Multi-criterion Water Quality Analysis of the Danube River in Serbia: A Visualisation Approach

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Abstract

17 River quality analysis is an important activity which, in Serbia, has been performed using the

18 Serbian Water Quality Index (SWQI). This is a measure based on a weighted aggregation of

19 10 water quality parameters. In this work, alternative methods drawing on visualisation

20 approaches used in multi-criterion decision analysis are applied to the problem of evaluating

21 river quality in the Danube. Two methods are considered: one which constructs a graph using

22 the dominance relation combined with a further multi-criterion ranking method, *average rank*,

23 and the other in which the dimensionality of the data is reduced using PCA for visualisation.

24 Results for data collected in 2010 are analysed and compared with the corresponding SWQI

25 values for the river in that year, and we find that by employing these methods it is possible to

26 reveal more information within the data than is possible by using SWQI alone.

1. Introduction

28 Water quality plays a vital role in all aspects of human and ecosystem survival. All living and

29 industrial activities are controlled by physical, chemical, biological and microbiological

30 activities (Mahapatra *et al.,* 2011; Vasiliev *et al.,* 2014). Anthropogenic influences and

31 natural processes degrade surface waters and impair their use for drinking, industry,

32 agriculture, recreation and other purposes (Sánchez *et al.,* 2007). In aquatic environments

33 organisms are exposed to mixtures of pollutants whose effects are hardly interpreted and

34 predicted exclusively from chemical analyses. Moreover, the analyses of pooled chemicals,

35 present at different compounds, increase uncertainty when evaluating water quality

36 (Monferrán *et al.,* 2011). Hence, analysing the quality of river water requires a range of

37 quality indicators, from which an overall measure of quality can be produced. Evaluation of

38 water quality parameters is necessary to plan and develop better water resource management

39 (Mahapatra *et al.,* 2011). To establish water quality criteria, measures of chemical and

41   physical constituents must be specified, as well as methods for reporting and comparing

42   results of water analysis (Saxena and Gangal, 2010). In order to evaluate water quality

43   synthetically, many techniques have been introduced to monitor and evaluate the effects of

44   pollution: traditional methods, modelling approaches, water quality indices (WQIs, e.g.

45   Armitage *et al.* (1983) and Prati *et al.* (1971)), multivariate statistical techniques, such as

46   principal component analyses (PCA), artificial neural networks, artificial intelligence, fuzzy

47   logic, as well as combinations of some of them (Ma *et al.,* 2013; Othman *et al.* 2012;

48   Monferrán *et al.* 2011; Taner *et al.,* 2011; Saxena and Gangal, 2010; Simões *et al.* 2008;

49   Nasirian, 2007). The work presented in this paper is distinct from these examples in that none

50   of them are based on multi-criterion visualisation techniques constructed in terms of the

51   water quality parameters on which WQIs are based.

52   *Multi-criterion decision making* (MCDM) is a process by which a set of options can be

53   assessed according to a set of criteria. MCDM is often applied in cases where the selection of

54   a single choice from a set of alternatives is required, and provides techniques for drawing

55   together information from all of the criteria so that a *decision maker* can make an appropriate

56   selection. Often the criteria are in conflict with each other, and selecting an option which

57   performs well against one criterion means accepting poor performance on another criterion.

58   A range of MCDM techniques exist, and in this work we are concerned with those in which

59   alternatives are *ranked*, providing an ordering of the alternatives so that the best one can be

60   readily identified through visualisation. Visualisation of alternatives allows the decision

61   maker to observe how they relate to each other, for example, making use of spatial

62   information gleaned from the placement of alternatives in the visualisation, to better

63   understand the nature of the alternatives from which they must choose (e.g., Walker *et al*,

64   2013).

65   In addition to selecting the best alternative, it can also be useful to identify the worst

66   alternatives. Engineers often undertake activities such as constructing maintenance schedules.

67   It is not usually feasible to maintain all of the components of an infrastructure, so those

68   components most urgently in need of maintenance must be identified so that they can be

69   prioritised in the schedule. This too is often formulated as a MCDM task, and one of the

70   visualisation methods used in this study has been applied in this area (for ranking district

71   metered areas in a water distribution network (McClymont *et al.*, 2011) and for analysing the

72   performance of the wireless access points in a mobile telephone network (Walker, 2013) for

73   the purpose of constructing maintenance timetables). MCDM techniques of this variety are

74   particularly well suited to river quality analysis as they allow engineers and scientists to

75   identify regions of the river that have particularly poor quality so that remedial action can be

76   taken.

