will be used to analyze the spatial distribution of overall metal content in 1988.

Let $X = \{x_1, x_2, \cdots, x_n\}$ denote a finite set of n heavy metals. In our case, $X =$ { Mercury/Hg (x_1), Cadmium/Cd (x_2), Cromium/Cr (x_3), Copper/Cu (x_4), Nickel/Ni (x_5), Lead/Pd (x_6), Zinc/Zn (x_7) }.
Let S denote the universal set, $S = \{s_1, s_2, \cdots, s_m\}$ of m sampled stations (or objects/points) in a marine environment, i.e., $m = 70$ in Liverpool bay, and $m = 198$ in Morecambe bay. Then let $x_i(s_j)$ be the concentration of the metal x_i measured at site s_j.

The following is a summarized overview of steps which shall be implemented to design the fuzzy model.

1. Construct a fuzzy membership function to measure a specific feature, i.e., 'the degree to which a site is considered to be contaminated'.

   (a) Decide upon a function to convert the metal concentrations from a specific scale to the unit interval. Then, determine the parameters needed by the function to express this feature. The shale values and the acceptable maximal concentration of a metal can be used to pinpoint the lower and upper boundaries of this feature, the 0 and the 1, respectively. This is done for each of the sampled metals.

   (b) Find the parameter values, e.g., by literature research or expert opinion.

   (c) Apply the function to convert the concentrations of each metal data set to a fuzzy set on S.

2. Aggregate the fuzzy sets for the metals to express 'the possibility that a given point or station is contaminated'.

(a) Construct or select a suitable set of aggregation operators. Here "suitable" should be related to the operator's interpretability in the domain context.

(b) Apply the operators to the fuzzy sets of metal elements to compute values for each point in S.

3. Use a formal or a subjective method to choose the most useful set of aggregated results.

4.4.4 Determining a Fuzzy Membership Function (FMF)

The concepts of contamination and pollution

Substances that occur in nature and exist naturally in the sea are called inputs [23]. Examples of inputs are metals in the runoff from metalliferous deposits, or particulate material from coastal erosion, e.g. coal. With so many natural inputs to the sea, the concentrations of substances vary widely from place to place in the marine environment.

Contamination is caused when an input from human activities increases the concentration of a substance in seawater, sediments, or organisms above the *natural background level* (i.e., average shale values) for that area and for the organisms [23]. Sometimes the locally elevated concentrations may be less than the concentration of the same substances in other areas where there is a large natural input.

Marine **pollution** is the introduction by man, directly or indirectly, of substances or energy to the marine environment resulting in deleterious effects such as: hazards to human health; hindrance of marine activities, including fishing; impairment of the quality for the use of sea water, and reduction of amenities [23]. The definition of contamination differs from the definition of pollution in that 'contamination' is the occurrence of inputs in the sea, while 'pollution' is the damaging effects these inputs have on the environment. Although the discovery of high concentrations of a substance may provide a warning signal, unless it is the result of human activities and is damaging, it does not constitute pollution. Generally, there can be no doubt about

the existence of pollution when the damage is severe, but there is often considerable difficulty in identifying damage from low levels of contamination caused by diffused, or sometimes, unknown inputs. Hence, measuring pollution is not an easy task to perform. Therefore, we focus this research on identifying mathematically the different **levels of contamination**.

Fuzzy membership function (FMF)

To construct the fuzzy sets we must select a function that scales the metal concentrations (in μg/g of sediment) to the unit interval, to denote the degree of contamination by a metal. We decided that the FMF must be an increasing function, with respect to the increasing levels of metal concentrations. Since we have seven metals measured on different scales, the FMF is a context specific function [51], i.e., different for each metal. Therefore, for each x_i, a fuzzy set A_i over S is defined corresponding to 'contamination with x_i' with an asymmetric left variant type function

$$\mu_{A_i}(x_i(s_j)) = \begin{cases} 0 & \text{, if } x_i(s_j) < L_i \\ \frac{x_i(s_j)-L_i}{T_i-L_i} & \text{, if } x \in [L_i, T_i] \\ 1 & \text{, if } x_i(s_j) > T_i \end{cases} \tag{4.72}$$

where L_i are background metal concentrations that are naturally present in sediments [70, 29], and T_i are upper guideline limits of metal concentrations from the U.K. Department of the Environment (DOE) Interdepartmental Committee for the Reclamation of Contaminated Land (ICRCL) list of trigger concentrations for environmental metal contaminants [5] as shown in Table 4.1. The upper trigger levels are those given by the ICRCL [5], whereas the average shale values were obtained from [29, 70].

Results

Using Equation (4.72) on the metal concentration data of Liverpool bay and Morecambe bay (1988), seven fuzzy sets are computed for each marine environment (see

Appendix (C)). Some summary statistics of the membership functions for both regions are given in Table 4.2. All major calculations were done with the aid of the packages, Octave and Matlab. Using Equation (4.72) metal concentrations are mapped to the unit interval $[0, 1]$, such that 0 and 1 fuzzy values correspond to **no** contamination and **full** contamination, respectively. Some data anomalies during the analysis process were encountered. Negative degrees of membership were reassigned the non-membership ($\mu_A(s_j) = 0$). These negative values occur because the lower bound of a metal set was less than the corresponding metal lower guideline. This is because within defining the concept of 'contamination', a degree of '0' is chosen to denote no contamination, but at the same time to indicate the existence of concentration levels equal to or below the benchmarks L_i (i.e., average shale values). In general, mean metal concentrations from Morecambe bay appear to be, on average, 27% less than metal concentrations found in Liverpool bay, in 1988 (Table 4.2).

Observing the resulting fuzzy sets in *Appendix (C)* and Table 4.2, the following features with respect to contamination can be seen for each marine environment.

Liverpool bay (1988)

- There is no evidence of contamination by the heavy metals chromium and nickel.
- All sampled sites register contamination with lead and zinc, compared to some sites are contaminated with mercury, cadmium and copper.

Morecambe bay (1988)

- There is no evidence of contamination by the heavy metals mercury, cromium and nickel.
- The majority of sites are contaminated with lead, whereas only a few sites register contamination with cadmium, copper and zinc.

Table 4.1: Contamination guidelines: Average shale and upper trigger limits on units

Metals	General limits Lower L_i	Upper T_i
Hg	0.4	20
Cd	0.3	15
Cr	90	1000
Cu	45	130
Ni	68	70
Pb	20	2000
Zn	95	300

Table 4.2: Some summary statistics of the membership functions of Liverpool and Morecambe bay data

Metals	LB(1988) Min.	Max.	MB(1988) Min.	Max.	(1) Mean LB	(2) Mean MB	Mean(2)-(1)
Hg	0.00	0.09	0.00	0.00	0.01	0.03	-0.01
Cd	0.00	0.15	0.00	0.06	0.02	0.00	-0.02
Cr	0.00	0.01	0.00	0.00	0.00	0.00	0.00
Cu	0.00	1.00	0.00	0.53	0.03	0	-0.03
Ni	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pd	0.03	0.60	0.00	0.12	0.11	0.02	-0.09
Zn	0.20	1.00	0.00	0.37	0.90	0	-0.90

4.4.5 Loading indices

Having designed the fuzzy sets, seven for each marine environment, the next step is to evaluate the possibility of a site being contaminated. We use fuzzy generalized aggregation operations to define overall loading (contamination) indices. Some information on the definition of environmental indices is introduced in [53].

Two groups of aggregating operators are used, ordinary operators and dependent operators. Operations that do not use external information (i.e., weights or information other than the fuzzy data sets at hand) we call *ordinary* operations. Operations which involve external parameters are called *dependent* operations.

Let $U = \{u_1, u_2, \cdots, u_m\}$ be the universal set of elements $u_j, \forall j = 1, \cdots, m$. The fuzzy aggregated set A_i on U is defined by assigning a degree of membership $a_{ij} = \mu_{A_i}(u_j)$ to each $u_j \in U$, with regard to overall contamination. Fifteen generalized aggregation operations are summarized in Table 4.3. These include intersection, union, mean, parameterized and weighted generalized aggregation operations, of which {3}, {4}, {6}, {7} and {8} were derived in Section 4.2. Not all of these operators were suited for the evaluation of a marine environment. Operations {14} and {15} were seen not suitable for the following reasons.

- A downside of the beta-gamma combination rule is that the parameters β and γ are not intuitively clear [66]. Even in the case of aggregating two fuzzy sets, it was recommended to obtain γ ($\beta = 1 - \gamma$) through predefined degrees of membership for some selected objects u. This requires external information from domain experts which was not available for our study. Another factor is, if some u from A_i has degree of membership $\mu_{A_i}(u) = 0$, then for any grade of compensation $\gamma \neq 1$ the resulting degree of membership is always $\mu_A(u) = 0$. In this case, the minimum, product and geometric mean generalized operations will suffice.

- The symmetric sum (4.8) is characterized as a balanced combination rule [66, 67]. This would be useful if we studied balancing environmental dam-

Table 4.3: Generalized aggregation operations, where $S_i = \sum_{j_1=1}^{n-i+1} \sum_{j_2=j_1+1}^{n-i+2} \cdots \sum_{j_i=j_{i-1}+1}^{n} a_{j_1} \cdot a_{j_2} \cdots a_{j_i}$.

Operation	Generalized operation $\mathcal{A}(a_1, \cdots, a_n)$	External information
1. Minimum	$\min(a_1, \cdots, a_n)$	None
2. Algebraic product	$a_1 \cdot a_2 \cdot \cdots \cdot a_n$	None
3. Hamacher product	$\frac{\prod_{i=1}^{n} a_i}{\sum_{i=1}^{n} \prod_{j=1, j\neq i}^{n} a_j - (n-1) \prod_{i=1}^{n} a_i}$	None
4. Bounded difference	$\max\left(0, \sum_{i=1}^{n} a_i - (n-1)\right)$	None
5. Maximum	$\max(a_1, \cdots, a_n)$	None
6. Algebraic sum	$\sum_{i=1}^{n} (-1)^{i+1} S_i$	None
7. Hamacher sum	$\frac{\sum_{i=1}^{n} (-1)^{i+1} (i) \cdot S_i}{1 - \sum_{i=2}^{n} (-1)^{i} (i-1) \cdot S_i}$	None
8. Bounded sum	$\min\left(1, \sum_{i=1}^{n} a_i\right)$	None
9. Arithmetic mean	$\frac{1}{n} \sum_{i=1}^{n} a_i$	$w = [\frac{1}{n}, \cdots, \frac{1}{n}]$
10. Geometric mean	$(a_1 \cdot a_2 \cdot \cdots \cdot a_n)^{\frac{1}{n}}$	None
11. Competition jury	$\frac{1}{n-2}[\sum_{i=1}^{n} a_i - \{\min(a_1, \cdots, a_n) + \max(a_1, \cdots, a_n)\}]$	None
12. Fuzzy integral	$\max_{k=1}^{n}[\min(a_{i_k}, g(A_k)]$	$g = [g^{Hg}, g^{Cd}, g^{Cr}, g^{Cu}, g^{Ni}, g^{Pb}]$
13. Weighted average	$\frac{\sum_{i=1}^{n} a_i g(A_i)}{\sum_{i=1}^{n} g(A_i)}$	$g = [g^{Hg}, g^{Cd}, g^{Cr}, g^{Cu}, g^{Ni}, g^{Pb}]$
14. Beta-Gamma combination rule [25, 66]	$(\prod_{i=1}^{n} a_i)^{\beta} \cdot (1 - \prod_{i=1}^{n} (1 - a_i))^{\gamma}$	$\beta, \gamma \in [0, 1]$
15. Symmetric sum [66, 67]	$\left\{ \left(\frac{a_1}{1-a_1}\right)^{w_1} \cdot \left(\frac{a_2}{1-a_2}\right)^{w_2} \cdot \left(\frac{a_3}{1-a_3}\right)^{w_3} \cdots \right\}^{\frac{1}{w_1 + w_2 + w_3 + \cdots}}$	$\sum_{i=1}^{n} w_i = 1$

age against potential benefits. Also, symmetric sum is useful when there is no implicit assumption that certain degrees of membership are 'good' and others are 'bad'. Therefore, the symmetric sum is symmetric under reversal of definitions, such that one gets the same result by replacing a by $1-a$ and consequently a_i by $1-a_i$ $\forall i = 1, \cdots, n$.

None of these features are required in this study. In addition, Equation (4.8) is not defined if any of the a_i is equal to 1.

Therefore, our selection rested on operations {1} through {13}, from Table 4.3.

The computation of operators {1} to {11} does not require any external information, unlike the fuzzy integral {12} and weighted average {13}. Both of these generalized aggregating operators rely on defining the fuzzy densities (or weights) $g = [g_1, g_2, \cdots, g_7]$ where $g_i \in [0,1], \forall i = 1, \cdots, 7$. Here, we are concerned with the effect of a combination of metals. In order to represent this type of uncertainty, we could assign a value to each possible (nested) crisp subset of metals representing its importance. Therefore, using the notion of *fuzzy measure* we can express a group weight of each metal combination and take it into account in the aggregation. But to compute both operators {12} and {13}, we must determine the fuzzy densities.

Let $X = \{x_1, \cdots, x_7\}$ be the crisp set of metals, such that subscripts $i = 1, \cdots, 7$ denote: Hg, Cd, Cr, Cu, Ni, Pb, and Zn, respectively. To define the 7 fuzzy densities, the "*shale values*", L_i, were used. We assumed that the fuzzy densities should denote a metal's importance or weight with respect to contamination. The degree in which a metal concentration on average exceeds a benchmark value (i.e., shale values) is used to denote this. For Liverpool bay data (1988), the median of each metal set was taken to represent the metal concentration over all sites and to be compared with the benchmark. Similarly, the median of each metal in Morecambe bay (1988) was chosen to compute the fuzzy densities for this region. We chose the median to reduce the effect of accidental high concentrations (see Chapter 2). Examples of this, are the dumping of copper wires or lead batteries in the bay. Finally, a fuzzy density vector, $g = [g^{Hg}, g^{Cd}, g^{Cr}, g^{Cu}, g^{Ni}, g^{Pb}, g^{Zn}]$

for each region was computed as $\mu_{med} - \mu_{benchmark}$. These differences were scaled to $[0, 1]$, so that the smallest density is 0.05 and the largest is 0.95. The results are

$g_{lb} = [0.8, 0.94, 0.3, 0.86, 0.05, 0.9, 0.95]$

$g_{mb} = [0.89, 0.95, 0.2, 0.89, 0.05, 0.95, 0.94]$.

Using the fuzzy densities, g_{lb} and g_{mb}, to solve Equation (4.67), the root $\lambda = -1$ was calculated.

4.4.6 Index interpretation

In this section, we will summarize our interpretation of the resulting indices based on the aggregating operator used. This will be done within the context of overall metal contamination. Let the aggregated values of contamination $\in [0, 1]$ be linguistically interpreted as 'degrees of membership that fall between acceptable (aggregation value= 0) and unacceptable (aggregation value= 1) levels of overall contamination'.

Minimum {1} : One of the most standard combination rules used in environmental applications [12, 13, 11, 26, 41, 63, 66, 67, 68]. The minimum operator can be used to answer queries such as: "Where is there a reasonable possibility of finding areas in the bay where the sediments are generally contaminated throughout?" It gives for each site the smallest levels of contamination among the seven metals. Therefore, the minimum operator can be seen to reflect a definite contamination by all seven heavy metals in the region.

Algebraic product {2}, and geometric mean {10} : In some situations, environmental scientist would only consider the presence of heavy metal contamination, if all combined $\mu_{A_i}(u)$, $\forall i = 1, \cdots, 7$ are non-zero. In this case, the aggregate membership degrees in a set of unacceptable levels of contamination should be subject to the requirement that if any of $\mu_{A_i}(u) = 0$, the aggregate degree of membership is 0. In other words, if any of the metal contamination degrees of membership is totally acceptable, the total contamination is also acceptable. Hence, resulting JMF values of both operators can be said to reflect total unacceptable levels of overall metal contamination in the region.

Hamacher product {3} : The 2-place hamacher product

$$\mathcal{A}(a,b) = \frac{a \cdot b}{a + b - a \cdot b} \tag{4.73}$$

is an intersection type operator defined by (2), such that $\mathcal{A}(0,b) = 0, \forall b \in (0,1]$, but is undefined for $\mathcal{A}(0,0)$. Consider the n-place structure of this operator, Equation (4.19), and the defining properties of an n-place aggregation connective, Definition 7. This operator is not defined for the boundary condition, $\mathcal{A}(a_1 = 0, \cdots, a_n = 0)$ for $n \geq 2$. Therefore, redefining the generalized hamacher product is necessary,

$$\mathcal{A}(a_1, \cdots, a_n) = \begin{cases} 0 & \text{, if } \exists i \text{ such that } a_i = 0, \\ & \text{for } i = 1, \cdots, n \\ \frac{\prod_{i=1}^{n} a_i}{\sum_{i=1}^{n} \prod_{j=1, j \neq i}^{n} a_j - (n-1) \prod_{i=1}^{n} a_i} & \text{, otherwise} \end{cases}$$

The resulting aggregate degrees of membership can be interpreted as the relative degrees of totally unacceptable levels of contamination in the bay.

Bounded difference {4} : Degrees of membership, as a result of the bounded difference, can be used to interpret excess levels of overall metal contamination, above the unacceptable level of contamination $a_i = 1$, in the region.

Maximum {5} : The maximum operator can be used to answer queries such as: "Where is there a reasonable possibility of finding areas in the bay where sediments register a contamination by one or more of the seven heavy metals?" It gives the largest levels of contamination by one or more metals. This operator can therefore be used by a scientist as a prevention sign. That is, when the contamination by one or more of the seven metals is detected, it can be used to prevent additional or an increase in metal contamination in the area.

Algebraic sum {6} : The resulting sets can be interpreted as the aggregate membership degree of the difference of unacceptable levels of overall metal contamination from the total sum of metal contaminations, in the bay.

Hamacher sum {7} : As part of the hamacher family, redefining the hamacher sum in terms of boundary conditions is necessary. Similarly, consider the n-place structure of this operator, Equation 4.19, and the defining properties of an n-place aggregation connective, Definition 7. The 2-place hamacher product

$$\mathcal{A}(a,b) = \frac{a+b-2a\cdot b}{1-a\cdot b} \tag{4.74}$$

is a union type operator defined by (3), such that $\mathcal{A}(1,b) = 1, \forall b \in [0,1)$, but undefined for $\mathcal{A}(1,1)$. Therefore, using the property of associativity, the generalized hamacher sum is not defined for the boundary condition $\mathcal{A}(a_1 = 1, \cdots, a_n = 1)$ for all $n \geq 2$. Therefore, based on the property of symmetry and that $\mathcal{A}(1,b) = 1, \forall b \in [0,1)$, we redefine the Hamacher sum as

$$\mathcal{A}(a_1, \cdots, a_n) = \begin{cases} 1 & \text{, if } \exists i \text{ such that } a_i = 1, \text{ for } i = 1 \cdots n \\ \frac{\sum_{i=1}^{n}(-1)^{i+1}(i)\cdot S_i}{1-\sum_{i=2}^{n}(-1)^{i}(i-1)\cdot S_i} & \text{, otherwise} \end{cases}$$

The degrees of aggregate membership as a result of 4.4.6 can be interpreted as the relative difference of totally unacceptable levels of overall metal contamination from their summed contamination, in the sedimentary area of the bay.

Bounded sum {8} : The fuzzy set as a result of the bounded sum reflects the summation of unacceptable levels of overall metal contamination in the bay.

Arithmetic mean {9} : As a mean type aggregation, it has the ability to compensate the input data between values of acceptable and unacceptable levels of overall contamination. The arithmetic mean fuzzy set interprets the average levels of overall metal contamination in the bay.

Competition jury {11} : Like the arithmetic mean, it has the compensation ability. The competition jury considers in its computation only fuzzy degree of metal membership that fall between the extremes, i.e., the smallest and largest degrees of fuzzy membership. Therefore, the aggregate fuzzy set can be seen as the true average of overall metal contamination levels in the bay.

Fuzzy integral {12} : Because the fuzzy integral is based on the fusion of external information via fuzzy measures, the aggregate fuzzy set can be interpreted as follows: the interactive impact between unacceptable levels of combined metal contaminations in the bay.