77   In this work, we examine the quality of water in the Danube in Serbia. Due to its great

78   international importance, the Danube River has been the subject of numerous water quality

79   studies (Živadinović *et al.,* 2012; Micić *et al.,* 2011; Bird *et al.,* 2010; Kirschner *et al.,* 2009;

80   Micić and Hofmann, 2009; Maljević and Balać, 2007; Relić *et al.,* 2005).

81   Data was collected at a range of *stations*; in the MCDM context, these stations are the

82   alternatives, or *individuals*. A range of water quality parameters have been collected for each

83   of the stations at approximately monthly intervals for a year. These parameters are used as

84   criteria in order to compute the Serbian Water Quality Index (SWQI) which ranks stations

85   according to 10 criteria.

86   This paper presents an analysis of the water quality data using the criteria constructed under

87   the scheme. We use multi-criterion visualisation techniques, one based on methods for

88   ranking multi-criterion sets (Walker *et al.*, 2010) and the other employing principal

89   component analysis (Jolliffe, 2002). The visualisations are used to provide new insight into

90   the data, before which we discuss avenues of future work arising from this study.

91   2. Multi-criterion Visualisation

92   Visualisation is an active area of research within the MCDM community because of the

93   potential for revealing more about the characteristics of a multi-criterion dataset, or

94   *population* of individuals. Visualising a population of multi-criterion individuals is usually a

95   nontrivial task, since it is often the case that a large number of criteria must be incorporated

96   into the visualisation. In the case of a two or three dimensional population the task is

97   relatively straightforward: we must simply construct a scatter plot in two or three dimensions,

98   a visualisation approach with which most people are familiar and able to use. Unfortunately,

99   since most people are not able to comprehend four or more spatial dimensions visually, this is

100   not possible for populations comprising four or more criteria. It is therefore necessary to

101   develop techniques for visualising such populations, and one of two approaches can be taken:

102   either reduce the dimensionality of the population so that it can be visualised with a scatter

103   plot, or find a way of visualising all of the data in an intuitive fashion.

104   A range of methods have been developed for visualising a population in terms of the full set

105   of criteria. A considerable amount of work in visualising populations has been done in the

106   optimisation community; optimisation problems are often formulated in terms of a set of

107   problem objectives.

108   One of the early approaches developed was the *Pareto race* (Korhonen and Wallenius, 1988),

109   which enabled a decision maker to "drive" through the space of possible solutions to an

110   optimisation problem in order to steer an interactive optimisation procedure. More recently,

111   another method developed as part of an interactive optimisation framework was the *Pareto*

112   *navigator* (Eskelinen *et al.*, 2010).

113   Vilfredo Pareto defined the Pareto *dominance* relation; dominance is one of the most

114   frequently used methods for comparing multi-criterion individuals, and is used in MCDM so

115   that the relative quality of individuals can be considered without requiring a weighted

116   summation of their respective criterion values. The dominance relation will be formally

117   introduced shortly. Other techniques for visualising the complete criterion set are *heatmaps*

118   (Pryke *et al.*, 2006; Walker *et al.*, 2013), which represent individuals as the rows in a matrix,

119   criteria as the columns, and criterion values with colour (where "cool" colours indicate low

120   values and "warm" colours indicate high values). The alternative is to use a dimension

121   reduction method to identify a two or three dimensional representation of the individuals that

122   can be visualised with a scatter plot. Two varieties of dimension reduction can be used:

123   *feature selection* and *feature extraction*. In feature selection, the most representative features

124   are retained, and the remainder are discarded. In MCDM, this means finding the two or three

125   most important criteria; methods for doing this have been demonstrated (e.g. Saxena *et al.*,

126   2013). Under feature extraction, a completely new set of coordinates is identified which

127   represent the individuals. Common examples are PCA, which seeks to preserve as much of

128   the variance within the data as possible, and *multidimensional scaling* (MDS) which

129   preserves pairwise distances between individuals. MDS was recently used in combination

130   with a metric defined in terms of dominance to visualise multi-criterion populations (Walker

131   *et al.*, 2013). The application of other feature extraction techniques, *neuroscale* and

132   *generalised topographic mappings*, were examined by Fieldsend and Everson (2005), and

133   Obayashi (2002) demonstrated the use of *self-organising maps* for visualising criterion data.

134   Of particular relevance to this work are *interactive decision maps*, which have been used for

135   analysing river quality (Lotov *et al.*, 2004). Interactive decision maps are used to identify

136 *goal points*, regions of criterion space that are perceived to be of high quality. This is done by

137 allowing the decision maker to experiment with different combinations of criterion values to

138 find the most satisfactory trade-off possible. In their work, Lotov *et al.* (2004) present two

139 relevant analyses using interactive decision maps. The first tackles the problem of designing

140 wastewater treatment strategies that would enhance water quality, while the second optimises

141 the parameters of a water quality decision support system. Another relevant application of

142 multi-criterion visualisation was reported by Udias *et al.*, (2012) in which a watershed

143 management system was presented. Their visualisation was based on a combination of

144 interactive decision maps and 2-dimensional scatter plots. The scatter plots displayed the

145 overall quality in the ordinate axis and the monthly cost for each of four criteria in the

146 abscissa.

147 Each visualisation method has features that make them attractive for specific uses. For

148 example, heatmaps are useful because they incur no information loss and the original

149 criterion values can be recovered from the visualisation. Projection techniques, on the other

150 hand, incur information loss in that the original criterion values are discarded, however are

151 very useful for identifying spatial relationships in the data. In this work, in order to overcome

152 the shortcomings of existing approaches, we employ two methods. The first method uses

153 dominance and rank information to visualise the water quality stations in such a way that no

154 information is discarded. The second uses PCA to project the stations into two dimensions so

155 that they can be visualised using scatter plots, in order to compare the resulting spatial

156 arrangement with the dominance-based approach.

157 *2.1 Pareto Sorting Visualisation*

158 Ranking is an important component of MCDM framework, as well as in evolutionary

159 algorithms (EAs) used to solve multi-objective optimisation problems. The first method we

160   use draws on ranking methods from multi-objective EAs. One of the most common

161   approaches to ranking a population of multi-criterion individuals is *Pareto* or *non-dominated*

162   *sorting*, particularly well known for its use in the popular non-dominated sorting genetic

163   algorithm (*NSGA*) (Srinivas and Deb, 1994), and its successor *NSGA-II* (Deb *et al.*, 2002).

164   Non-dominated, or *Pareto* sorting is a technique that is based on the *dominance* relation.

165   Under dominance, an individual ***u*** *dominates* individual ***v*** if its criterion values u_m are no

166   worse than those of ***v***, and are better than ***v*** on at least one criterion. More formally:

167
$$u \prec v \Leftrightarrow \forall m(u_m \leq v_m) \wedge \exists m(u_m < v_m) \qquad (1)$$

168   If an individual exists such that it is dominated by no other individuals within the population,

169   it is called *non-dominating*. A pair of individuals where neither dominates the other are called

170   *mutually non-dominating*. Pareto sorting follows a simple procedure by which a partial

171   ordering of solutions is constructed. This begins by identifying all of the individuals in the

172   population that are non-dominated. Those individuals are the strongest, and are assigned to

173   the first Pareto *shell* before being temporarily discarded. The removal of shell 1 individuals

174   means that a new subset of the individuals in the population are non-dominated (those

175   previously dominated only by shell 1 individuals). These become the second Pareto shell, and

176   are themselves discarded from the population, leaving a third subset of non-dominated

177   individuals. This procedure continues until the entire population has been assigned to a Pareto

178   shell.

179   A visualisation method was presented in Walker *et al.* (2010) that uses dominance

180   information and the partial ordering resulting from Pareto sorting to construct a visualisation

181   of a population. The population is cast as a directed graph, such that individuals are nodes

182   arranged into columns according to their Pareto shell (each column represents a shell) and

183   edges are used to show dominance relations between individuals in adjacent shells.

184 ## *2.2 Average Rank*

185 The Pareto sorting visualisation furnishes us with a way of discriminating between

186 individuals in different Pareto shells, however it provides limited information about the

187 difference between individuals in the same shell. We therefore enhance the visualisation with

188 a complementary ranking method. Additionally, while dominance is capable of distinguishing

189 between individuals comprising a small number of criteria, it is known that individuals

190 comprising a large number of criteria (often called "many-objective" or "many-criterion"

191 individuals) are likely to be mutually non-dominating (Farina and Amato, 2003). As such,

192 various alternative schemes for ranking multi-criterion populations have been developed; one

193 of these methods is *average rank* (Bentley and Wakefield, 1998). In order to calculate the

194 average rank $\bar{r}_i$ of an individual y_i the population is ranked *M* times, once for each criterion.