Weighted average {13} : The fuzzy set as a result of the weighted (fuzzy densities) average can be viewed as the weighted average of unacceptable overall metal contamination in the bay.

Probability of species death index (PSD) {14} : Previously, we only considered loading indices that measure the level of contamination (concentration) within the sedimentary surface of a marine environment. But, what about the effect of metal contamination on organisms living in the sedimentary area? And can we construct a loading index that measures this effect, using only the limited information at our disposal?

If we want to look at the harmful effect of metal contamination on species, that exist in the sediment, then we can use the fuzzy sets constructed using (4.72) and interpret the degrees of membership as probabilities. Let a_i denote the probability that metal i will lethally harm an organism present in the sediment surface of Liverpool bay. Then the probability that an organism will survive a harmful effect of contamination by the i^{th} metal is $(1 - a_i)$. If we assume that the metals have independent effects, the probability that an organism in Liverpool bay will survive the effect of overall metal contamination, is equal to $\prod_{i=1}^{n=7}(1 - a_i)$. Then "the probability that species will not survive contamination by overall heavy metal loading" is

$$\mathcal{A}(a_1, a_2, \cdots, a_n) = 1 - \prod_{i=1}^{n=7}(1 - a_i). \tag{4.75}$$

We will call this index (Equation (4.75)) the "*probability of species death*" (PSD). This index is not included in our analysis because taking the probabilities a_i to be $\mu_{A_i}(s_j)$ is an unrealistic guess. We have included it here for completion.

4.4.7 Spatial distribution of metal contamination: A visual representation

Using MATLAB, all thirteen generalized aggregating operators were computed. In some cases, environmental data is sampled or surveyed over a grid of regularly spaced points [12] while in other cases this has not been possible [13, 51, 41]. In the case of irregularly sampled data, interpolation is necessary. In short, interpolation results in surfaces being smoothed, to obtain a regular pattern of data distribution [57, 75]. The most natural output of the results of these studies is to represent them visually on a 2-D geographical grid.

Interpolation

In the data set, X refers to the geographical longitude location of the sampled point, Y to the latitude location of the sampled point, and Z is the measured property at the (X, Y) location. Because the data is made up of irregularly spaced data points, a method to interpolate scattered data is used. In [51], the "linear" interpolation method (default interpolation method in MATLAB when using the command "griddata") was used. It could be expected that a change in the method used will have an effect on the visual representation of the loading indices. According to [75], an ideal interpolation method for the display of spatial data should produce a continuous and smooth surface. We compared the visual outcome of all available methods in MATLAB, suitable for interpolating non-collinear or scattered data points ('linear', 'nearest neighbor', 'cubic' and 'v4' interpolation methods). Best results were obtained using the 'MATLAB 4 griddata method' better known as 'v4' and the default 'linear' interpolation. Linear interpolation is recommended for faster interpolation when X and Y are equally spaced and monotonic. We found that both these methods gave the smoothest graphical outcomes. The only difference between them is the ability of the 'v4' method to cover all sampled sites in its interpolation and also extrapolate to areas outside the sampled region. This factor did not have an effect on the visual outcome over the sampled region when using the 'linear' or 'v4'

Table 4.4: Upper and lower limits of longitude (X) and latitude (Y) of Liverpool bay (1986-1992) and Morecambe bay (1988) sampled data. For Liverpool bay values of X are in minutes west of 3^oW of Greenwich and for Y in minutes north of 53^oN of Greenwich, while Morecambe bay values of X are in degrees west of Greenwich and for Y in degrees north of Greenwich.

Liverpool bay	1986		1987		1988		1989		1990	
	X	Y	X	Y	X	Y	X	Y	X	Y
Minimum	-42	26.9	-42	26.9	-41.9	25.4	-44.4	25.8	-44.4	25.2
Maximum	-13.7	36.4	-13.7	36.4	-12	36.4	-13.27	35.8	-15.1	36.2

Liverpool bay	1991		1992	
	X	Y	X	Y
Minimum	-41.9	26.9	-42	25.3
Maximum	-13.1	35.7	-12.4	35.7

Morecambe bay	1988	
	X	Y
Minimum	-3.4	53.9
Maximum	-2.8	54.2

methods. Figure 4.3 gives a visual comparison between the four methods applied on one loading index.

Grid resolution

After selecting the method of interpolation, a decision must be made about the appearance of the grid. In other words, select the most suitable number of grid nodes, on which the loading indices are interpolated, which determines the grid resolution.

In MATLAB the grid resolution is defined by two parameters a and b, the offsets on X and Y, respectively. To determine the values of the upper and lower limits for both X and Y axis of the grid, we use the data (1986 to 1992 for Liverpool bay and 1988 for Morecambe bay) as a guide. Table 4.4 shows the different range of X and Y for all sampled years. X and Y values of the grid for Liverpool bay are in minutes, while for Morecambe bay the X and Y values are in degrees. This is because we proceeded with the raw data provided. Using the summarized information from

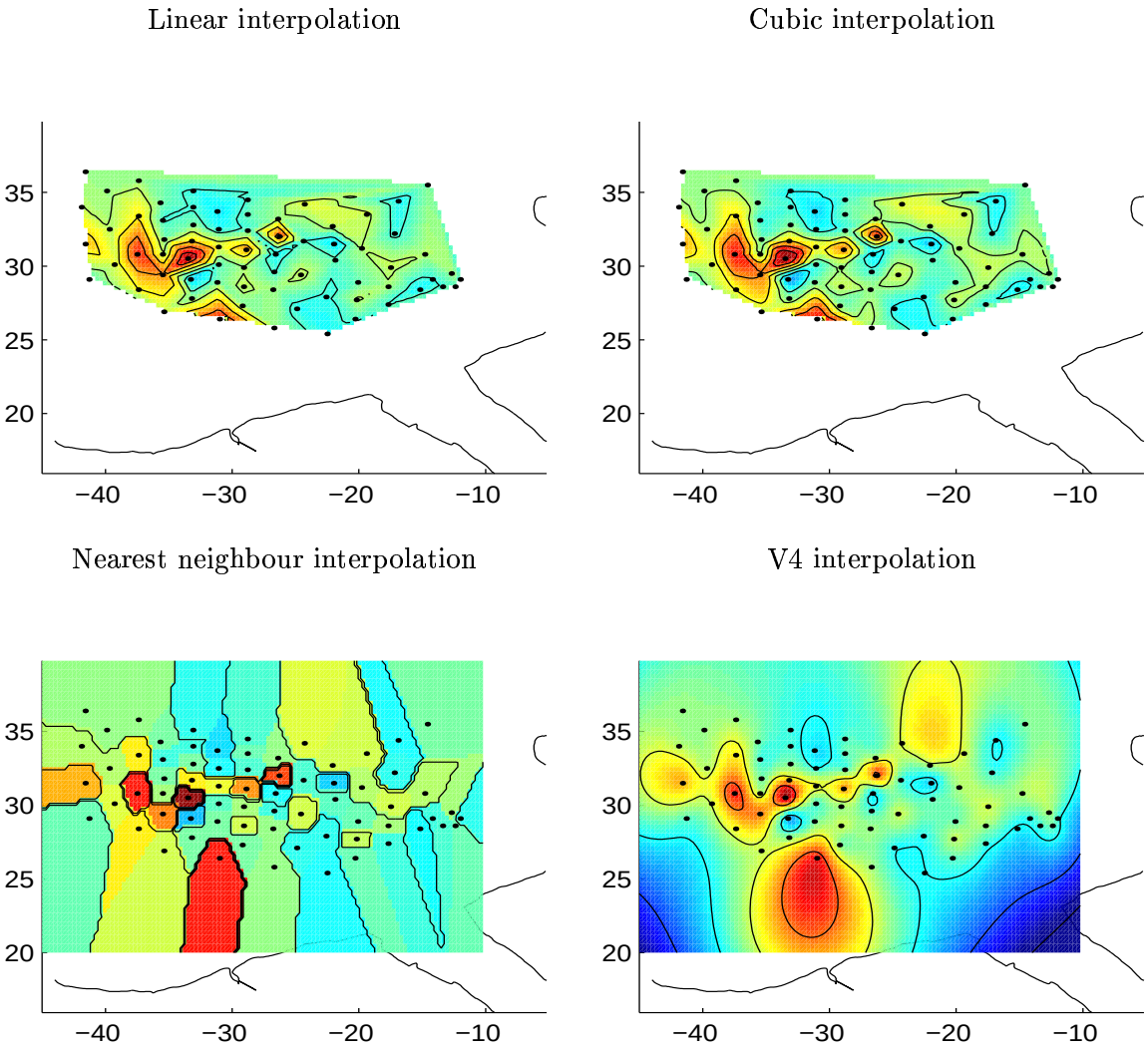


Figure 4.3: A comparison of interpolation methods using shaded contour plots of a selected loading index (Maximum) from Liverpool bay 1988

Table 4.4, we selected our limits. Arrays, $X = -45 : a : -10$ and $Y = 20 : b : 40$ for Liverpool bay data were used, while $X = -3.4 : c : -2.8$ and $Y = 53.85 : d : 54.25$ were used for Morecambe bay data. The default values for Liverpool bay, $a = b = 1$, were initially used. Then varying a and b we determine the number of grid nodes and see the effect it has on the visual output. Similarly, this was also done for parameters c and d, the offsets on X and Y, respectively, for Morecambe bay. For Liverpool bay, we varied a and b (in minutes) ($a = b$) assigning them values $\cdots 0.1, 0.2, \cdots 1.0, \cdots$, and observed the visual change in the appearance of the graph. In the end, we found that information held by a loading index is preserved for $a, b \in [0.3, 1.0]$. The smoothest graphs were found for $a = b$ between 0.3 and 0.5. The same procedure was done for Morecambe bay. We found the best grid resolution for values of c and d (in degrees) between 0.008 and 0.01.

In [12], the concept of α-level fuzzy sets was used to answer a query related to land evaluation. Based on the maximum aggregation connective, the 0.6-level fuzzy set was constructed to show those large parts of the study area in which the possibility of sand occurring somewhere in the soil profile exceeds 0.6. Therefore, we can use different α-levels, where $\alpha \in (0, 1]$, to distinguish areas of moderate to high overall metal contamination with respect to a certain loading index. Or, to answer queries such as:

"*Are there areas in Liverpool bay of suspected unregulated dumping of sewage and industrial material?*"

Different α-cuts can be used, $\alpha = 0.5, 0.6, 0.7, \cdots, 1.0$, to observe the gradual change of moderate ($\alpha = 0.5$) to highly ($\alpha = 1.0$) contaminated areas. Here we will not use this method of distinguishing between the spatial distribution of moderate to high contamination levels, because this will confine our analysis to specific indices. That is, we can only look at those indices that have loading $LI(u_j) > \alpha$, for $j = 1, \cdots, m$.

Visual comparison of loading indices

Colour shaded contour plots were used to visualize the loading indices. The different colour shades are retrieved from MATLAB's *colormap*. A colormap is a matrix of real numbers between 0 and 1, which define the different colors used for plotting. Color scaling is done using the MATLAB command '*caxis*'. *Caxis* controls the mapping of the data values to the colormap. By default, MATLAB computes the color limits, for the colormap, automatically using the minimum and maximum data values. For the preassigned color map in MATLAB, HSV, the value of 1 is colored bright red, and the value of 0 is colored in dark blue. For example, if the values of the loading index span the interval 0.01 to 0.10, the bright red (1) will be assigned to 0.10 and the dark blue (0) will be assigned to 0.01. For another loading index, spanning the interval 0.20 to 0.80, bright red will be assigned to 0.80 and dark blue will be assigned to 0.20. Thus a direct visual comparison of the strength of contamination will not be possible across different plots. To enable a cross-plot comparison, we set '*caxis*' to the unit interval, i.e., *caxis* ([0,1]). By this, dark blue will always be assigned to 0 and bright red to 1. Figures 4.4 - 4.14 show the distribution of metal loading indices in Liverpool bay and Morecambe bay, respectively. The following conclusions can be drawn:

Liverpool bay (1988)

1. The minimum, product, bounded difference and Hamacher product indices produced the lowest index values. The bounded difference and Hamacher product registered no contamination, i.e., loading index values at all sampled data points $u \in U$ as a result of both aggregation operators registered no contamination ($LI(u_j) = 0, \forall j = 1, \cdots, m$).

2. The maximum and the fuzzy integral indices pinpoint isolated regions of high overall metal contamination.

3. The geometric mean, arithmetic mean, competition jury and weighted average indices produced similar distribution of index values ranging $\in [0, 0.4)$.

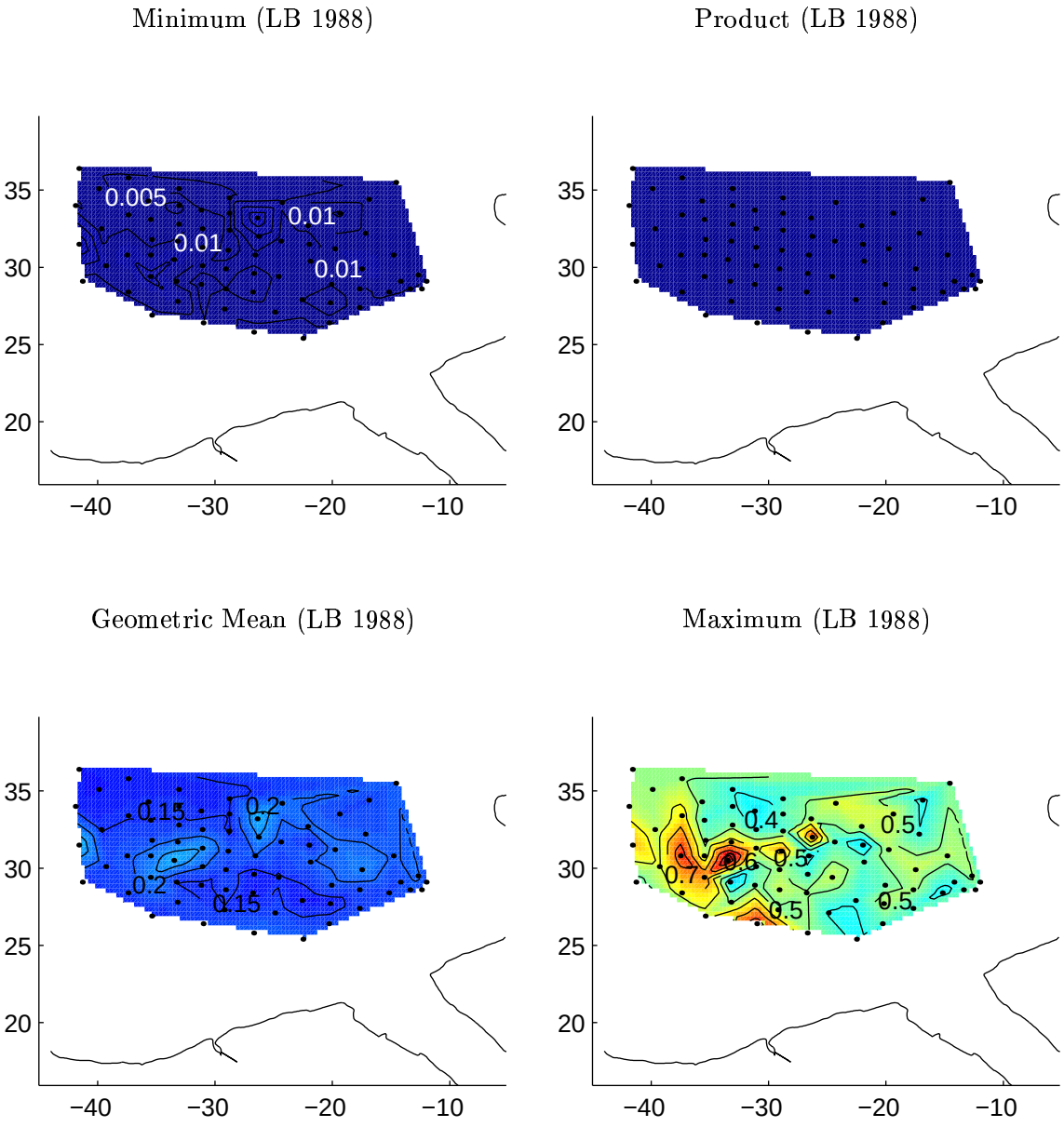


Figure 4.4: Shaded contour plots of selected aggregation connectives for Liverpool bay 1988

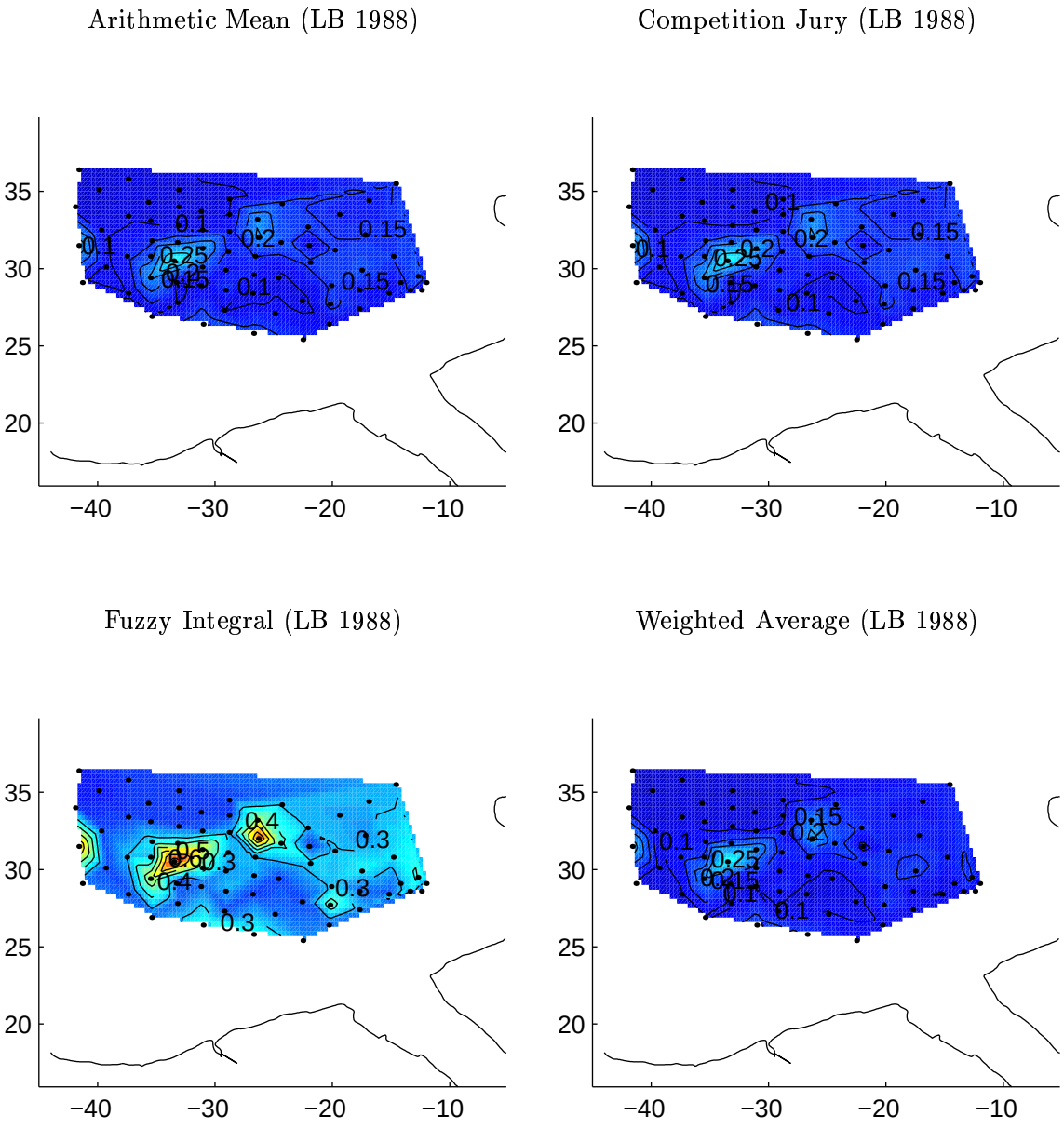


Figure 4.5: Shaded contour plots of selected aggregation connectives for Liverpool bay 1988 (continued)