195 This converts the population to *rank-coordinates*, such that each criterion is on the scale 1 to

196 *N*; the best individual has a score of 1, and the worst has a score of *N*. Then, an average of the

197 rank-coordinate values for the individual is taken:

198
$$\bar{r}_i = \frac{1}{M} \sum_{m=1}^{M} r_{im}$$
(2)

199 Other multi-criterion ranking methods can be employed instead of average rank; several were

200 demonstrated in Walker *et al.*, (2010), and were found to provide complementary rankings to

201 the partial ordering resulting from Pareto sorting. In fact, any colour scheme can be used. In

202 the next section, we also colour the nodes according to the classification of the stations under

203 SWQI.

204 ## *2.3 Principal Component Analysis*

205 A widely used visualisation method is Principal Component Analysis (PCA) (Jolliffe, 2002),

206 and we use it here to perform multi-criterion analyses. PCA is well suited to reducing the

207   dimensionality of multi-criterion individuals. It has, for example, been used to reduce the

208   dimensionality of populations of solutions in evolutionary algorithms (e.g., Deb and Saxena,

209   2005). In terms of water quality analysis, Astel *et al.* (2007), Kowalkowski *et al.* (1971) and

210   Vega *et al.* (1998) presented visualisations of water quality using PCA. Other studies have

211   used PCA for reasons other than visualisation, such as data clustering. Examples include

212   Koklu *et al.* (2010), Simeonov *et al.* (2003), Singh *et al.* (2004), Alberto *et al.* (2001) and

213   Zhang *et al.* (2010).

214   PCA projects data points into a low-dimensional space such that their new low-dimensional

215   representation retains as much of the variance contained within the original, high-dimensional,

216   data as possible. The low-dimensional space does not comprise any of the original criteria. In

217   the context of MCDM, each individual is a data point, and the original dimensions are the

218   criteria. Projecting the individuals into a low-dimensional space should therefore preserve as

219   much of the original variance within in the criteria, so that the most important information is

220   preserved. The principal components are identified by first computing the covariance matrix

221   of the data. Given the covariance matrix, the principal components are the eigenvectors

222   corresponding to the eigenvalues, which correspond to the original criteria, with largest

223   magnitude. In this study, as the goal is to produce a visualisation, the first two principal

224   components are retained. Having projected the individuals onto the first two principal

225   components, they can be visualised with a two-dimensional scatter plot.

226   ## 3. Case Study

227   We apply the methods described above to the analysis of water quality in the Serbian

228   stretches of the Danube; this region of the river is 588km long and constitutes 20.6% of the

229   total 2857km river (Fig 2a). Data is collected for eleven monitoring stations along the river,

230   shown in Fig. 2b. The available data is for 2010, and was collected at monthly intervals with

231   some exceptions. Number of measurements for each constituent was following: 1) Bezdan

232   station: 11 measurements for 8 constituents, 10 for Oxygen Saturation and BOD; 2) Bogojevo

233   station: 9 measurements for all constituents; 3) Bačka Palanka station: 8 measurements for all

234   constituents except 7 for BOD; 4) Novi Sad station: 12 measurements for all constituents; 5)

235   Slankamen station: 11 measurements for all constituents; 6) Čenta station: 11 measurements

236   for all constituents; 7) Smederevo station: 12 measurements for all constituents; 8) Banatska

237   Palanka station: 10 measurements for all constituents; 9) Veliko Gradište station: 12

238   measurements for all constituents; 10) Dobra station: 12 measurements for all constituents

239   except 11 for BOD; 11) Radujevac station; 12 measurements for all constituents. E. Coli

240   criterion is omitted from this study, because of small number of measurements in all stations.

241   Where a station was omitted from data collection, it is omitted from the results presented

242   herein. No attempt was made to impute missing values.

243   The parameters collected in the study (Jakovljević, 2012) are used to calculate the Serbian

244   Water Quality Index (SWQI). SWQI is an environmental indicator, developed by Serbian

245   Environmental Protection Agency and based on the Water Quality Index method (Scottish

246   Development Dept., 1976). SWQI uses ten quality parameters: oxygen saturation,

247   biochemical oxygen demand (BOD_5), ammonium, pH, total nitrogen oxides, orthophosphate,

248   suspended solids, temperature, conductivity and most probable number of coliform bacteria

249   (E. Coli/MPN). Each of these parameters has value q_i (the water quality of the i-th parameter)

250   and weight unit w_i (the weight attributed to the i-th parameter). Parameters have varying

251   degrees of importance on the overall water quality, specified by an appropriate weight (w_i)

252   where the sum of all weights is 1. By summarizing the products of all quality parameters (q_i)

253   and all weights (w_i) an index is created representing a weight sum of all parameters (q_i).

254   (Veljković, 2013; Veljković et al., 2010; Veljković et al., 2008). SWQI is then calculated as

255   the sum of $q_i \times w_i$. The maximum value of each parameter is shown in Table 1.

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263   **Table 1: SWQI parameters and their corresponding maximum** $q_i \times w_i$ **value (Veljković et al., 2010).**

Parameter (unit)	Maximum $q_i \times w_i$ value
Oxygen Saturation (%)	18
BOD$_5$ (mg/l)	15
Ammonium (mg/l)	12
pH	9
Total Nitrogen oxides (mg/l)	8
Orthophosphates (mg/l)	8
Suspended solids (mg/l)	7
Temperature (°C)	5
Conductivity (μS/cm)	6
E. Coli (MNP/100 ml)	12
$SWQI = \sum(q_i \times w_i)$	100

264

265   For each SWQI range a descriptive quality indicator has been defined ranging from very poor

266   (0–38), poor (39–71), good (72–83), very good (84–89), and excellent (90–100) (Veljković et

267   al., 2008). Parameter values are shown in Table 2.

268

269   **Table 2: Parameters concentration corresponding to** $q_i \times w_i$ (*Scottish Development Department, 1976*)

Water quality ($q_i \times w_i$)	Oxygen saturation (%)		BOD (mg/l)		Ammonium (mg/l,)		E.coli (coli/100ml)		Suspended solids (mg/l)
18	93-109		-		-		-		-
17	88-92	110-119	-	-	-		-		-
16	85-87	120-129	-	-	-		-		-
15	81-84	130-134	0	0.9	-		-		-
14	78-80	135-139	1.0	1.9	-		-		-
13	75-77	140-144	2.0	2.4	-		-		-
12	72-74	145-154	2.5	2.9	0	0.09	0	249	-
11	69-71	155-164	3.0	3.4	0.10	0.14	250	999	-
10	66-68	165-179	3.5	3.9	0.15	0.19	1000	3999	-
9	63-65	180 +	4.0	4.4	0.20	0.24	4000	7999	-
8	59-62	-	4.5	4.9	0.25	0.29	8000	14999	-
7	55-58	-	5.0	5.4	0.30	0.39	15000	24999	0-9
6	50-54	-	5.5	6.1	0.40	0.49	25000	44999	10-14
5	45-49	-	6.2	6.9	0.50	0.59	45000	79999	15-19
4	40-44	-	7.0	7.9	0.60	0.99	80000	139999	20-29
3	35-39	-	8.0	8.9	1.00	1.99	140000	249999	30-44
2	25-34	-	9.0	9.9	2.00	3.99	250000	429999	45-64
1	10-24	-	10.0	14.9	4.00	9.99	430000	749999	65-119
0	0-9		15.0+		10.00+		750000+		120+

270

Water quality ($q_i \times w_i$)	pH	Total nitrogen oxides (mg/l)	Orthophosphate (mg/l)	Conductivity (μS/cm)	Temperature (°C)
18	-	-	-	-	-
17	-	-	-	-	-
16	-	-	-	-	-
15	-	-	-	-	-