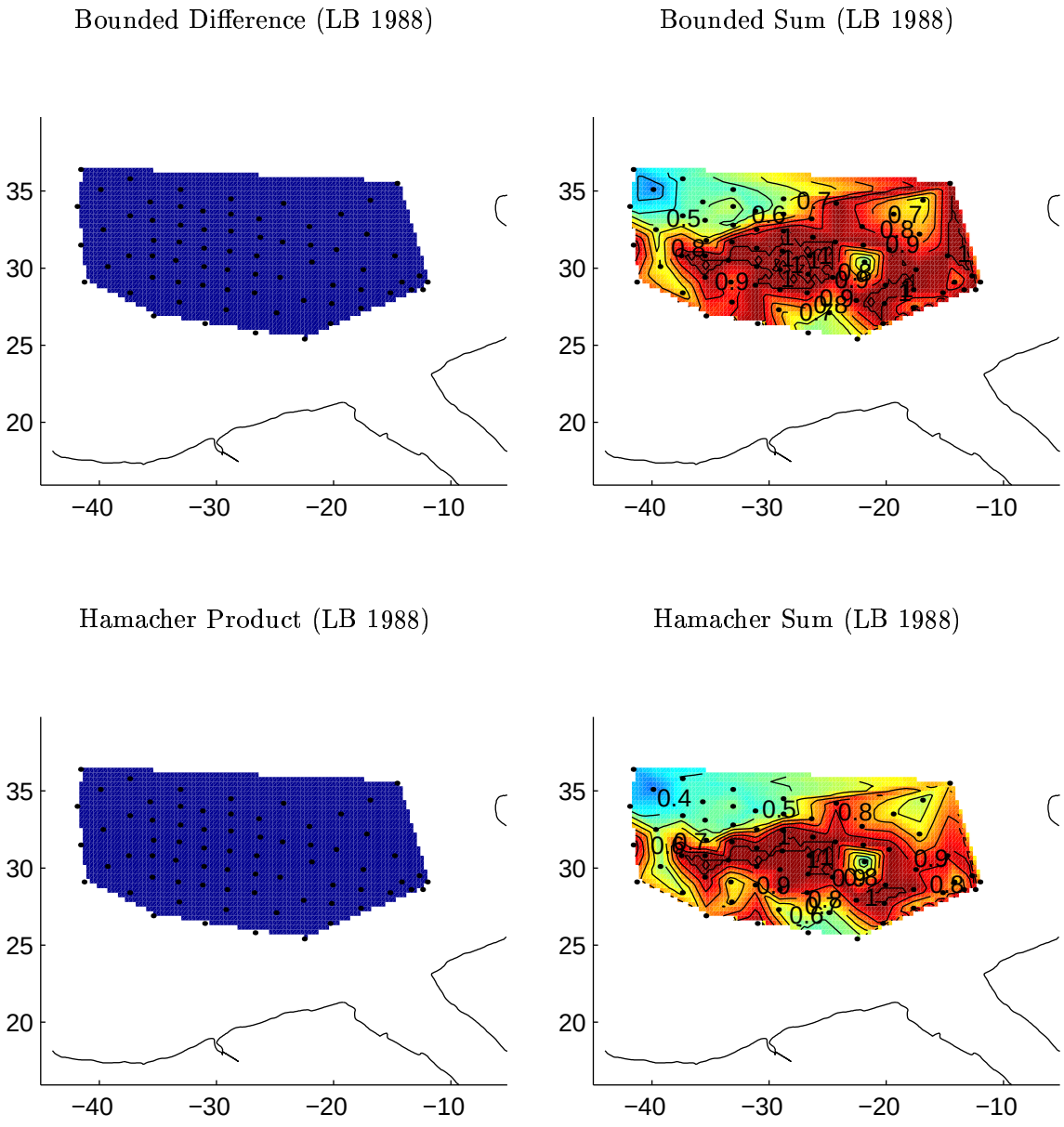


Figure 4.6: Shaded contour plots of selected aggregation connectives for Liverpool bay 1988 (continued)

4. The bounded sum, Hamacher sum and algebraic sum gave similar graphical distribution of overall metal contamination. These indices assume that the largest part of Liverpool bay is contaminated ($LI(u_j) \geq 0.7$), which is an overly pessimistic estimate, not corresponding to reality. The graphical distribution of the maximum index, one of the commonly used aggregations, pinpoints at least two regions of high contamination and so does the fuzzy integral index.

Morecambe bay (1988)

1. The minimum, product, geometric mean, bounded difference and Hamacher product indices did not register any overall metal contamination.

2. Only a very small level of overall metal contamination is registered by the remaining indices.

3. All graphical distribution of loading indices seem to support the expectation that Morecambe bay is in general a clean and uncontaminated region.

From the mathematical and graphical observation of the thirteen aggregate membership functions, we excluded the following indices.
From Figures 4.4 to 4.14 we see that many loading indices have almost identical distribution patterns. Therefore, we can eliminate the indices that require more calculations, and do not have a straightforward interpretation. We decided to leave out the bounded difference, bounded sum, Hamacher product, Hamacher sum, and algebraic sum and keep a set of indices,
$\{LI_{min}, LI_{prod}, LI_{gm}, LI_{max}, LI_{avg}, LI_{cj}, LI_{FI}, LI_{WA}\}$.

To select a small set of most different indices from the group of remaining indices, a mathematical approach is required. Such an approach in fuzzy set theory is by using similarity measures [76]. This issue will be discussed in the next chapter.

4.4.8 Conclusion

A fuzzy model has been applied for the study of contamination by seven heavy metals of Liverpool bay and Morecambe bay. We found that some aggregate membership

functions were not suited to model the concept of metal contamination. Within the scope of our environmental study, some functions are easier to interpret than others. Eight loading indices were subjectively selected, although thirteen in total were initially considered.

We were able to identify regions of high contamination outside the designated dumping area (SI), in Liverpool bay. This was done by comparing outcomes of the maximum and fuzzy integral generated loading indices. Three regions, in Liverpool bay, registered a moderate to high contamination impact as a result of the interaction between combined metal loading. All mean type aggregating operators gave in average a low overall metal contamination in both regions. Outcomes of overall metal distribution in Morecambe bay, supported the hypothesis that the region is generally clean.

In Chapter 5, measures of similarity will be used to find a set of distinct indices out of the selected eight which can easily be implemented in this area of study.

We considered n-place aggregation operators as combination rules, and introduced methods of generalizing associative aggregation operators. A selection of thirteen aggregation operators were applied for the evaluation of loading indices of two marine environments, Liverpool bay and Morecambe bay (in 1988). Finally, based on graphical observation, eight out of the thirteen indices were selected, which were based on the following aggregation operators: Minimum, Product, Geometric mean, Maximum, Average, Competition jury, Fuzzy integral, and Weighted average.

Algebraic Sum

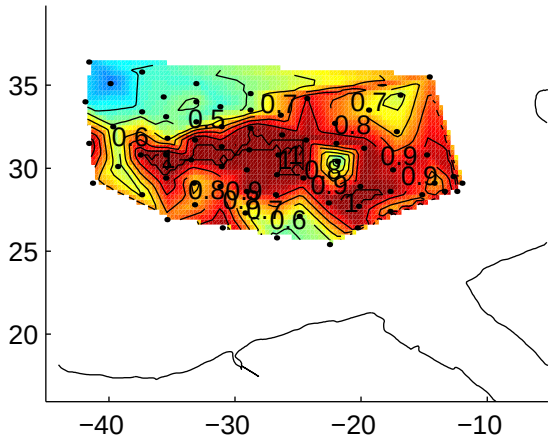


Figure 4.7: Shaded contour plots of selected aggregation connectives for Liverpool bay 1988 (continued)

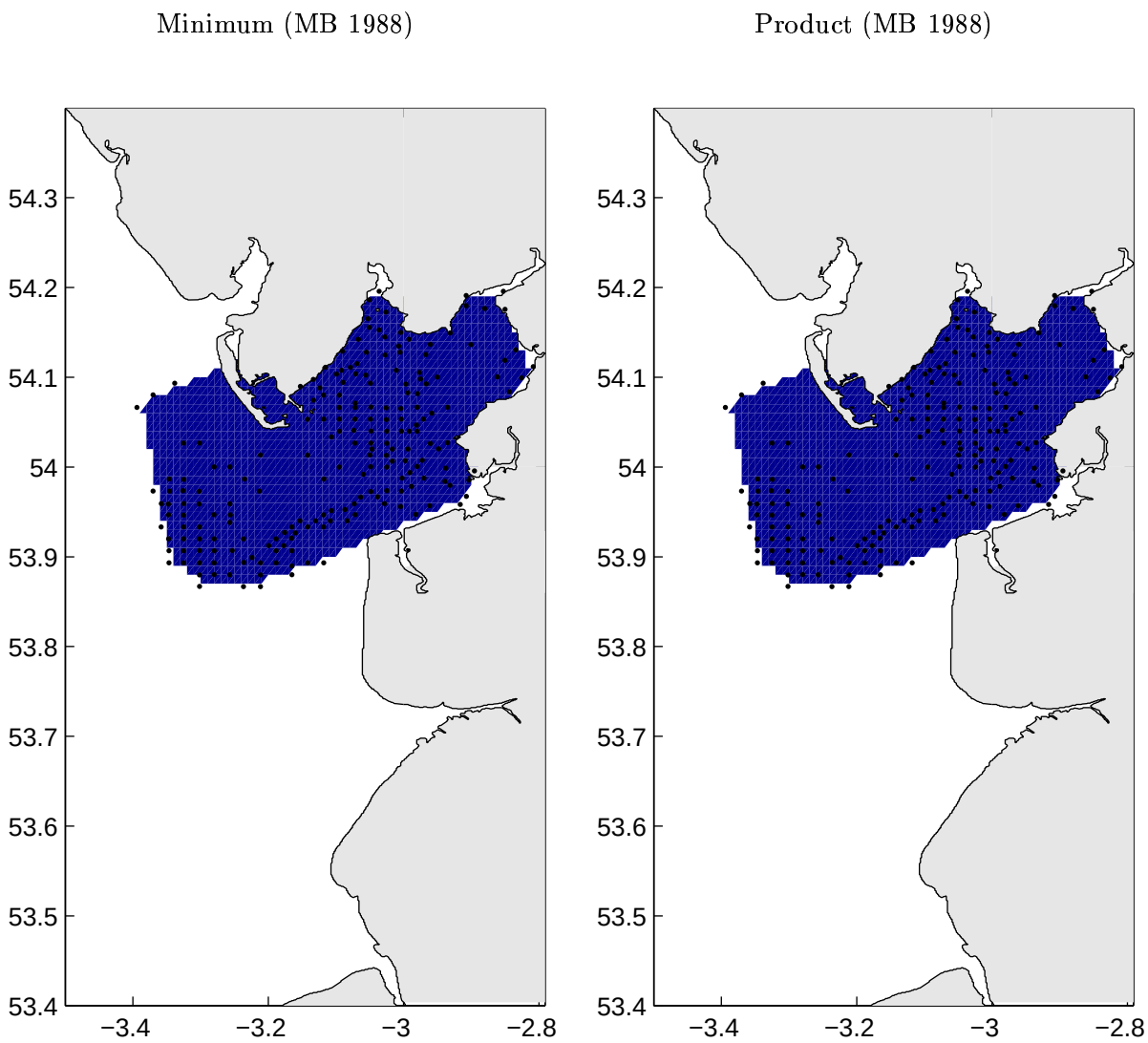


Figure 4.8: Shaded contour plots of selected aggregation connectives for Morecambe bay 1988

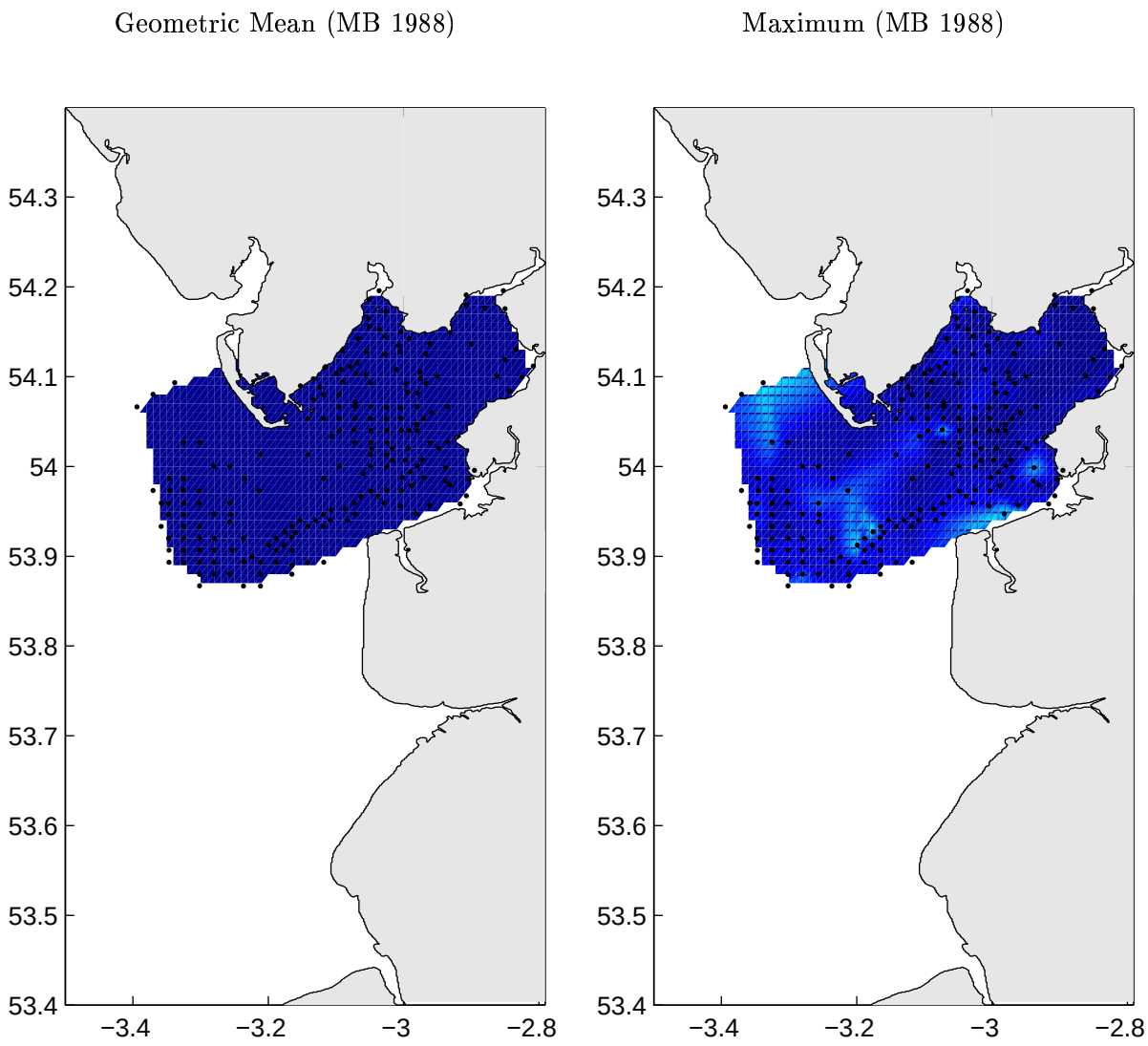


Figure 4.9: Shaded contour plots of selected aggregation connectives for Morecambe bay 1988 (continued)

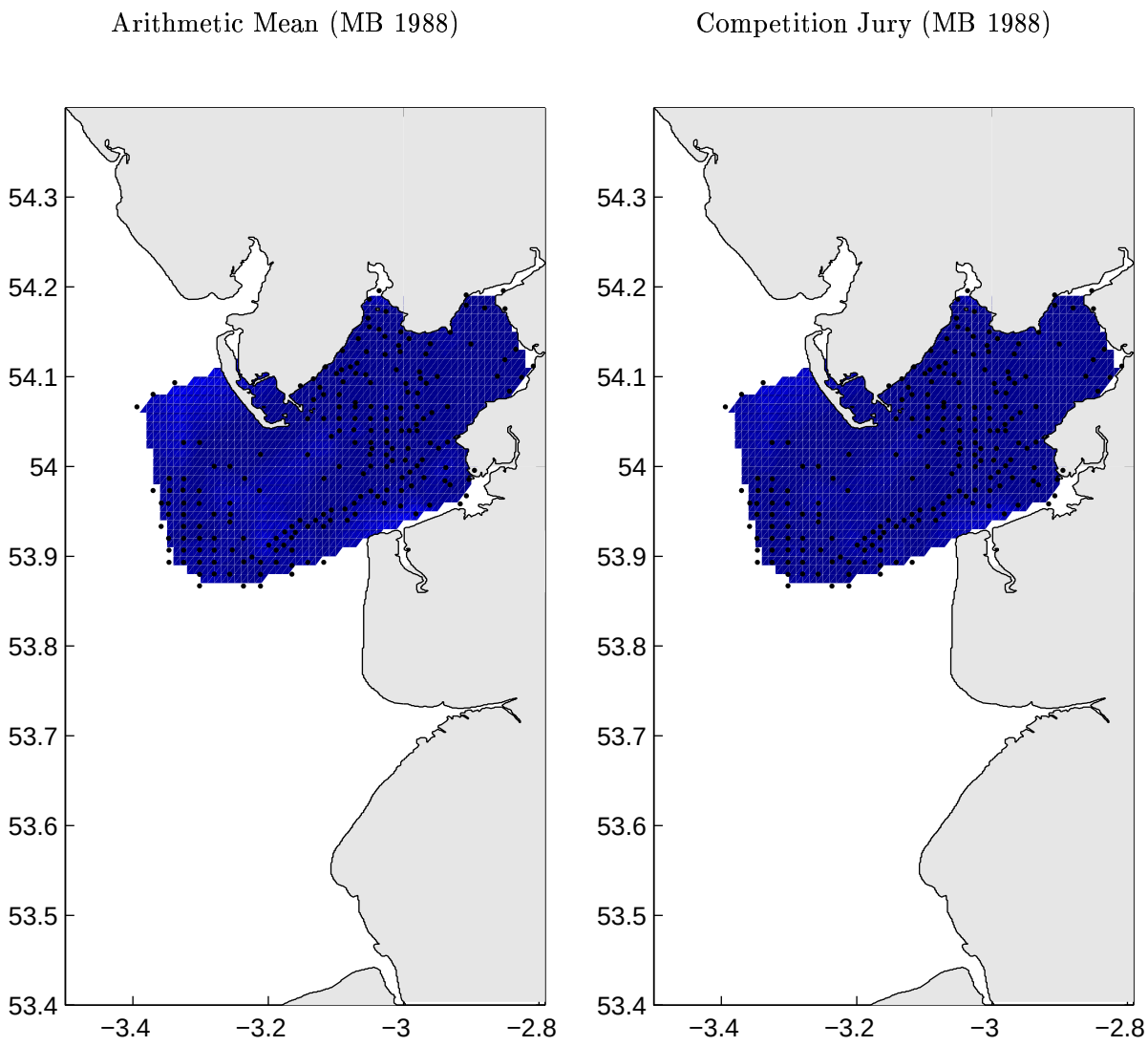


Figure 4.10: Shaded contour plots of selected aggregation connectives for Morecambe bay 1988 (continued)