14	-		-		-		-		-
13	-		-		-		-		-
12	-		-		-		-		-
11	-		-		-		-		-
10	-		-		-		-		-
9	6.5-7.9		-		-		-		-
8	6.0-6.4	8.0-8.4	0	0.49	0	0.029	-		-
7	5.8-5.9	8.5-8.7	0.50	1.49	0.030	0.059	-		-
6	5.6-5.7	8.8-8.9	1.50	2.49	1.060	0.099	0-49	50-188	
5	5.4-5.5	9.0-9.1	2.50	3.49	0.100	0.129	189	190-239	0-17.4
4	5.2-5.3	9.2-9.4	3.50	4.49	0.130	0.179	240	289	17.5-19.4
3	5.0-5.1	9.5-9.9	4.50	5.49	0.180	0.219	290	379	19.5-21.4
2	4.5-4.9	10.0-10.4	5.50	6.99	0.220	0.279	380	539	21.5-22.9
1	3.5-4.4	10.5-11.4	7.00	9.99	0.280	0.369	540	839	23.0-24.9
0	0-34	11.5-14	10.00+		0.370+		810+		25+

271

According to the Regulation – Official Gazette 1978, all surface waters in Serbia are categorized in four classes (class I – best water quality). Parameters from Regulation were used as input parameters for SWQI calculation. Maximum Concentration Level (MCL) is defined for each of these classes; this is shown in Table 3. MCL values have been established by the Regulation 1978 and they have been constant. There were no their changes, as well as maximum $q_i \times w_i$ values have not changed during the time. This is an important for calculation of long term trends by SWQI method.

279

280 **Table 3: Correlation between SWQI and Maximum Concentration Level (MCL), *(Veljković et al., 2010).***

281 **Temperature and conductivity are omitted as they are not used in water quality characterisation using MCL.**

Parameter (unit)	Max $q_i \times w_i$ value	MCL Class I	MCL Class II	MCL Class III	MCL Class IV
Oxygen saturation (%)	18	90-105	70-90	50-75	30-50
			105-115	115-125	125-130
BOD (mg/l)	15	2	4	7	20
Ammonium (mg/l)	12	0.1	0.1	0.5	0.5
pH	9	6.8–8.5	6.8–8.5	6–9	6–9
Total Nitrogen Oxides (mg/l)	8	10	10	15	15
Orthophosphate (mg/l)	8	0.005	0.005	0.01	0.01
Suspended solids (mg/l)	7	10	30	80	100
Temperature (°C)	5	-	-	-	-
Conductivity (µS/cm)	6	-	-	-	-
E.coli (coli/100ml)	12	200	10000	20000	20000
$\sum(q_i \times w_i)$=WQI	100	85–84	69–71 74–71	44–48 56–52	35–36 51–46

4. Results

282

283 The two visualisation methods described above are now applied to the case study data. Due to

284 its absence in many cases, the E. Coli criterion is omitted from these results. The results

285 presented herein are based on the remaining 9 SWQI parameters. In all cases, the criteria

286 were arranged for minimisation, such that small criterion values are preferred to large ones

287 when stations are ranked. This is in some ways an arbitrary choice, but was made because in

288 a ranking of N items 1 is generally the best rank and N is the worst. The methods were

289 applied to all of the populations (one for each month that data was collected), and we begin

290 by illustrating the features of each visualisation.

4.1   Rank-based Visualisation

292 Figure 3 illustrates the population describing the water quality stations in February 2010. The

293 left-hand plot shows the data visualised as a Pareto shell graph. The stations sort into four

294 Pareto shells; the most powerful (best) station is Smederevo, which is in shell 1 and has the

295 best average rank (light colours indicates a good average rank; dark colours indicates a poor

296 average rank). Generally, the ordering of individuals according to Pareto sorting corresponds

297 to that average ranking; stronger individuals are on the left-hand side of the visualisation and

298 weaker individuals are on the right-hand side. This corresponds to the findings presented in

299 Walker *et al.*, (2010). That said, according to the Pareto sorting Veliko Gradište is the

300 weakest station, Bezdan (shell 2) has the worst average rank of any in the population. This

301 highlights a useful feature of the method first observed in Walker *et al.*, (2010), whereby it is

302 possible for an individual with an extremely poor average rank to be placed in a high Pareto

303 shell. In order for this to happen, the individual must have a very strong score on one of the

304 criteria, making it very hard for other individuals to dominate it; this means that the

305 individual is likely to be placed into a strong Pareto shell. If the remainder (and majority) of

306 the criterion values are extremely poor, the overall average rank for the individual will be

307 very poor. In fact, Bezdan has a very strong score on the BOD criterion, and poor scores on

308 the other eight criteria. By combining the two ranking methods we prevent stations from

309   being unduly rewarded for extreme criterion values, as was demonstrated by Walker *et al.*

310   (2010).