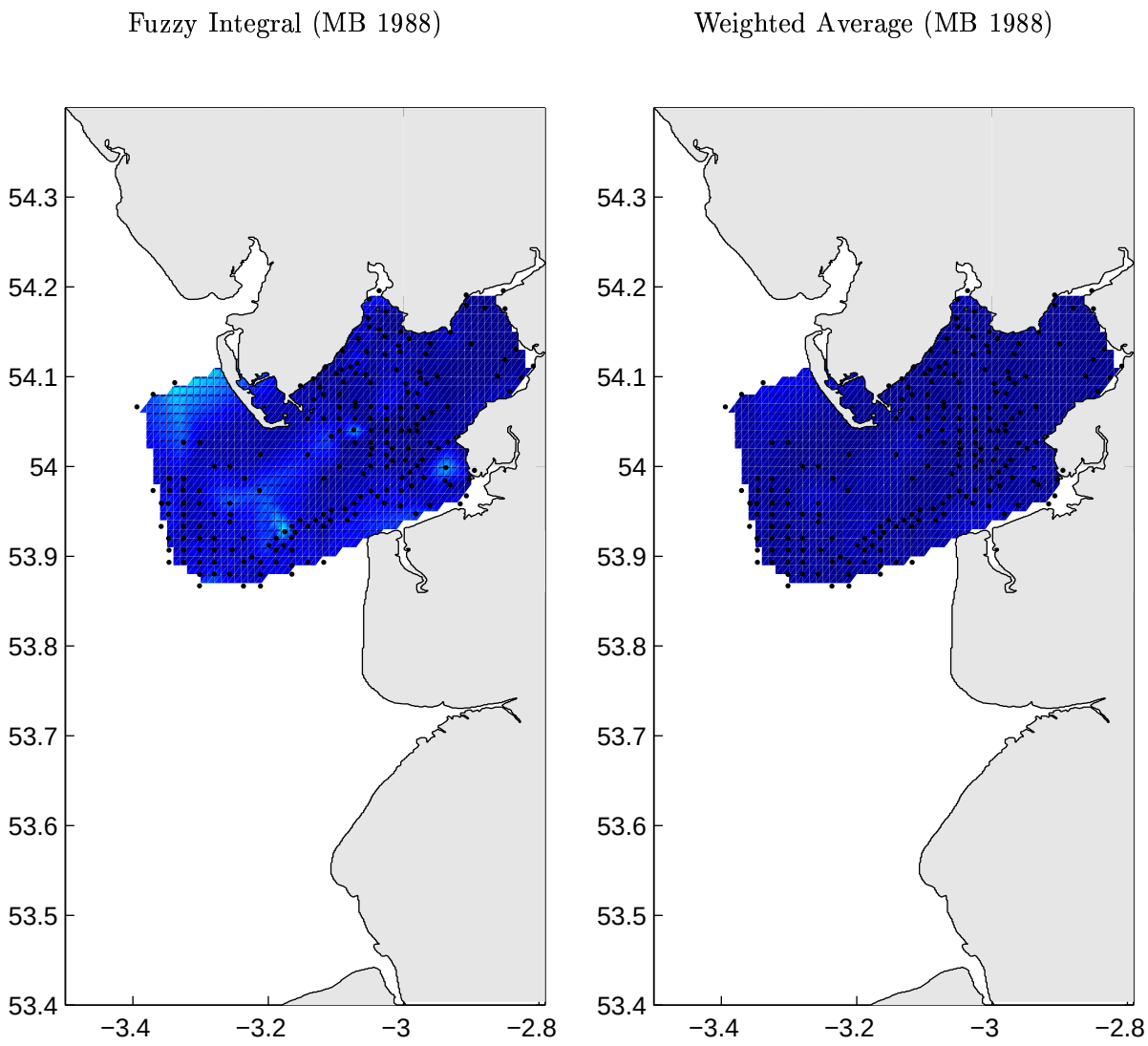


Figure 4.11: Shaded contour plots of selected aggregation connectives for Morecambe bay 1988 (continued)

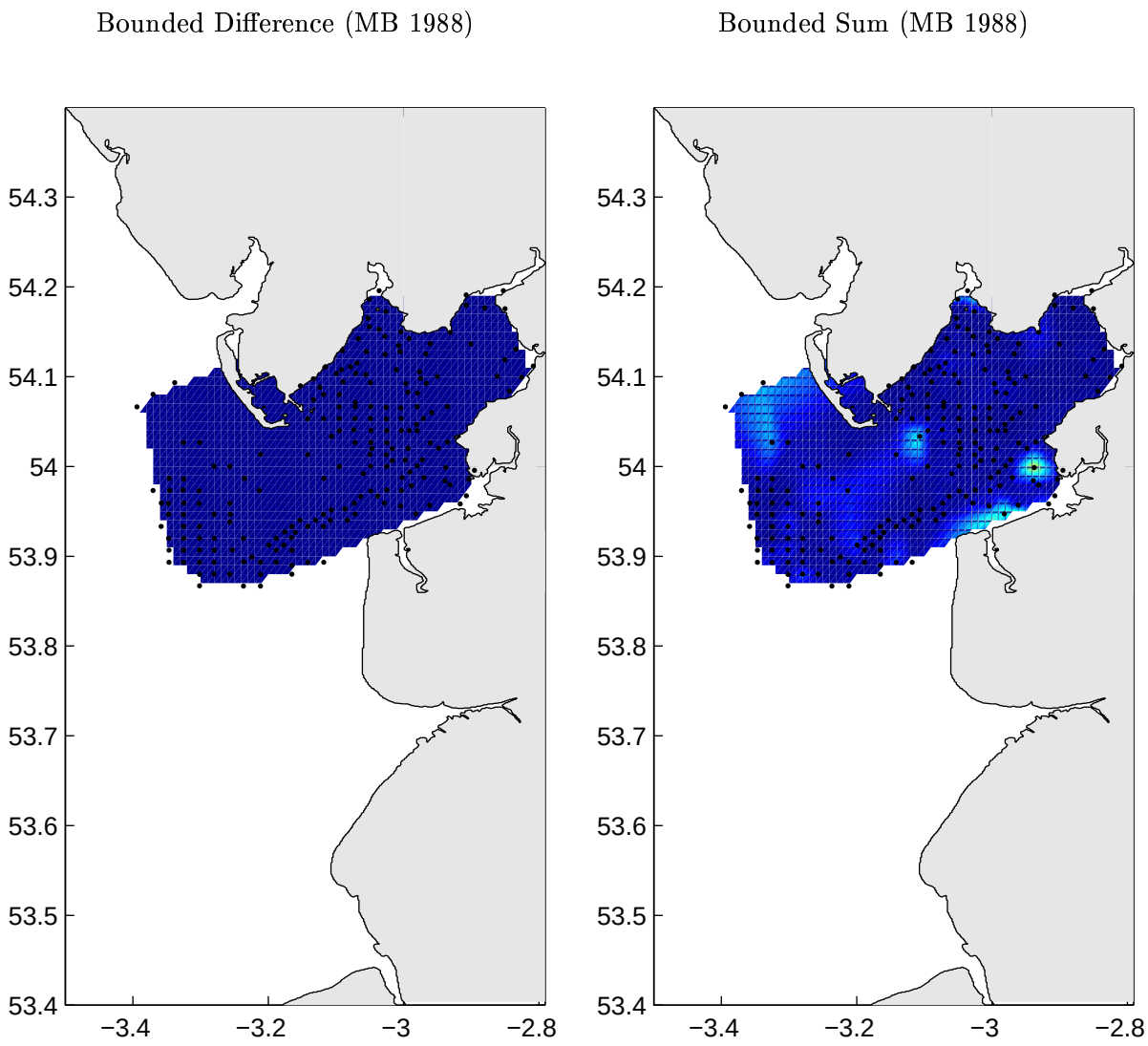


Figure 4.12: Shaded contour plots of selected aggregation connectives for Morecambe bay 1988 (continued)

Hamacher Product (MB 1988)

Hamacher Sum (MB 1988)

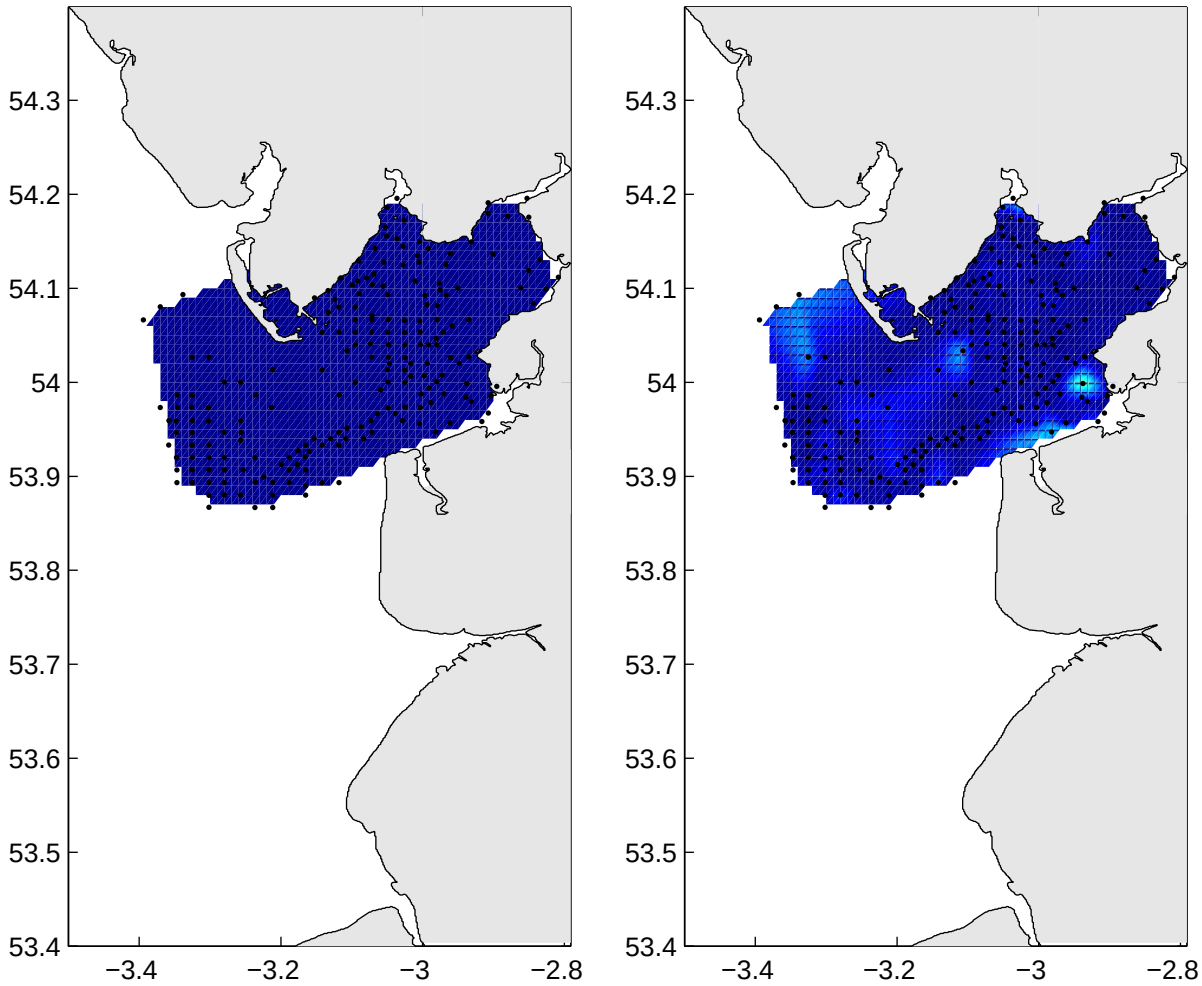


Figure 4.13: Shaded contour plots of selected aggregation connectives for Morecambe bay 1988 (continued)

Algebraic Sum

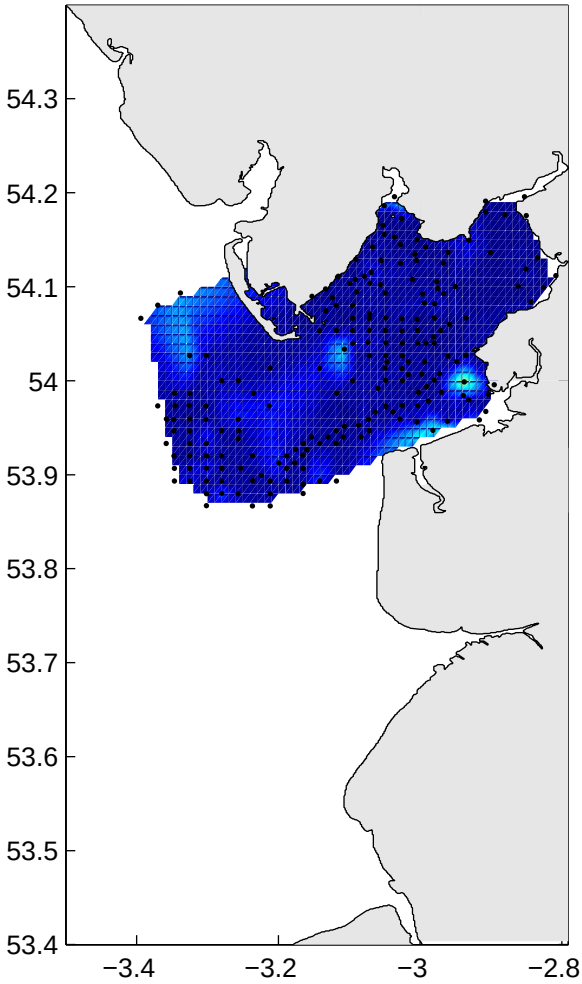


Figure 4.14: Shaded contour plots of selected aggregation connectives for Morecambe bay 1988 (continued)

Chapter 5

Similarity Measures

After formulating metal loading indices of an environmental region, the next step is to quantify the degree of similarity between the chosen eight indices: *minimum, product, geometric mean, maximum, average, competition jury, fuzzy integral,* and *weighted average.* Based on the similarity, we suggest selecting a subset of loading indices.

Scalar measures of similarity are fuzzy operations that define weak or strong equalities between two fuzzy sets.

The interpretation of similarity in everyday language is 'having characteristics in common' or 'shape is alike, but size and position may be different'. This is different to the definition of similarity based on equality between fuzzy sets. Then in the same way that fuzzy sets allow for gradual transition between full membership and non-membership, a similarity measure captures a gradual transition between equality and non-equality.

5.1 Definitions and Properties

A similarity measure $\mathcal{S}$ indicates the degree to which two fuzzy sets A and B on the same universal set U are equal or similar, i.e.,

$$\mathcal{S}(A,B) = \text{ degree } (A = B), \quad \text{where } \mathcal{S}(A,B) \in [0,1].$$

Therefore, for a discrete finite universe U, given that: $|U| = m$, $\mathcal{P}(U)$ denoting the class of all fuzzy sets on U and $\mathcal{C}(U)$ the class of all crisp sets on U, we define the following:

Definition 13 (Similarity Measure). *A function $\mathcal{S} : \mathcal{P}(U) \times \mathcal{P}(U) \longrightarrow [0,1]$ is called a similarity measure on $\mathcal{P}(U)$, if $\mathcal{S}$ satisfies the following general properties [27, 47, 80]:*

1. $\mathcal{S}(A,B) = \mathcal{S}(B,A), \quad A,B \in \mathcal{P}(U)$.
2. $\mathcal{S}(E,E) = 1$, $E \in \mathcal{P}(U)$.
3. *If $A \subseteq B \subseteq C$, $\forall A,B,C \in \mathcal{P}(U)$, then $\mathcal{S}(A,B) \geq \mathcal{S}(A,C)$ and $\mathcal{S}(B,C) \geq \mathcal{S}(A,C)$. Note that, $A \subseteq B \subseteq C$ implies that $\mu_A(u) \leq \mu_B(u) \leq \mu_C(u) \quad \forall\ u \in U$.*

In general, the larger the value of $\mathcal{S}(A,B)$, the more similar A and B are.

Related with the concept of similarity measure, the dissimilarity measure of two fuzzy sets, used by many researchers, is a measure that describes the difference between fuzzy sets. The following is the axiom definition of a dissimilarity measure of fuzzy sets .

Definition 14 (Dissimilarity Measure). *A function $D : \mathcal{P}(U) \times \mathcal{P}(U) \longrightarrow [0,1]$ is called a dissimilarity measure on $\mathcal{P}(U)$, if D satisfies the following general properties:*

1. $D(A,B) = D(B,A)$, *for* $A,B \in \mathcal{P}(U)$
2. $D(E,E) = 0$, $\forall\ E \in \mathcal{P}(U)$

3. *If* $A \subseteq B \subseteq C$, $\forall\ A, B, C \in \mathcal{P}(U)$, *then* $D(A,B) \leq D(A,C)$ *and* $D(B,C) \leq D(A,C)$.

Examples of dissimilarity measures are given at the end of this section.

Many measures of similarity among fuzzy sets have been proposed in the literature [27, 19, 31, 61, 64].

The motivation behind many of these measures is either geometric (i.e., based on a geometric distance model) or set-theoretical (i.e., based on the operations of union and intersection) [19, 61, 83]. In the geometric based measures, the fuzzy sets are represented as points in some coordinate space such that the distance among the sets corresponds to the metric distance between the respective points. Sometimes the assessment of similarity may be better described as a comparison of features rather than as a computation of metric distance between points. In this instance, similarity may be better modeled by a function that is not a geometric distance but a set-theoretic function.

In [83], noted it was argued that geometric representations may be appropriate for certain studies, but not for others. For example, consider the set of countries (objects), $\delta = \{(a, \text{Belgium}),\ (b, \text{U.K.}),\ (c, \text{Mexico}),\ (d, \text{U.S.A})\}$ and the set of features, $\Delta = \{(A, \text{Geographical proximity}),\ (B, \text{Economy}),\ (C, \text{Political aspect}),\ (D, \text{Culture}),\ (E, \text{Heritage}),\ (F, \text{History})\}$ where features C, D, E and F are qualitative features. In this case, the assessment of similarity between such objects may be better described as a function of their common and distinctive features, i.e., a set theoretic approach, than representing the objects as metric distances between the respective points.

In Pappis et al. [61] and Chen et al. [19], measures of similarity of fuzzy sets (coming from both approaches) are presented and compared. The authors point out that although several properties were common to these measures, there exist notable differences between the similarity measures (in terms of properties). As a result of this, care should be taken when selecting a measure for a particular application. A summary of both studies done in [19, 61] is given in [54]. The following are

examples of similarity measures based on the two approaches.

5.1.1 A measure based on the set-theoretic approach (Type [1])

1. Cardinality-ratio measure:

$$\mathcal{S}_C(A,B) = \frac{|A \cap B|}{|A \cup B|} \tag{5.1}$$

Since the measure is undefined for $A = B = \phi$, we can redefine Equation (5.1) as follows

$$\mathcal{S}_C(A,B) = \begin{cases} 1 & A = B = \phi, \\ \frac{|A\cap B|}{|A\cup B|} = \frac{\sum_{i=1}^{m} \min(\mu_A(u_i),\mu_B(u_i))}{\sum_{i=1}^{m} \max(\mu_A(u_i),\mu_B(u_i))} & \text{otherwise.} \end{cases} \tag{5.2}$$

i.e, $\mathcal{S}_C(A,B)$ is the ratio of the relative cardinality of the intersection and the union, (set-theoretical approach). When $\frac{|A\cap B|}{|A\cup B|} = 0$, A and B are called separable fuzzy sets. If $\frac{|A\cap B|}{|A\cup B|} = 1$ and A, B are non-empty crisp sets, then $A = B$ [27].

Another example of a set-theoretic based similarity measures is the symmetrical difference measure [27, 51],

$$\begin{aligned} \mathcal{S}_{SD}(A,B) &= 1 - \|A \triangle B\| \\ &= 1 - \frac{\sum_{i=1}^{n} \max\{\min\{\mu_A(u_i)\}, \mu_{\bar{B}}(u_i), \min\{\mu_{\bar{A}}(u_i)\mu_B(u_i)\}}{n} \end{aligned} \tag{5.3}$$

where $\mu_{A\triangle B}(u) = \max\{\mu_{A\cap\bar{B}}(u), \mu_{\bar{A}\cap B}(u)\}$, $u \in U$. The fuzzy set $A \triangle B$ accounts for the elements that approximately belong to A and not to B, or conversely to B and not to A. The symmetrical difference is defined based on a definition of similarity adopted by other authors [31, 72, 77]. This measure differs in that it does not always hold for property (2) of Definition 13. That is, $\mathcal{S}(E,E) = \max_{A,B\in\mathcal{P}(U)} \mathcal{S}(A,B)$, $\forall\ E \in \mathcal{P}(U)$. In our case, these functions are not suitable as similarity measures in this type of application.

5.1.2 Measures based on the geometric distance model (Type [2])

A particular class of distance functions some measures are based on, what is known as the Minkowski r-metric. The Minkowski r-metric is a one parameter class of distance functions defined as follows [31, 83, 19].

Let $a = (a_1, a_2, \cdots, a_n)$ and $b = (b_1, b_2, \cdots, b_n)$ be two points in an n-dimensional space, then

$$d_r(a,b) = \left[\sum_{i=1}^{n} |a_i - b_i|^r\right]^{1/r}, r \geq 1. \tag{5.4}$$

Some cases of this metric are,

- The city-block distance, $r = 1$,

$$d_1(a,b) = \sum_{i=1}^{n} |a_i - b_i| \tag{5.5}$$

- The Euclidean distance, $r = 2$,

$$d_2(a,b) = \left(\sum_{i=1}^{n} |a_i - b_i|^2\right)^{1/2} \tag{5.6}$$

- As r approaches ∞, Equation (5.4) approaches the dominance metric in which the distance between points a and b is determined by the difference between features along only one dimension – that dimension for which the value $|a_i - b_i|$ is greatest. That is,

$$d_\infty(a,b) = \max_i |a_i - b_i| \tag{5.7}$$

Let A and B be two fuzzy sets on $\mathcal{P}(U)$. Then the following similarity measures are based on the geometric model,

1. Difference-sum ratio measure based on the difference and the sum of grades of membership [72]

$$d_D(A,B) = 1 - \frac{\sum_{i=1}^{n} |\mu_A(u_i) - \mu_B(u_i)|}{\sum_{i=1}^{n} (\mu_A(u_i) + \mu_B(u_i))} = 1 - \frac{|A \bigtriangledown B|}{|A| + |B|} \tag{5.8}$$

to account for $A = B = \phi$, Equation (5.8) can be redefined as

$$d_D(A,B) = \begin{cases} 1 & A = B = \phi, \\ 1 - \frac{\sum_{i=1}^{n} |\mu_A(u_i) - \mu_B(u_i)|}{\sum_{i=1}^{n} (\mu_A(u_i) + \mu_B(u_i))} & \text{otherwise.} \end{cases} \tag{5.9}$$

Equation (5.8) can also be written as follows

$$\begin{aligned} d_D(A,B) &= 1 - \frac{\sum_{i=1}^{n} \max(\mu_A(u_i), \mu_B(u_i)) - \min(\mu_A(u_i), \mu_B(u_i))}{\sum_{i=1}^{n} (\mu_A(u_i) + \mu_B(u_i))} \\ &= 1 - \frac{|A \cup B| - |A \cap B|}{|A| + |B|} \end{aligned} \tag{5.10}$$

2. Symmetrical difference measures [27, 31]

   (a)

$$\begin{aligned} d_{SD1}(A,B) &= 1 - \max_{u_i \in U} |\mu_A(u_i) - \mu_B(u_i)| \\ &= 1 - height(A \bigtriangledown B) \end{aligned} \tag{5.11}$$

   (b)

$$d_{SD2}(A,B) = 1 - \|A \bigtriangledown B\| = 1 - \frac{\sum_{i=1}^{n} |\mu_A(u_i) - \mu_B(u_i)|}{n} \tag{5.12}$$

   where $\|A \bigtriangledown B\|$ denotes the relative cardinality of the symmetrical difference $A \bigtriangledown B$. The fuzzy set $A \bigtriangledown B$ denotes the elements that belong more to A than to B or conversely. Also, owing to the symmetrical difference, $A = B$ if and only if $A \bigtriangledown B = \phi$.

The following similarity measure we refer to as the Vector-product measure. This measure was defined by Chen [31]

$$\mathcal{S}_V(A,B) = \frac{A \cdot B}{\max(A \cdot A, B \cdot B)} \tag{5.13}$$

such that $A \cdot B$ expresses the inter-product of A and B taken as vectors of membership degrees. Or, taking into account that both A and B can be empty sets, $A = B = \phi$

$$\mathcal{S}_V(A,B) = \begin{cases} 1 & A = B = \phi, \\ \frac{A \cdot B}{\max(A \cdot A, B \cdot B)} & \text{otherwise.} \end{cases} \tag{5.14}$$

Then this measure can be written as,

$$\mathcal{S}_V(A,B) = \begin{cases} 1 & A = B = \phi, \\ \frac{\sum_{i=1}^{m} \mu_A(u_i) \cdot \mu_B(u_i)}{\max(\sum_{i=1}^{m} \mu_A(u_i)^2, \sum_{i=1}^{m} \mu_B(u_i)^2)} & \text{otherwise.} \end{cases} \tag{5.15}$$

Also related to the concept of similarity measures, Wang et al. (1995) presented a definition of **approximate equality** between fuzzy sets A and B, for the three measures given by Equations (5.1), (5.11) and (5.8) [61, 73]. Consider the similarity measure $\mathcal{S}_C$ of Equation (5.1). For two fuzzy sets, A and B are said to be equal to "*degree* α" with respect to $\mathcal{S}_C$, denoted $A \sim_{\alpha}^{\mathcal{S}_C} B$, if and only if $\mathcal{S}_C(A,B) \geq \alpha$, where $\alpha \in [0,1]$. Similarly, definitions of 'equality to degree α' with respect to the measures (5.11) and (5.8) can also be introduced.

5.1.3 Proximity measures

In [31], a general definition of another class of similarity measures was given known as Proximity measures. Most of the measures introduced up to now, give consideration to the relation between A and B, and have no concern about the relation between their complement sets $\bar{A}$ and $\bar{B}$. *Proximity Measures* are measures that take into account the similarity between two fuzzy sets as well as the similarity between their complements.

Definition 15 (Proximity Measure). *: A similarity measure $\mathcal{S}$ is called a proximity measure, if*

$$\mathcal{S}(A,B) = \mathcal{S}(\bar{A},\bar{B})$$

.

Examples of such measures already introduced are Equations (5.11) and the similarity measure based on the general Minkowski function, i.e.,

$$\mathcal{S}_r(A,B) = 1 - \frac{1}{n}\left(\sum_{i=1}^{n} |\mu_A(u_i) - \mu_B(u_i)|^r\right)^{1/r} \tag{5.16}$$

with special cases for $r = 1$ (5.12) and $r = 2$. Additional examples are:

1. The proximity measure defined by Bhandari and Pal [31].

$$\begin{aligned}\mathcal{S}_{pm_1}(A,B) &= 1-\frac{1}{2n\ln 2}\sum_{i=1}^{n}(\mu_A(u_i)-\mu_B(u_i))\ln\frac{1+\mu_A(u_i)}{1+\mu_B(u_i)} \\ &\quad +(\mu_B(u_i))-(\mu_A(u_i))\ln\frac{2-\mu_A(u_i)}{2-\mu_B(u_i)} \qquad (5.17)\end{aligned}$$

2. Fan and W. Xie (1999) proposed generating proximity measures through ordinary similarity measures using the following operations:

$$\mathcal{S}_{pm_2}(A,B)=\min\{\mathcal{S}(A,B),\mathcal{S}(\bar{A},\bar{B})\} \qquad (5.18)$$

$$\mathcal{S}_{pm_3}(A,B)=\frac{1}{2}\left(\mathcal{S}(A,B)+\mathcal{S}(\bar{A},\bar{B})\right) \qquad (5.19)$$

[31].

5.2 Similarity measures for environmental data

In fact-based studies such as this one, a clear explanation of the context in which the membership functions are defined, must be given. In summary, metal concentrations were mapped via a membership function, Equation (4.72), into degrees of membership in the unit interval $[0,1]$, corresponding to "contamination with the metal x_i". Therefore within each fuzzy set A_i,

- a degree of membership $= 0$, would reflect the level of harmless and naturally found metal concentrations within the environment, i.e., **no contamination**.
- a degree of membership $= 1$, would correspond to the largest amount of metal concentrations considered to pose the greatest levels of harm within environmental guidelines, i.e., **full contamination**.
- degrees of membership in the interval $(0,1)$, would reflect a gradual transition between no contamination and full contamination of metal concentrations.

Table 5.1: Six examples of pairs of fuzzy sets and the desired similarity values

Example	$\mu(x_1)$	$\mu(x_2)$	$\mu(x_3)$	Similarity
$T1$	1.0	0.2	0.8	Moderate
	1.0	0.1	0.2	$0.50 \leq \mathcal{S}^{T1}(A,B) \leq 0.55$
$T2$	0.0	0.1	0.0	Moderately high
	0.0	0.9	0.0	$0.65 \leq \mathcal{S}^{T2}(A,B) \leq 0.75$
$T3$	1.0	0.1	1.0	Moderately high
	1.0	0.9	1.0	$0.65 \leq \mathcal{S}^{T3}(A,B) \leq 0.75$
$T4$	0.8	0.5	0.2	Low
	0.1	0.6	0.4	$\mathcal{S}^{T4}(A,B) \leq 0.5$
$T5$	0.0	0.1	0.3	Low
	0	0.9	0.8	$\mathcal{S}^{T5}(A,B) \leq 0.5$
$T6$	0.0	0.0	0.0	Low
	0.1	0.3	0.2	$\mathcal{S}^{T6}(A,B) < \mathcal{S}^{T5}(A,B) \leq 0.5$

In Table 5.1, data example pairs are used to reflect specific practical properties, from an environmental point of view (with respect to contamination)[1]. Let $X = \{x_1, x_2, x_3\}$ be the universal set. Six example pairs of fuzzy sets A and B are shown in Table 5.1, rows (1) through (6) denoted Ti, for $i = 1, ..., 6$. The six example pairs are constructed to reflect these practical properties mathematically and account for, (i) matching singletons and their complement, e.g., T2 and T3, (ii) separated fuzzy sets, e.g., T6, (iii) fuzzy sets A and B for which $\exists u_i \in U$, such that $\mu_A(u_i) = \mu_B(u_i)$, e.g., T1 and T5, and (iv) fuzzy sets A and B that do not fall in the other types, e.g., T4. In addition, the (intuitively) reasonable value of the similarity is expressed verbally and an interval is suggested for each example. Therefore, the suggested ordering of the intuitive values of a similarity measure are as follows:
T2 and T3 $>$ T1 $\geq$ T4 $\geq$ T5 $>$ T6.

Within our framework in defining the concept of 'contamination', a degree of '0' is chosen to denote no contamination, but at the same time indicates the existence of concentration levels equal to or below the benchmark (i.e., average shale values). A degree of '1' is chosen to denote the highest level of contamination, but also to indicate the existence of very high concentration levels equal to or far above the upper guidelines. In other words, in interpreting the concept of contamination, a value of 0 is as important as a fuzzy value of 1. This theoretically desirable property can be satisfied if:

$$\mathcal{S}(A, B) = \mathcal{S}(\bar{A}, \bar{B}) \quad \forall A, B \in \mathcal{P}(U).$$

Therefore, we require a similarity measure which is also a proximity measure. Table 5.2, compares some similarity measures and this desired property. Comparative studies of similarity measures and their individual properties can be found in [19, 54, 61, 72]. Observing Table 5.2 we find that two out of the five measures satisfy the desired property. They are measures (5.11) and (5.12). But which one is best suited to our data? To make an overall judgment on the performance of (5.11) and (5.12),

[1]The data examples were derived intuitively after some trial and error, and comparison with different data structure using various similarity measures

Table 5.2: A desirable property of similarity measures

Similarity measures	$\mathcal{S}(A,B) = \mathcal{S}(\bar{A},\bar{B})$
Type [1]	
$\mathcal{S}_C(A,B)$ (5.1)	No
Type [2]	
$d_D(A,B)$ (5.8)	No
$d_{SD1}(A,B)$ (5.11)	Yes
$d_{SD2}(A,B)$ (5.12)	Yes
Others	
$\mathcal{S}_V(A,B)$ (5.13)	No

we shall include similarity measures from other types, to test the practical properties. Table (5.3) shows the values of the four similarity measures, (5.1), (5.13), (5.11), and (5.12), on the six example pairs and gives a short comment for each. Observations can be made by comparing the intuitive similarity values, from Table (5.1), with the calculated similarities, in Table (5.3), of the six data examples for each measure.

Generally, we can see that the results of the four measures of similarity were not satisfactory to a certain extant and some discrepancies in the results exist. Measures (5.1) and (5.13) seem to produce results consistent with the desired intervals of similarity for data examples (T1) and (T3) to (T5), i.e., $T3 > T1 > T4 > T5$. On the other hand, they did not comply with the desired intervals for matching singletons and separated fuzzy sets in data examples (T2) and (T6), respectively. As for the symmetrical difference based measure (5.11), it produced values different from the desired ordering of similarity values. The same holds for (5.12).

Therefore, taking into consideration all four similarity measures and their results on the six data examples, in the next section we propose a new measure of similarity based on the desirable theoretical and practical properties.

Table 5.3: The values of the four similarity measures for the six examples examples from Table 5.1

Similarity measures	T1	T2	T3	T4	T5	T6	Remarks
$\mathcal{S}_C$ Cardinality-ratio, (5.1)	0.65	0.1	0.72	0.44	0.24	0	Does not comply with the desired intervals; poor result on T2 and T6
$\mathcal{S}_V$ Vector-product, (5.13)	0.7	0.1	0.74	0.5	0.23	0	Similar to $\mathcal{S}_C$.
$\mathcal{S}_{SD1}$ Symmetrical difference, (5.11)	0.4	0.2	0.2	0.3	0.2	0.7	Do not correspond to the desired ordering.
$\mathcal{S}_{SD2}$ Symmetrical difference, (5.12)	0.77	0.73	0.73	0.7	0.57	0.8	Similar to $\mathcal{S}_{SD1}$
$\mathcal{S}_*$ **The proposed measure**, (5.20)	0.61	0.67	0.67	0.52	0.46	0.33	Close to the desired intervals and consistent with the order of preference.

5.2.1 A new measure of similarity $\mathcal{S}_*$

Proposition 6. *The function* $\mathcal{S}_* : \mathcal{P}(U) \times \mathcal{P}(U) \longrightarrow [0,1]$, *based on the symmetrical difference ratio is*

$$\mathcal{S}_*(A,B) = 1 - \frac{\| A \bigtriangledown B \|}{height(A \bigtriangledown B)}$$

$$= 1 - \frac{1}{m} \left\{ \frac{\sum_{i=1}^{m} |\mu_A(u_i) - \mu_B(u_i)|}{\max(|\mu_A(u_i) - \mu_B(u_i)|)} \right\} \tag{5.20}$$

Equation 6 is a similarity measure on $\mathcal{P}(U)$ satisfying the properties:

1. $\mathcal{S}(A,B) = \mathcal{S}(B,A), \;\; A,B \in \mathcal{P}(U)$.

2. $\mathcal{S}(E,E) = 1$, $E \in \mathcal{P}(U)$.

3. If $A \subseteq B \subseteq C$, $\forall A,B,C \in \mathcal{P}(U)$, then $\mathcal{S}(A,B) \geq \mathcal{S}(A,C)$ and $\mathcal{S}(B,C) \geq \mathcal{S}(A,C)$. Note that, $A \subseteq B \subseteq C$ implies that $\mu_A(u) \leq \mu_B(u) \leq \mu_C(u)$ $\forall \; u \in U$.

4. $\mathcal{S}(A,B) = \mathcal{S}(\bar{A},\bar{B}), \;\; A,B \in \mathcal{P}(U)$.

As the denominator is undefined for $A = B$, we extend (5.20) to be

$$\mathcal{S}_*(A,B) = \begin{cases} 1, & \text{if } A = B \\ 1 - \frac{\|A \bigtriangledown B\|}{height(A \bigtriangledown B)}, & \text{otherwise} \end{cases}$$

This proposed similarity measure is based on the maximum symmetrical difference.

The next step is to check the performance of (5.20) on the data examples. In Table 5.3, the bottom row shows that values of the proposed measure for the six examples are consistent with the desired values.

In the next section, the proposed similarity measure, designed here for environmental type data, will be applied on data from Liverpool and Morecambe bay.

5.3 Application of similarity measure $\mathcal{S}_*$ to Liverpool bay and Morecambe bay data of 1988

For our study, we wish to reduce the number of loading indices that contain similar information of metal distribution in a marine environment. This reduction will be performed with the help of the similarity measure $\mathcal{S}_*$ and statistical analysis using hierarchical relational data clustering. The main question we want to address is

- How many different groups of informative loading indices can we find in the set of constructed indices and subsequently, which index do we choose as a representative of its group?

Eight loading indices were calculated for the data in Liverpool bay and Morecambe bay collected in 1988 (details in Chapter 4). Many operators are applicable, although these eight were selected because of their desirable properties. LI_7: Fuzzy integral and LI_8: Weighted average, take into account the importance of each metal with respect to contamination. On the other hand from an environmental aspect, the common operators; LI_1: Minimum, LI_2: Product, LI_3: Geometric mean, LI_4: Maximum, LI_5: Arithmetic mean, and LI_6: Competition jury, produce most intuitive and interpretable indices of their type.

For this study, we wish the measure of similarity to help us in reducing the number of loading indices by replacing a group of indices containing similar information with one single index. Having picked the similarity measure, (5.20), the next question is "How many different groups of loading indices shall we consider?"

Results of implementing the proposed measure $\mathcal{S}_*$ (5.20) to Liverpool and Morecambe bay are listed in Tables 5.4 and 5.5, respectively. The similarities for the Morecambe bay are higher than those for the Liverpool bay region. This is an indication of the lower contamination in Morecambe bay, which can be seen visually as the blue contour shades in Figure 4.8 to 4.14 , and quantitatively in *Appendix (C)*. That is, since there are large areas in the bay which are not contaminated, and hence all loading indices have low values across these areas, the similarity measure

takes high values.

Hierarchical relational clustering, using single linkage, complete linkage and average linkage were applied to identify clustering among the eight loading indices. The results of classifying the indices into 2, 3, 4 and 5 clusters are listed in Tables 5.6 and 5.7 for Liverpool bay and Morecambe bay, respectively. Comparing the results in Table 5.6 and Table 5.7,

- Clustering all eight loading indices into three and four clusters produced the same grouping of indices for both regions.
- Relational clustering was able to identify the group consisting of $\{LI_4,\ LI_7\}$, and keep the two together for 2, 3, and 4 clusters, for both regions.
- The loading indices $\{LI_1,\ LI_2,\ LI_3\}$ were identified as a unique group for all clusters.

This shows that the proposed measure gives stable results, and also indicates a natural grouping of the indices based mainly on the "degree of optimism" of the aggregation. Similarities between the 8 loading indices for both Liverpool bay and Morecambe bay can be seen by comparing the shaded contour plots in Figures 4.4-4.14 for each region separately. The loading indices of the minimum and product have similar overall metal spatial distribution. This is true for both Liverpool bay and Morecambe bay. For the remaining indices, it is difficult to make a visual difference between the clusters of indices. It is impossible to distinguish between the indices for Morecambe bay, whereas we can easily group the indices for Liverpool bay into 2 groups: {maximum, fuzzy integral} and {minimum, product, geometric mean, competition jury}.

Another objective method for grouping similarity measures between the eight loading indices is by using a *similarity tree* [82]. A similarity tree is similar to a dendogram, used to represent the similarity relation of a finite number of elements. In the tree, each level shall represent an α-cut of the similarity relation between the indices. The sets of indices on specific α-levels can be considered as similarity classes

Table 5.4: Measures of similarity $\mathcal{S}_*(A,B)$, of all 8 paired loading indices of Liverpool bay.

$(S*)$	LI_2	LI_3	LI_4	LI_5	LI_6	LI_7	LI_8
LI_1	1	1	0.27	0.58	0.76	0.27	0.57
LI_2	1	1	0.27	0.58	0.76	0.27	0.57
LI_3		1	0.27	0.58	0.76	0.27	0.57
LI_4			1	0.31	0.32	0.8	0.32
LI_5				1	0.37	0.28	0.54
LI_6					1	0.29	0.29
LI_7						1	0.3
LI_8							1

Table 5.5: Measures of similarity $\mathcal{S}_*(A,B)$, of all 8 paired loading indices of Morecambe bay.

	LI_2	LI_3	LI_4	LI_5	LI_6	LI_7	LI_8
LI_1	1	1	0.9	0.91	0.98	0.89	0.91
LI_2	1	1	0.9	0.91	0.98	0.89	0.91
LI_3		1	0.9	0.91	0.98	0.89	0.91
LI_4			1	0.9	0.9	0.97	0.9
LI_5				1	0.9	0.9	0.91
LI_6					1	0.9	0.9
LI_7						1	0.9
LI_8							1

Table 5.6: Hierarchical clustering of the 8 loading indices using calculated similarities $\mathcal{S}_*(A,B)$ for Liverpool bay.