311   Figure 4 presents the visualisations shown in Figure 3, this time coloured according to the

312   quality rating assigned to each station using SWQI. With the exception of three stations

313   (Smederevo, Čenta and Radujevac) all are "good". Of the three that are not, two are "very

314   good" and one (Smederevo) is "excellent". This corresponds with the ranking induced by

315   average rank, under which the strongest station was Smederevo, followed by Radujevac and

316   Čenta. This is a useful result, as it shows that the average rank procedure allows for

317   comparison between individuals that were incomparable under the SWQI scheme without

318   conflicting with the partial ordering produced under SWQI. Average rank scores for the

319   stations throughout the year are shown in Table 4. Note, that these scores do not take account

320   of the absence of some stations from the data in some months, which causes artificially low

321   average rank scores (this is particularly prevalent in December, where the measurement of

322   just five stations results in a maximum average rank of 5). Figure 6 presents the distribution

323   of average ranks graphically; in order to facilitate comparison of stations, the average rank

324   values shown in Table 4 have been ranked, placing them on the scale 1, ..., N (for N stations

325   in a given month) and then normalised to the range (0, 1).

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330   **Table 4: Monthly average rank scores for water quality stations.**

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Bačka Palanka	-	-	11	9	8	11	3	4	6.5	10	-	-
Banatska Palanka	7.5	5	10	5	6	7	-	10	8	8	10	1
Bezdan	4.5	9	3	10	10	5	6	7	6.5	11	2	-
Bogojevo	-	-	5	3	7	4	2	6	1	7	8	-
Čenta	7.5	3.5	5	8	9	10	5	3	3	5	5.5	-
Dobra	4.5	7	1	4	4	3	8	8	10	1	3.5	2.5
Novi Sad	9	6	5	11	11	6	8	9	5	3	3.5	5
Radujevac	2	2	9	2	3	2	8	1	2	9	1	4
Slankamen	3	3.5	8	6.5	5	8.5	10	2	4	5	5.5	-
Smederevo	1	1	7	1	1	8.5	1	5	11	5	7	-
Veliko Gradište	6	8	2	6.5	2	1	4	11	9	2	9	2.5

331

332   Radujevac had the highest quality according to Pareto sorting. It achieved rank 1 on nine

333   occasions and rank 2 twice. One of these two occasions was February, in which it was

334   dominated by Smederevo. Radujevac in turn dominated Dobra and Veliko Gradište. The

335   SWQI values for these four stations agree with the ordering according to dominance:

336   Smederevo is rated excellent, Radujevac is very good, while Dobra and Veliko Gradište are

337   rated good. The parameter that causes this relationship is BOD. In the case of Smederevo, the

338   BOD result was 2mg/l (14 according to SWQI and class I according to the maximum

339   concentration level (MCL)). Radujevac had BOD of 2.8mg/l (12 according to SWQI, class II

340   MCL), while Dobra and Veliko Gradište measured 4.8mg/l (8 under SWQI and class III

341   MCL) and 5.3 mg/l (7 under SWQI, class III MCL). The average rank results support this

342   ordering too: Smederevo and Radujevac are the best two individuals in the population, while

343   Dobra and Veliko Gradište are two of the worst. This agreement between the Pareto sorting

344   method and well understood measures such as SWQI and MCL is reassuring, as it provides a

345   simple approach to visualising the relationship between stations in a context with which

346   engineers and scientists are familiar. This, when combined with its ability to compare stations

347   without requiring WQIs to be weighted, illustrates the potential of the visualisation method

348   for analysing multi-criterion water quality data. That said, if weights are available, as is the

349   case here, then they can be incorporated via the colouring approach taken (e.g., there is an

350   optional provision for incorporating weights into average rank).

351   The other occasion in which Radujevac was dominated was October, when it was dominated

352   by Veliko Gradište. Both stations were rated very good under SWQI, however Veliko

353   Gradište's Ammonium value was better than that of Radujevac (0.05mg/l, or 12 according to

354   SWQI and MCL class I-II, in the case of Veliko Gradište; 0.19mg/l, or 10 under SWQI and

355   MCL class III-IV in the case of Radujevac). Interestingly, however, Radujevac has a poor

356   average rank. This, in concert with the fact that Radujevac does not dominate anything in the

357   next shell, indicates overall poor quality. By observing the average rank results for the rest of

358   the year we can see that its performance according to average rank was poor in five months.