Number of Clusters	Grouping
2	(LI_4, LI_7),$(LI_1, LI_2, LI_3, LI_5, LI_6, LI_8)$,
3	(LI_4, LI_7),(LI_1, LI_2, LI_3, LI_6), (LI_5, LI_8)
4	(LI_4, LI_7),(LI_1, LI_2, LI_3, LI_6), (LI_5), (LI_8)
5	(LI_4, LI_7),(LI_1, LI_2, LI_3), (LI_6),(LI_8),(LI_5)

Table 5.7: Hierarchical clustering of the 8 loading indices using calculated similarities $\mathcal{S}_*(A,B)$ for Morecambe bay

Number of Clusters	Grouping
2	(LI_4, LI_5, LI_7, LI_8), (LI_1, LI_2, LI_3, LI_6)
3	(LI_4, LI_7),(LI_1, LI_2, LI_3, LI_6),$(LI_5, , LI_8)$,
4	(LI_4, LI_7),(LI_1, LI_2, LI_3, LI_6),(LI_5),(LI_8)
5	(LI_4),(LI_7),(LI_1, LI_2, LI_3, LI_6),(LI_5),(LI_8)

Figure 5.1: Similarity tree of the 8 loading indices of Liverpool bay

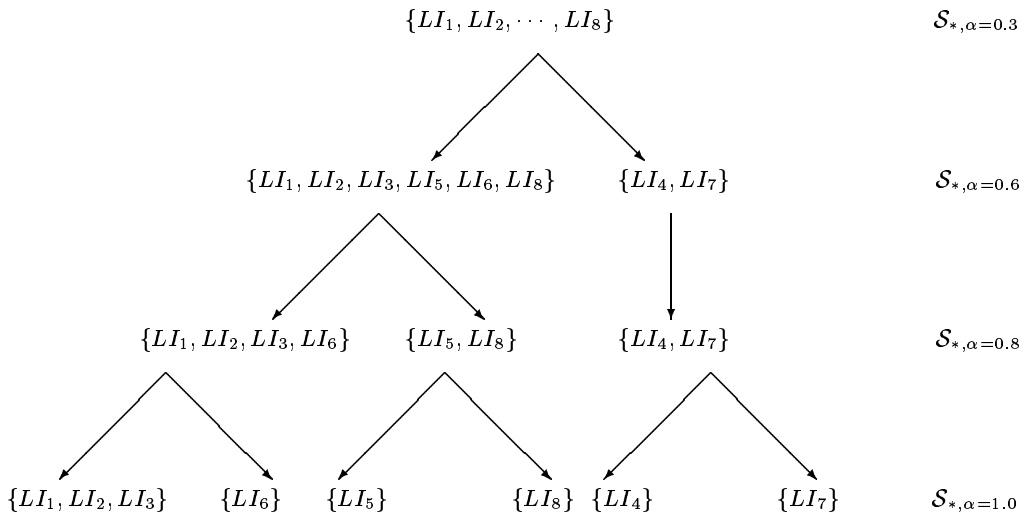
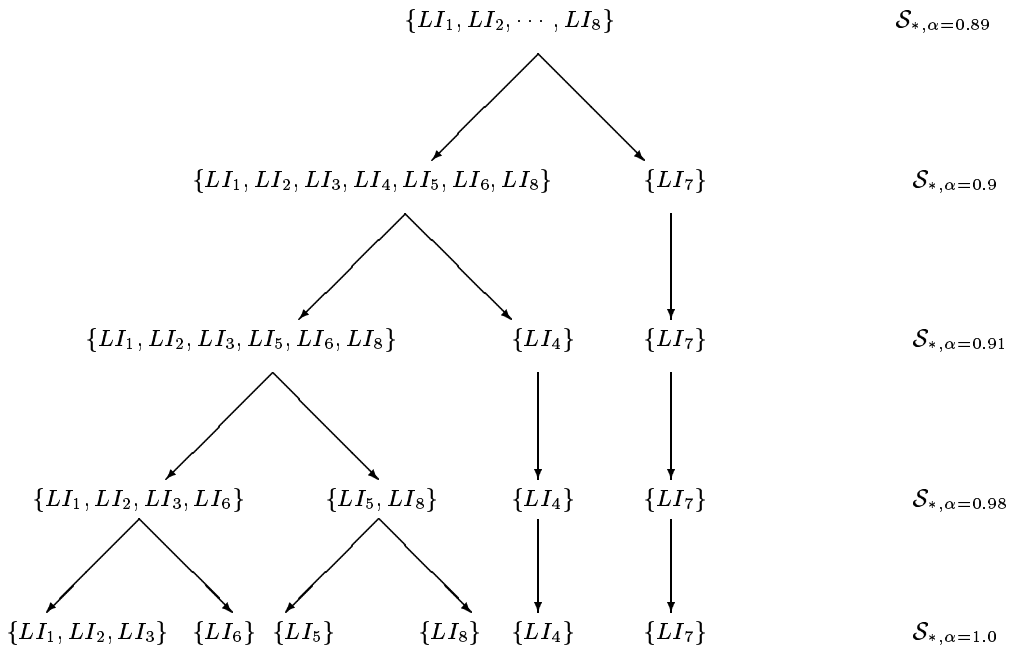


Figure 5.2: Similarity tree of the 8 loading indices of Morecambe bay



of α-level. The first step is to select the values for the α-cuts. Rounding the similarity measures in Table 5.4 to the first value after the decimal, we chose α levels at 0.3, 0.6, 0.8, and 1.0. As for similarities in Table 5.5, we chose α values equal to 0.89, 0.9, 0.91, 0.98, and 1.0. The next step is to group the indices from the first 0.3-level, $\{LI_1, LI_2, \cdots, LI_8\}$, into two classes at the 0.6-level. classes at the second 0.6-level. The first class is grouped such that $\{(LI_i, LI_j) | \mathcal{S}_*(LI_i, LI_j) \geq 0.6, i, j = 1, \cdots 8\}$ and the second such that $\{(LI_i, LI_j) | \mathcal{S}_*(LI_i, LI_j) < 0.6, i, j = 1, \cdots 8\}$. Similarly, this is done for $\alpha = 0.8$ and $\alpha = 1.0$. This process of grouping is applied on each class of indices at each α-level. Figure 5.1 and Figure 5.2 show the similarity trees for the eight loading indices for Liverpool bay and Morecambe bay, respectively. Similarity trees for both regions of the eight indices give the same result at the $\alpha = 1$-level.

Therefore, we can summarize our findings for both classification methods as follows. As a result of cluster analysis, the eight indices were classified into four groups for Liverpool bay and Morecambe bay. They are, {minimum, product, geometric mean, competition jury}, {average}, {maximum, fuzzy integral}, and {weighted average}. Using the similarity tree method, the loading indices were classified into six groups for both regions: {minimum, product, geometric mean}, {competition jury}, {average}, {maximum}, {fuzzy integral}, and {weighted average}. We also wish to take into account our subjective visual classification of the indices. Because it is impossible to visually group the spatial distribution of indices for Morecambe bay, we will only consider classification of Liverpool bay indices. We found that the spatial distribution of the eight indices can be visually classified into 4 groups: {minimum, product}, {geometric mean, average, competition jury, weighted average}, {maximum} and {fuzzy integral}. Comparing the results of these different grouping approaches, we found that the loading indices were classified in two out of the three approaches into five groups:
{minimum, product, geometric mean}, {maximum}, {average} ,{fuzzy integral}, and {weighted average}. Only the competition jury based index differed in its classification in all three approaches.

Based on this outcome, we choose our index representatives as, the *Minimum*, *Maximum*, *Average*, *Fuzzy integral* and *Weighted average*.

5.4 A general methodology for designing and selecting loading indices in a marine environment

As a conclusion of this pilot study, the following generic methodology is suggested for constructing and selecting loading indices in marine environment.

1. Identify the contaminants and collect a data set of measurements of these contaminants across the region of interest (Chapter 1).
2. Specify the lower and upper limits for each contaminant.
3. Calculate the membership degrees of the fuzzy sets over the set of sites.
4. Using fuzzy aggregation operators, calculate a set of loading indices (Chapter 4). Many operators are applicable at this stage, not only the initial thirteen discussed, and the eight used in Chapter 4.
5. Calculate pairwise similarities between the loading indices using a similarity measure (we recommend $\mathcal{S}_*$ for the reasons explained in the text).
6. Run relational clustering for several number of clusters to find groups of similar indices. (We found out that hierarchical clustering procedures with single linkage, average linkage, and complete linkage led to the same grouping.)
7. Display the results, e.g., by color contour plots, and select one loading index from each group.
8. Use the selected indices to characterize the region of interest. We believe that the indices will be grouped according to the "level of optimism" involved in the aggregation. It is important to select indices which are interpretable in terms of the domain context. For example, the meaning of minimum, maximum and average aggregation can be explained to the environmental user.

After applying the above methodology to Liverpool bay and Morecambe bay, for data collected in 1988, we conclude that the results of implementing the proposed measure of similarity (and the grouping approach) can be seen to be in agreement with observed visual similarities between the loading indices (Figures 4.4 to 4.14.

Therefore, we find $\mathcal{S}_*$ appropriate for the type of environmental data considered here.

5.5 Conclusion

We used the concept of a similarity measure to identify similarity relationships between the eight loading indices: *minimum, product, geometric mean, maximum, average, competition jury, fuzzy integral,* and *weighted average.* A set of desirable theoretical and practical properties were identified for environmental data and a new similarity measure was proposed, $\mathcal{S}_*$. The similarity measure, $\mathcal{S}_*$, was then applied to Liverpool bay and Morecambe bay data of 1988 to identify similar information of spatial distribution held by the loading indices. The proposed similarity measure was found to give stable results and indicate a natural grouping of the indices based on the "degree of optimism" of the aggregation.

Using hierarchical clustering and the idea of a similarity tree (in addition to a subjective comparison), we were able to select a set of five indices: *minimum, maximum, average, fuzzy integral* and *weighted average.* These characterize a marine environment from different aspects and are interpretable in a domain context.

A new similarity measure was proposed based on a set of desirable properties for environmental data. Using two classification approaches we were able to reduce the indices from eight (based on graphical observation of similarity) to five: *minimum, maximum, average, fuzzy integral* and *weighted average.*

Chapter 6

Further analysis of a marine environment: Liverpool bay

Based on graphical observation and quantitative analysis of pair-wise similarity between thirteen loading indices, a final selection of five indices was made. The chosen indices were based on the *minimum, maximum, average, fuzzy integral* and *weighted average* aggregation operators. Using these indices, we want to compare the change in the metal loading distribution of annually sampled metal concentrations.

6.1 Introduction: Annual data

In Chapter 2, preprocessing of annually sampled metal data sets was carried out. We handled missing observations and detected suspected outliers within the data sets. This was done for each metal set, from 1986-1992, for Liverpool bay, and for Morecambe bay in 1988. So far only data sets sampled in 1988 have been used. The annually sampled data sets differ in the number of sampled sites ranging from $m = 58$ in 1986, $m = 54$ in 1987, $m = 70$ in 1988, $m = 61$ in 1989, $m = 26$ in 1990, and $m = 40$ in 1991 and 1992. Also, we found a difference in the geographical location of some sampled sites, including those sites that make up the designated

dumping site (SI), i.e., SI= { J07, J09, J11, K08, K09, K10, K11, K12, L09, L10, L11, L12}. Because of these differences it is not appropriate to compare the loading distributions directly. Even if we wish to look only at the dumping region (SI) and ignore the spatial fluctuations of the stations' coordinates, the comparison is not straightforward because not all sites in SI are sampled every year. For example, only 50% of SI sites are sampled in 1990, compared to 100% of SI sites sampled in 1988. We chose for our analysis only those years, 1986-1989, in which $m \geq 50$ stations.

The chapter is sectioned as follows: analysis of annual contamination, and temporal change in metal concentrations is introduced in Section 6.2. Representative indices, based on the minimum, maximum, average, fuzzy integral and weighted average aggregation operations, will be used to carry out further analysis on the distribution of overall metal contamination for a given sampled year in Liverpool bay. In section 6.3 we conclude our findings for this chapter.

6.2 Temporal changes of regions of high and low contamination

We discuss and analyze the dynamics of Liverpool bay system using different approaches. In Chapter 4, Section 7, we suggested the use of α-cuts, that can be implemented on certain loading indices, to extract regions that exhibit moderate to high levels of metal contamination. Here we consider a process that distinguishes between, what we call, *clean* and *highly contaminated* regions of Liverpool bay for each sampled year. In addition to this, an approach is defined to compare the average annual change in overall metal contamination. But first, we shall construct a priori set of contamination by sewage and industrial waste based on the designated area for dumping, SI.

6.2.1 Ideal contamination index (IC)

Observing the annually sampled data sets processed and presented in Chapter 2, each site is distinguished by a symbol (e.g., L09) and assumed to have a constant geographical location (X =longitude,Y =latitude). However, when comparing the latitude and longitude coordinates of a site in one year with its coordinates from another year, we found that the coordinates for some sampled sites were not consistent throughout the years. For example, the site G07 has coordinates $(-41.6, 29.1)$ in 1986 and 1987, $(-41.3, 29.1)$ in 1988, and $(-44.4, 29.1)$ in 1989. Because of this, it was necessary to smooth out the differences in the geographical locations (X, Y) from one year to the other. As a result, we averaged the coordinates for each site sampled over the seven years. The total number of sites sampled over the years 1986-1992 and their averaged coordinates are given in *Appendix (B)*. Sites that fell within, or on the boundaries of, the designated dumping area SI are: J07, J09, J11, K08, K09, K10, K11, K12, L09, L10, L11, L12. To distinguish these sites from other non SI sites, we will denote their coordinates as $s_{SI}(X, Y)$ (see *Appendix (B)*.

Next we wish to construct a priori knowledge (or set) reflecting the importance of sampled sites in Liverpool bay, with respect to contamination, using the set of averaged sites (*Appendix (B)*). To do so, an appropriate function is needed that maps all $m = 94$ site coordinates $s(x, y)$ to a single value. This value should represent the concept of "*the importance of sampling stations to contamination*". Since, the highest contamination should be concentrated within SI, i.e., the designated dumping region, we can redefine the concept as "*the importance of sampling stations to SI*". Therefore, we require a function that can associate the coordinates of each sampled station $s_j(x, y)$ and the stations that fall within SI. To simplify the calculations, we averaged all sites that belong to the dumping region $SI(x, y)$ into one site, $\bar{s}_{SI}$ with coordinates $(\bar{x}_{SI}, \bar{y}_{SI}) = (-35.25, 31.72)$. A distance function $d : \Re^2 \longrightarrow \Re^+$ was chosen to compute the relationship between the dumping area $\bar{s}_{SI}$ and all sampled sites s_j with coordinates (x_j, y_j). We chose the commonly used Euclidean distance

measure,

$$d(\bar{s}_{SI}, s_j) = \sqrt{(\bar{x}_{SI} - x_j)^2 + (y_{SI} - y_j)^2} \tag{6.1}$$

Distances for sampled sites located in the dumping area SI, $d(\bar{s}_{SI}, s_{SI})$, ranged from 0.15 to 3.955. Distance values calculated for all sampled sites $s_j, j = 1, \cdots 94$ (including sites within the dumping region SI) ranged between $[0.15, 23.40]$. Therefore, on average, the closer the calculated distances are to values in the interval $[0.15, 3.955]$, the closer a sampled site is to the dumping region.

The next step is to construct an ideal fuzzy set (or crisp set) of contamination in Liverpool bay, based on data sampled between 1986 and 1992. When we say ideal, we make the assumption of an ideal situation where (i) dumping occurs only in the designated area and (ii) waste is not influenced by natural phenomena such as tidal movement. Therefore, we want to formulate a fuzzy (or crisp) set of importance for sampled sites $s_j(x, y)$ with respect to their distance from $s_{SI}(x, y)$. For this, the chosen membership function must have the following features:

1. For $d(\bar{s}_{SI}, s_j) \leq 3.955$, the fuzzy degree of membership must be 1,
   $\mu_{Fuzzy}(d(\bar{s}_{SI}, s_j)) = 1$.
   Otherwise, $\mu_{Fuzzy}(d(\bar{s}_{SI},\ s_j)) \in [0, 1)$.

2. The fuzzy membership function should be a decreasing function with respect to the increasing distance $d(\bar{s}_{SI}, s_j)$ from the dumping region SI.

3. In an area designated for the disposal of sewage and industrial waste, ideally the greatest degree of membership should exist in the dumping site SI, with decreasing degrees of membership for sites outside the dumping area.

Considering these points, we chose the fuzzy membership function as a right asymmetric function, based on Equation (3.29), to denote the concept of ideally perceived contamination in Liverpool bay. The function is used to define how close a sampled site s_j is to the designated dumping area SI, $d(\bar{s}_{SI}, s_j)$ (an ideal centre). Hence, our

fuzzy membership function is

$$\mu(d(\bar{s}_{SI}, s_j)) = \begin{cases} 1 & , d(\bar{s}_{SI}, s_j) < b \\ \frac{1}{1+c[d(\bar{s}_{SI}, s_j)-b]^2} & , d(\bar{s}_{SI}, s_j) \geq b \end{cases} \tag{6.2}$$

The parameters b and c are given the values 3.955 and 0.026, respectively. The parameter b denotes the '*ideal center*' chosen as the maximum distance within the dumping area. As for the parameter c, the dispersion index, for a chosen $b = 3.955$ of the fuzzy set of ideal contamination, a value of $c = 0.026$ gives a cross-over point at distance 10.15, where $\mu(d(\bar{s}_{SI}, s_j)) = 0.5$. The cross-over point was calculated as, $\frac{1}{m}\sum_j^{m=94} d(\bar{s}_{SI}, s_j)$. In addition to this, an ideal crisp membership set can be computed by the following formula,

$$\mu(d(\bar{s}_{SI}, s_j)) = \begin{cases} 1 & , d(\bar{s}_{SI}, s_j) \in \leq 3.955 \\ 0 & ,\text{Otherwise} \end{cases} \tag{6.3}$$

The resulting crisp and fuzzy ideal sets are presented in Figure 6.1. The computed ideal data sets are listed in *Appendix (C)*. Both sets of weights can be used as future reference for contamination with respect to the dumping area SI.

Recall the fuzzy membership function of Equation (4.72), defined by the data set of metal concentrations $x_i(s_j)$, the average shale values, L_i, and upper trigger levels, T_i. Using annually sampled metal data sets from 1986 to 1989 and Equation (4.72), we plotted the spatial distribution of metal contamination in Liverpool bay, shown in Figures 6.2-6.6, using the five chosen loading indices. The minimum, average and weighted average indices exhibit very low metal loading. Interestingly, the highest values of metal loading were not produced by the maximum index but by the fuzzy integral index, i.e., when the importance of each heavy metal was taken into account. On the other hand, on average, we can say that the sampled region of Liverpool bay is not contaminated. This is evident by observing both the average and weighted average indices.

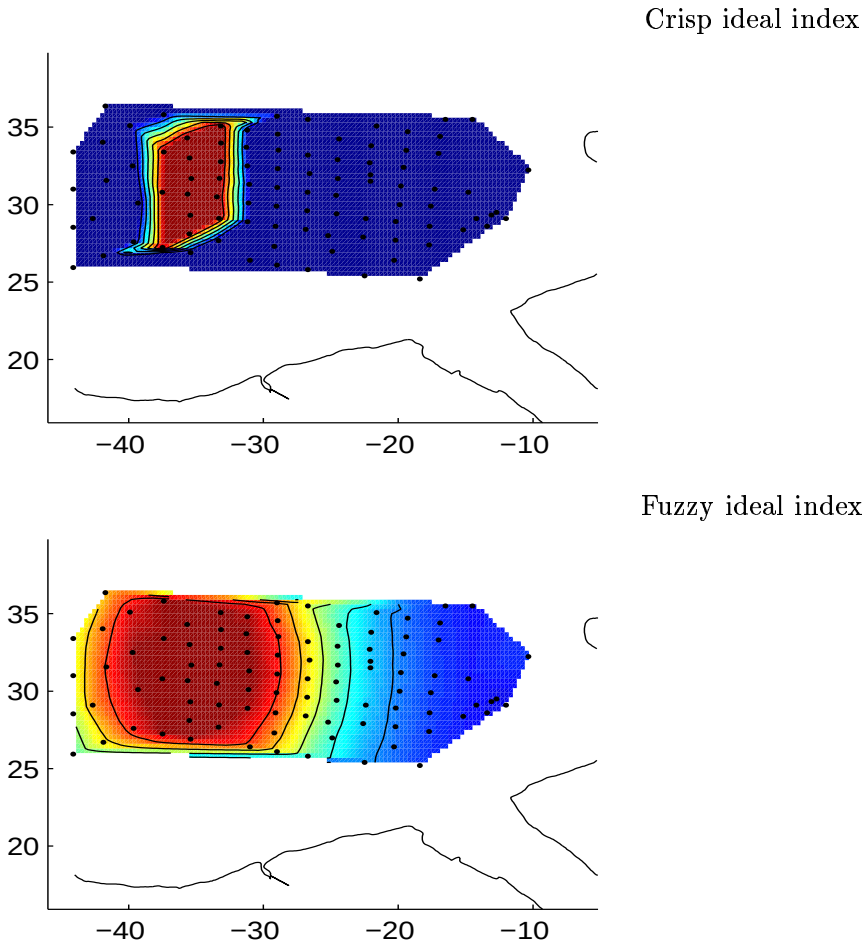


Figure 6.1: Crisp and fuzzy ideal contamination indices of total sampled stations in Liverpool bay

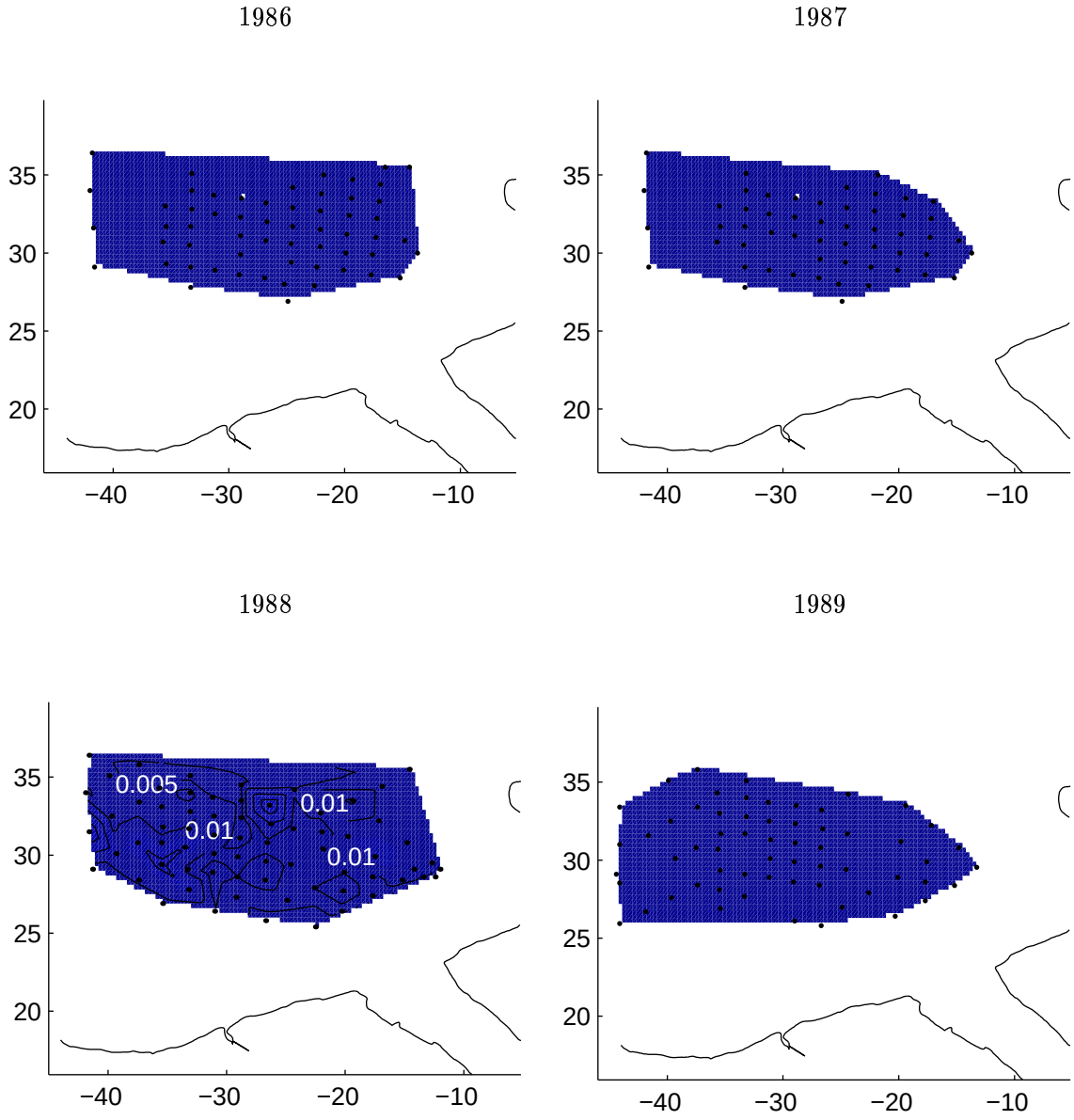


Figure 6.2: Shaded contour plots of the Minimum aggregation connective for Liverpool bay from 1986 to 1989

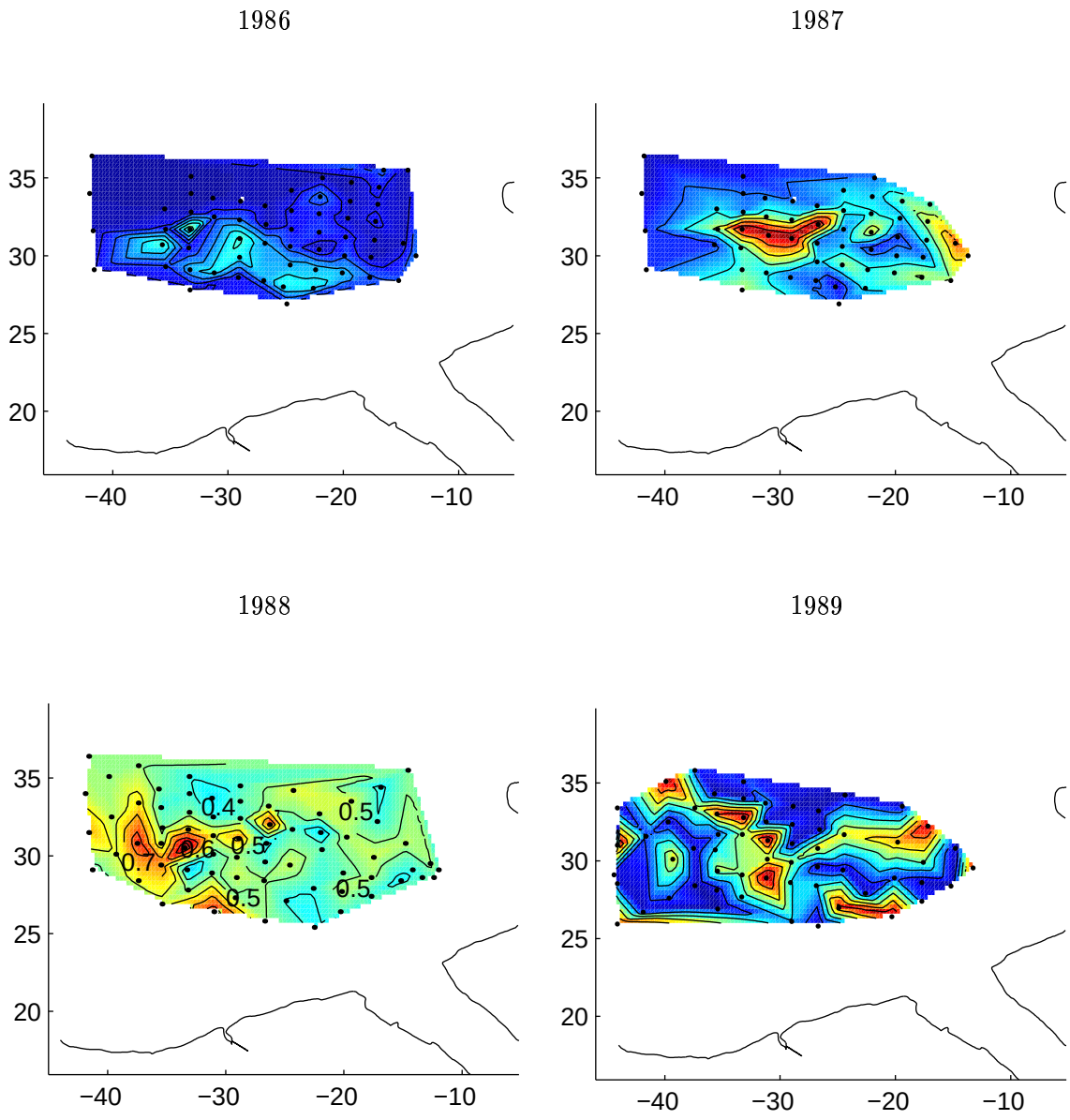


Figure 6.3: Shaded contour plots of the Maximum aggregation connectives for Liverpool bay from 1986 to 1989

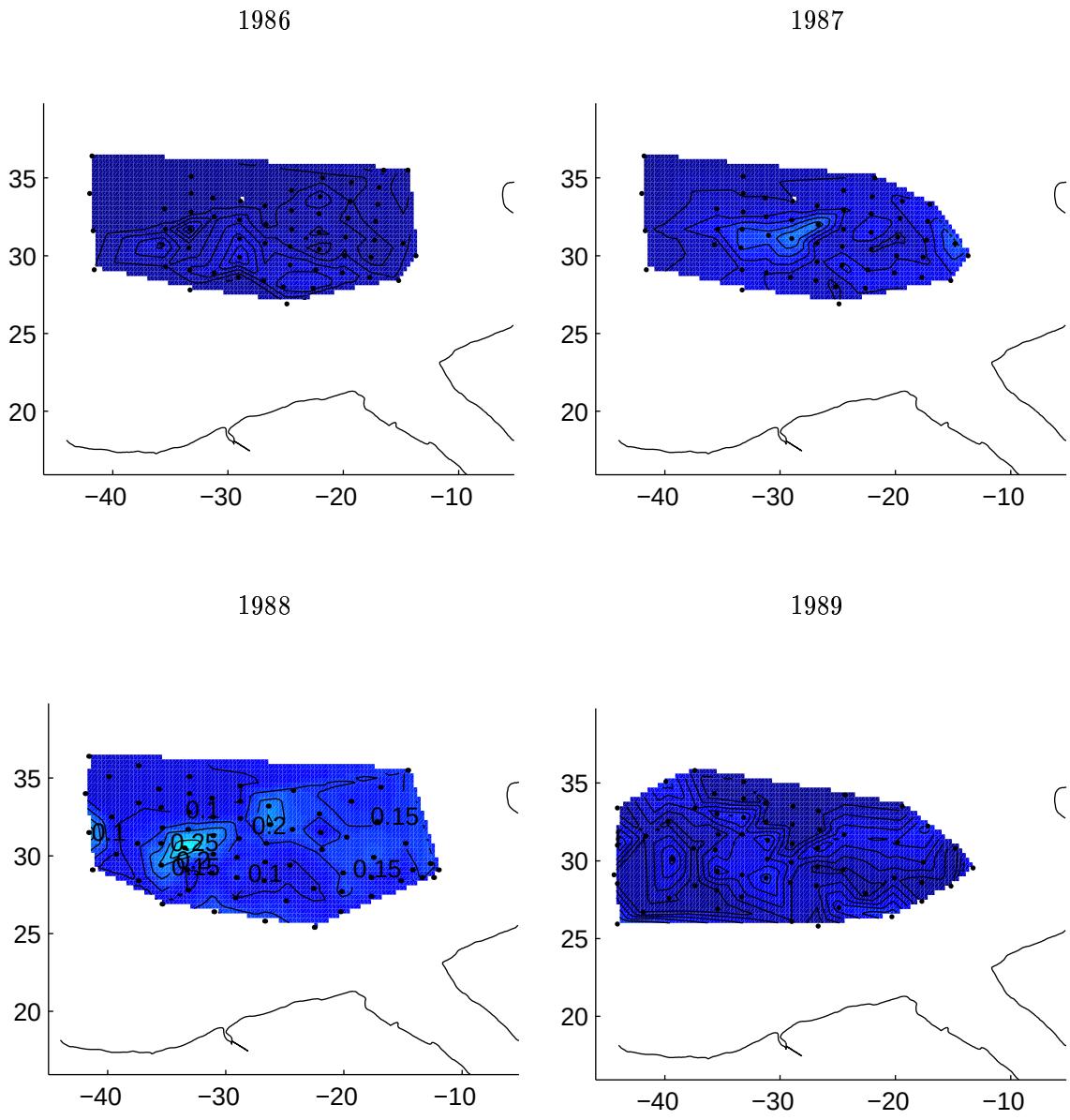


Figure 6.4: Shaded contour plots of the Average aggregation connective for Liverpool bay from 1986 to 1989

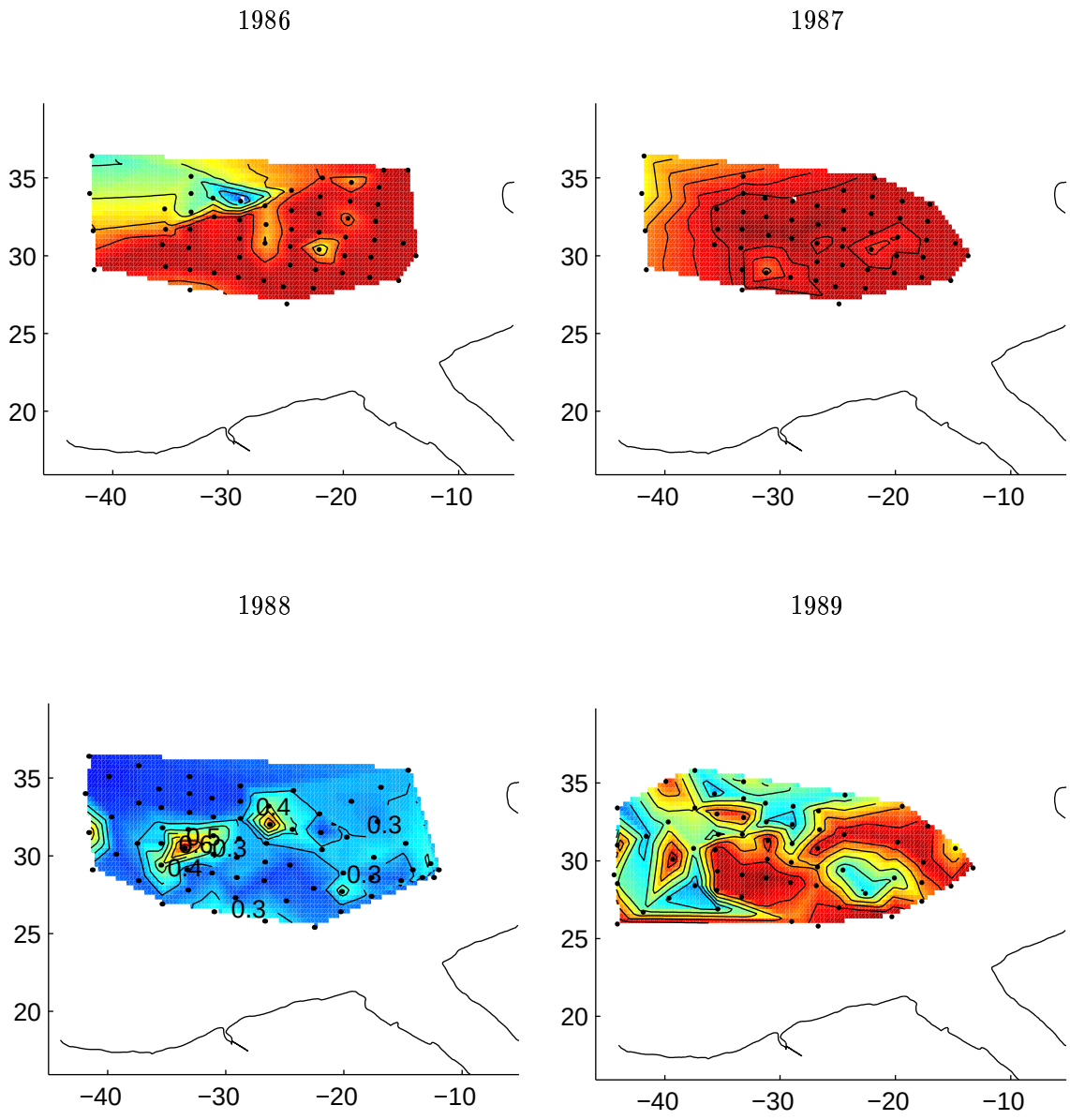


Figure 6.5: Shaded contour plots of the Fuzzy integral aggregation connective for Liverpool bay from 1986 to 1989

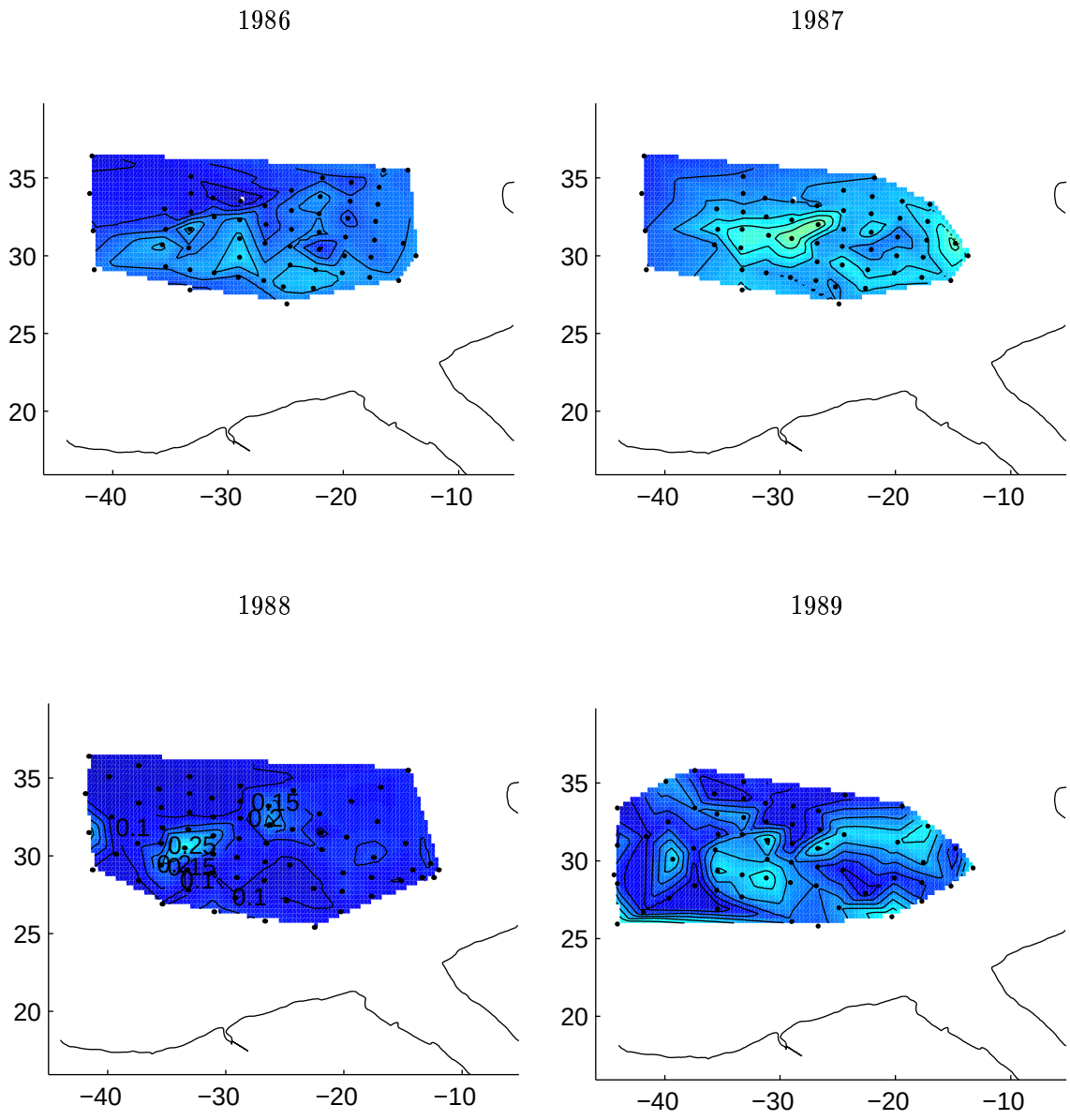


Figure 6.6: Shaded contour plots of the Weighted average aggregation connective for Liverpool bay from 1986 to 1989

6.2.2 A single representative index value (SRV)

In previous sections, we analyzed sampled data from 1986-1989. Here we make use of the data sampled in 1990-1992. This data was left out in the previous analysis because of the insufficient sample size. We suggest a single value representing each loading index on average, thereby disregarding the size of the annual sample sets. We call this value the "single representative value"

$$SRV_{LI}(u) = \|LI_u\| = \frac{1}{m}\sum_{j=1}^{m} LI(u_j) \tag{6.4}$$

The resulting value $SRV_{LI}(u)$ will represent the distribution of overall metal contamination by the loading index LI_u for a given sampled year.

Equation (6.4) was applied to the five representative loading indices constructed for the annually sampled data, 1986 to 1992. Figure 6.2.2 plots the minimum, maximum, average, fuzzy integral and weighted average SRV's for 1986-1992. The graphs show that the contamination is generally decreasing. We can see that there was a definite rise in contamination levels in 1987 (compared to 1986), which then fell again in 1988. The fuzzy integral loading index produced the largest values of averaged contamination for all sampled years 1986-1992. Thus, this index can be used as a warning sign.

6.2.3 'Clean' and 'Highly contaminated' regions of Liverpool bay

In Liverpool bay, the area 'SI' is designated for sewage and industrial waste disposal. Based on this, we partition the sampled region into two or more distinct regions of supposed low and high contamination. Then we compare these regions with respect to contamination levels. We will use metal sets sampled from 1986-1992 to classify sites into two regions, called "clean" and "highly contaminated".

We distinguish between *clean* and *highly contaminated* regions, by separating the metal concentrations, and consequently the sites, based on the 1st and 3rd data quartiles (or 25th and 75th percentile) denoted 1Q and 3Q, respectively. Using the 1st and 3rd quartile of each metal data set, for each year (Table 6.1), we classified

Table 6.1: Descriptive statistics of annual metal data (1986-1989), with respect to the 25th and 75th percentile

Metal Data		Hg	Cd	Cr	Cu	Ni	Pb	Zn
1986	1Q	0.79	0.108	18.27	45.42	28	101.25	247
	3Q	1.4	0.29	25.15	63.4	34.75	158.5	351
1987	1Q	0.88	0.67	70.65	62.95	38.02	156.5	295.75
	3Q	1.44	2.02	93.52	82.95	43.97	216.25	392.25
1988	1Q	0.16	0.36	54.25	43.25	34	104.25	195.75
	3Q	0.77	0.75	73.75	71.5	45	258.75	316.25
1989	1Q	0.34	0.24	61.98	45.62	25.12	74.6	181.56
	3Q	0.53	0.65	75.49	93.24	29.2	143.8	286.14
1990	1Q	0.23	0.12	20.13	15.4	18.98	54.5	74.98
	3Q	0.66	0.32	32.73	27.93	25.38	92.08	174.35
1991	1Q	0.36	0.03	47.38	13.43	30.3	47.25	85.55
	3Q	0.89	0.08	84.85	23.33	38.8	90.28	150.38
1992	1Q	0.36	0.03	1.3	13.43	30.3	47.25	85.55
	3Q	0.69	0.06	2.1	23.33	36.6	90.28	150.38

a site as belonging to the *clean* or *highly contaminated* region. The classification procedure was conducted as follows:
We count in how many of the seven metal data sets, the measurements for this site is below the first quartile 1Q. Let $N_1(s_j)$ denote this number. Also, denote by $N_3(s_j)$ the number out of seven of the metal data sets for which the metal concentration measured at s_j is larger than the third quartile 3Q. If $N_1(s_j) > N_3(s_j)$, then s_j classed as a site of low contamination. All sites for which $N_1(s_j) = N_3(s_j)$ are considered in both groups.

Table 6.2 shows the total number of sites sampled over the years 1986-1992 and their averaged coordinates. Sites shown in Table 6.2 are classified into two types, *clean* and *highly contaminated*. They are marked with the superscripts, $+$ and $*$, respectively. The remaining sites belong to both types.

The next step is to apply SRV to the *clean* sites and *highly contaminated* sites separately for the five chosen loading indices. The SRV over 1986 to 1992, for both regions, are plotted together for each loading index. This is shown in Figure 6.2.3. It is generally expected that a plot of SRVs of a *highly contaminated* region would have greater SR values than that of a *clean* region for any given loading index. There is a slight decrease in *highly contaminated* SR values, from *clean* SR values, for the maximum, average and weighted average indices between 1990 to 1992. This could be due to the small number of sampled stations in 1990 to 1992. Looking at the *highly contaminated* plots, the highest contamination from 1986-1992 for all indices occurred in 1987. This supports the outcome when comparing the spatial distribution of loading indices from 1986 to 1989 (Section 6.1) for the detection of overall metal contamination.

6.3 Conclusion

Coordinates of stations sampled from one year to another did not match for some years. By averaging similar stations sampled from one year to the other, we were able to construct a model set (fuzzy and crisp) of contamination by sewage and

Table 6.2: Total sampled sites from 1986-1989.

sites (86-89)	Symbol	$\overline{X}$	$\overline{Y}$
1	$F06^{+}$	-44.1	25.9
2	$F08^{*}$	-44.1	28.5
3	$F10^{*}$	-44.1	31.0
4	$F12^{*}$	-44.1	33.4
5	$G05^{*}$	-41.9	26.7
6	G07	-42.2	29.1
7	G09	-41.7	31.6
8	$G11^{*}$	-42.0	34.0
9	$G13^{*}$	-41.7	36.4
10	$H06^{*}$	-39.6	27.6
11	H08	-39.3	30.1
12	$H10^{*}$	-39.7	32.5
13	H12	-39.9	35.1
14	$J07^{*}$	-37.4	28.4
15	$J09^{+}$	-37.5	30.8
16	J11	-37.4	33.4
17	$J13^{*}$	-37.4	35.8
18	$K06^{*}$	-35.4	26.9
19	$K07^{+}$	-35.5	28.1
20	$K08^{+}$	-35.4	29.3
21	$K09^{+}$	-35.6	30.7
22	$K10^{+}$	-35.4	31.7
23	$K11^{*}$	-35.5	33.0
24	$K12^{*}$	-35.7	34.3
25	$L07^{+}$	-33.3	27.8

$+$ *clean* sites

$*$ *highly contaminated* sites

Table 6.3: Continued: Total sampled sites from 1986-1989

sites (86-89)	Symbol	$\overline{X}$	$\overline{Y}$
26	$L08^{+}$	-33.3	29.1
27	$L09^{+}$	-33.4	30.5
28	$L10^{+}$	-33.3	31.7
29	$L11^{*}$	-33.2	32.8
30	$L12^{*}$	-33.2	34
31	$L13^{*}$	-33.2	35.1
32	$M06^{+}$	-31.0	26.4
33	M08	-31.2	28.9
34	$M09^{+}$	-31.1	30.1
35	$M10^{+}$	-31.0	31.3
36	M11	-31.2	32.5
37	$M12^{*}$	-31.3	33.7
38	$M13^{*}$	-31.2	34.8
39	N05	-29.0	26.1
40	$N07^{*}$	-29.2	27.3
41	$N08^{+}$	-29.1	28.6
42	$N09^{*}$	-29.0	29.9
43	$N10^{+}$	-29.0	31.1
44	$N11^{*}$	-28.9	32.3
45	$N12^{*}$	-28.9	33.5
46	$N13^{*}$	-28.8	34.5
47	$N14^{+}$	-29	35.7
48	$NW24^{+}$	-13.3	29.5
49	P06	-26.7	25.8
50	P08	-26.9	28.4

Table 6.4: Continued: Total sampled sites from 1986-1989

sites (86-89)	Symbol	$\overline{X}$	$\overline{Y}$
51	$P09^{+}$	-26.8	29.6
52	$P10^{+}$	-26.7	30.8
53	P11	-26.6	32.0
54	$P12^{*}$	-26.7	33.2
55	$P14^{*}$	-26.7	35.5
56	$Q07^{*}$	-24.9	27.0
57	Q08	-25.2	28.0
58	$Q09^{+}$	-24.6	29.4
59	$Q10^{*}$	-24.6	30.6
60	$Q11^{+}$	-24.5	31.7
61	$Q12^{+}$	-24.5	32.9
62	$Q13^{*}$	-24.4	34.2
63	$R06^{*}$	-22.5	25.4
64	$R08^{+}$	-22.6	27.9
65	$R09^{+}$	-22.4	29.1
66	$R10^{*}$	-22.0	30.4
67	$R11^{+}$	-22.1	31.5
68	$R12^{*}$	-22.1	32.7
69	R13	-22.0	33.8
70	$R14^{*}$	-21.8	35.0
71	S07	-20.3	26.4
72	$S08^{+}$	-20.2	27.7
73	$S09^{+}$	-20.1	28.9
74	$S10^{*}$	-19.9	30.0
75	$S11^{+}$	-19.8	31.2

Table 6.5: Continued: Total sampled sites from 1986-1989

sites (86-89)	Symbol	$\overline{X}$	$\overline{Y}$
76	S12	-19.6	32.4
77	$S13^{+}$	-19.4	33.5
78	$S14^{*}$	-19.3	34.7
79	$T06^{*}$	-18.4	25.2
80	T08	-17.7	27.4
81	T09	-17.7	28.6
82	T10	-17.6	29.9
83	$T11^{*}$	-17.3	31.0
84	T12	-17.2	32.2
85	T13	-17.0	33.3
86	$T14^{*}$	-16.9	34.4
87	$T15^{+}$	-16.5	35.5
88	$U09^{+}$	-15.2	28.4
89	$U11^{+}$	-14.8	30.8
90	$U15^{*}$	-14.5	35.5
91	YY01	-14.2	29.1
92	$YY02^{+}$	-12.7	29.5
93	$YY03^{*}$	-12.0	29.1
94	YY04	-13.4	28.6

industrial waste (including heavy metals) over all sampled stations from 1986 to 1992. Analysis of Liverpool bay from 1986 through to 1989 was carried out with respect to the distribution of overall metal loading, based on adopted lower limits of average shale values within the earth's crust [70] and UK upper trigger levels [5]. We found the region showed no evidence of contaminated throughout the sampled years. An unexpected rise in the level of contamination was seen in 1987, compared to 1986, detected by the maximum and fuzzy integral indices.

In field research it is normal that sampling schedule is not exactly matched from one year to another. This is because of the restrictions imposed by financial and environmental factors. Using the *single representative value* approach we were able to use all annually sampled data from 1986 to 1992 to compare the rise and fall of metal contamination levels over the seven years. This was done for each of the five indices. Based on the same approach, analysis was carried on two distinct areas of Liverpool bay, those that continuously registered very high levels of a metal concentration and those that registered very low levels of a metal concentration. A comparison of the highly contaminated regions supported the previous outcome that Liverpool bay in 1987 contained the highest contamination of all annually sampled years.

Based on 1986 to 1989 sampling of metals, the environmental region of Liverpool bay is generally not contaminated. On the other hand, samples of metals collected from the same region in 1987 registered an unexpected increase in metal loading compared to sampled years from 1986 to 1992.

Chapter 7

Conclusion

In this final chapter, we summarize the results from the work. Also, we make some suggestions for improvements of future data collection procedures.

7.1 Summary and research inference

The large amount of environmental data available demands advanced processing methods to extract interpretable and useful information. We were presented with data about metal concentrations in sediments sampled in Liverpool bay between years 1986 and 1992. The task was to find a way to extract from this data information about the degree and the spread of contamination in Liverpool bay. As a benchmark of a "clean" environment we were given data about the same metals sampled from sediments in Morecambe bay.

The use of fuzzy set operations was suggested in many environmental applications ranging from soil fertility assessment, inland evaluation, and evaluation of a marine environment. Fuzzy sets and their combination via the standard intersection, standard union and weighted average operations have been applied in these studies.

The data collected from Liverpool bay contained missing and outlying observations. For our type of data we found that 'missing' refers to 'undetectable' concen-

trations of a metal. The absence of metal values were replaced by the minimum level of a metal concentration detectable by the instrument used for trace metal analysis. In observational data analysis, the need to investigate subjective (e.g., human error, physical limitation of field equipment) and statistical evidence, for the existence of outliers, may be desired. Two statistical tests, Grubb's test and Chebyshev's inequality, were used based on whether the data sets approximated to normality or not. Stations which registered outliers were removed from the data sets since the reason behind these outlying observations could not be explained by the domain expert.

On a preliminary basis, a study on Liverpool bay and Morecambe bay was conducted on data sampled in 1988. An asymmetric left variant function was chosen as an appropriate function to present the concept of contamination with respect to increasing levels of metal concentrations. Thus seven fuzzy sets were defined across the set of sampling sites. Before the aggregation of these sets, to form an overall index of contamination, we introduce the necessary concepts from fuzzy set theory. Two methods for designing and generating n-place aggregation operators were suggested and applied to formulate a set of possible indices of contamination, called here "loading indices". Both methods relied on the associativity of the 2-place aggregation operator being extended. The minimum, maximum, and algebraic product were easily extended. The hamacher product, hamacher sum, bounded difference, bounded sum, and algebraic sum required more complicated algebraic manipulation. In addition to these eight, the arithmetic mean, competition jury, geometric mean, fuzzy integral, and weighted average were also used, three of which use external information in the form of weights. Finally, a graphical representation was constructed for all indices via MATLAB. The overall metal distribution from Morecambe bay supported the hypothesis that the region is not contaminated, unlike Liverpool bay which showed some signs of contamination. Aggregation operators of the hamacher product, hamacher sum, bounded difference, bounded sum, and algebraic sum did not produce feasible results, and hence were not used. Thus we use further eight

out of the thirteen formulated indices: *minimum, product, geometric mean, maximum, average, competition jury, fuzzy integral,* and *weighted average.* Some of these indices produced similar visual results. We decided to quantify the degree of similarity between the indices using similarity measures and discard indices showing similar information. Because of the variety in similarity measures, it was important to specify our requirements from a practical point of view. A similarity measure $\mathcal{S}_*$ based on symmetrical difference was introduced and tested against other similarity measures. The measure appeared to be suitable for our task. Finally, we applied $\mathcal{S}_*$ to both Liverpool bay and Morecambe bay, and then used two grouping methods hierarchical relational clustering and similarity tree. Using outcomes of the two approaches and also comparison by eye, the set of recurring groups of loading indices were finally chosen. Five distinct groups were found, {minimum, product, geometric mean}, {maximum}, {average}, {fuzzy integral}, and {weighted average}, from which we chose five index representatives: *Minimum*, *Maximum*, *Average*, *Fuzzy integral* and *Weighted average.*

A generic methodology for designing and selecting loading indices of contamination in a marine environment was produced. The availability of annually sampled data from Liverpool bay between the years of 1986 until 1992 inclusive, presented us with the opportunity to compare the change in metal loading distribution. We use a single representative index value $SRV_{LI}(u)$, calculated as the relative cardinality of the index LI_u to represent the distribution of overall metal contamination by that index for a given sampled year. Application of $SRV_{LI}(u)$ on the five representative indices yielded a general view on the annual fluctuation of metal contamination levels over seven years, from 1986 to 1992. Also, we partitioned the whole sampled region into two areas, clean and highly contaminated, and showed graphs of the temporal changes in these areas. Our analysis lead us to conclude that there is no evidence to support that the area of Liverpool bay during the period from 1986-1992 was not contaminated with heavy metal loading.

7.2 Discussion and recommendations

From an analyst point of view, we found that the collection of data can be improved. The following points are some recommendations in regards to future data collection (sampling).

1. The number of points sampled from one year to another should be similar. This would help to produce a clearer comparison for the distribution of specified environmental feature within a region between sampled years.

2. To assess contamination based on human inputs of substances from surrounding industries in a region, it would be best to coordinate data collection with the time these inputs are dumped. For instance, data collection can be organized to take place before and after dumping of inputs. The time of sampling should be assigned by a domain expert who has sufficient knowledge with regards to environmental changes and when these inputs are dumped.

3. A change in the distribution of contamination over time (on a monthly basis, within one year) can be carried out. Consistent sampling at specific time intervals should be done and logged accurately. This data can then be used in relation with other factors (e.g., tidal movement, dumping of inputs/time, $\cdots$etc.) to view the gradual change in overall contamination levels over time within one year.

These requirements are logical but not very straightforward to implement because

- The extent of the sampling programme depends largely on budgetary constrains.

- If the weather is poor during the sampling week then smaller number of samples can be taken. Operation in more than "Force 4" wind conditions is extremely hazardous.

It is essential, however, to estimate in the future analysis the time variability of the contamination pattern and its relationship with the dumping activities and the seasonal variation of the other inputs.

7.3 Summarized contributions

The contributions of the research can be summarized as follows

- Theory Part:

    1. Extending 2-place aggregation operators to n-place operators using associativity. (Chapter 4, Section 2)
    2. Definition of a new measure of similarity suitable for environmental data. (Chapter 5, Section 2)

- Application Part:

    3. Developing a general methodology for designing a collection of loading indices (*contamination indices*) using fuzzy aggregation for a marine environment, and for environmental data in general. (Chapter 5, Section 4)
    4. Analyzing the contamination of Liverpool bay and Morecambe bay regions using the proposed methodology. (Chapter 2 - Data preprocessing, Chapter 4, Section 4, and Chapter 5, Section 3)

- Impact to ecological sciences:

    1. We were able to bring fuzzy set theory to be used almost directly by the domain expert and provide a toolbox and a logical interpretation for the methods in it.
    2. Explicating the need for a standardized procedure for data collection and a more systematic approach, e.g., monitoring the type and significance of disposal activities and the time of taking the samples.

List of Publications related to the thesis:

1. L.I. Kuncheva and J. Wrench and L.C. Jain and A.S. Al-Zaidan. A fuzzy model of heavy metal loadings in Liverpool bay. *Environmental Modelling and Software*, 15(2):161–167, 2000.

2. A.S. Al-Zaidan. Constructing a loading index of heavy metals, based on c-means and fuzzy sets, in Liverpool bay. Master's thesis, University of Wales, Bangor, 1998.

3. A.S. Al-Zaidan and L.I. Kuncheva. Selecting fuzzy connectives to represent heavy metal distribution in Liverpool bay. KES2000 Conference proceedings, August 2000.

4. Da Ruan and Janusz Kacprzyk and Mario Fedrizzi (eds). *Soft computing for risk evaluation and management: Applications in technology, environment and finance*, volume 76:355-374 of *Studies in fuzziness and soft computing*. Physica-Verlag, 2001.

Letter of support:

The following question was asked of the domain expert. What do you think of this fuzzy set approach in dealing with and analyzing metal concentrations?
He answered as follows: 'Where there is multivariate data, I think that it provides a number of advantages':

1. It reduces a large data matrix to an easily understandable form.

2. The concept of loading index is directly relevant to ecological impact. In the case of Liverpool Bay sediments, for example, organisms in the surface sediments experience the combined effect of all metals; that is there is likely to be an additive effect which the loading index goes some way to summarize.

3. The frequency distribution of most metals is skewed towards higher values. Calculation of loading index tends to normalize the data (central limit the-

orem?) this allows standard parametric test to be applied. Again the approach simplifies the data handling making the output easier to interpret - especially compared to other methods such as principal component analysis and cluster analysis.

4. In many environmental data sets there are inevitable outlying values; such values arise from the fact that one cannot exert complete control over the system under investigation (compare Liverpool Bay with the very controlled nature of laboratory experiments). The use of loading indices introduces a robustness whereby the pattern generated from the data is not unduly affected by outliers. For example, the pattern of the 2000 data is not affected by inordinately high values of Cu at some stations.

5. The application of loading index produces realistic patterns which are easy to interpret. Comparison of the patterns for the 1988 and 2000 data by the domain expert, for example, showed a consistency with known events (reduction of sludge disposal) and correspond with the natural characteristics of Liverpool Bay.

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