359   In three of these cases, March, July and December, its SWQI rating is good, the worst

360   classification assigned to a station in those months. That said, when considering the

361 distribution of normalised ranks in Figure 6, Radujevac has the best overall quality according

362 to average rank. While it might be tempting to interpret Smederevo as the best station (it

363 achieves rank 1 in five months, more than any other station) its ranking in some months is

364 particularly poor. Radujevac, on the other hand, has more consistent performance. It appears

365 in the top three positions in the ranking in all but four months of the year.

366 One of the important utilities of this type of analysis is that hydrologists can use them to

367 observe stations with low quality, so that efforts can be made to improve river quality at those

368 locations. Two stations with poor performance under Pareto sorting were Veliko Gradište and

369 Bogojevo. Veliko Gradište was in rank 1 on 8 occasions, rank 2 twice, and on one occasion

370 was the sole member of rank 4. Though it achieved a good rank in some of the months, its

371 lower rank on other occasions reduced its overall quality. On the occasion it appeared in rank

372 4, it had one of the lowest average ranks for that month (February). Bogojevo was in rank 1

373 on 7 occasions, rank 2 twice and rank 4 once. Bačka Palanka also achieved poor results.

374 Though it was in rank 1 on 5 occasions, there was also a month in which it appeared in ranks

375 2, 3 and 4, respectively. This corresponds to relatively low quality SWQI results. It was

376 predominantly classified "good" under SWQI, and was classified "very good" just once; most

377 of the other stations achieved a "very good" classification multiple times. In June it was

378 classified "poor", the worst possible classification under SWQI. Novi Sad was the worst

379 station according to Pareto sorting. It appeared in rank 1 only once, and was mainly placed

380 into rank 2. It was also placed into ranks 3 and 4 on one occasion each.

381 Beyond analysing the relative performance of individual months, considering the

382 visualisations for the year as a whole also offers useful insight. Under SWQI, the months

383 with lowest water quality are the summer months, June to September, inclusive. June is the

384 only month in which stations were classified "poor", and both July and August are entirely

385 comprised of "good" classifications, with no station achieving "very good" or "excellent".

386   Examining the Pareto shell visualisations for these months shows that they are also the

387   months in which the overall structure of the dominance graph is flattest. Figure 7 shows the

388   distribution of values throughout the year for the temperature and oxygen saturation

389   parameters. As can be seen, there is a significant peak in the values for the summer months,

390   which implies that these parameters have significant influence on the overall structure of the

391   population; we can infer a large degree of conflict between these parameters and one of the

392   other parameters, as the increased temperature appears to cause the stations in the data to

393   become mutually non-dominating. In order to properly evaluate this result it would be

394   necessary to collect data over a number of years, and currently this data is unavailable.

395   ### *4.2   PCA Visualisation*

396   We also applied PCA to the data, in order to produce two dimensional scatterplots of the data.

397   In this work we did not consider the data a time series; rather, each month was treated as its

398   own case, unrelated to the other data. One of the potential difficulties with using PCA is that

399   a loss of information is incurred. The data was projected onto the first two principal

400   components, which, as explained earlier, represent the stations in a new coordinate space that

401   may be, but is not necessarily, correlated with the original criterion values. Inspection of the

402   eigenvalues indicates in all cases between 89 and 99% of the variance in the data was

403   contained in the first two eigenvectors. This means that the majority of the information in the

404   data has been retained for all 12 months.

405   As with the Pareto sorting visualisations, the data is presented in terms of both average rank

406   and SWQI classification. The lower panel of Figure 3 illustrates the PCA projection of the

407   data for February, and examining the clustering reveals an interesting result. The data can be

408   broadly grouped into four clusters. The first cluster contains four stations: Čenta, Slankamen,

409   Bezdan and Novi Sad. Examining the Pareto shell visualisation of February (Figure 2) shows

410   that these four stations form a cluster in terms of their dominance relations too. Slankamen

411   and Čenta are Pareto optimal, and both Bezdan and Novi Sad are dominated by Čenta.

412   Bezdan is also dominated by Čenta. The second cluster includes Radujevac, Banatska

413   Palanka and Smederevo. Smederevo is Pareto optimal, and dominates both Radujevac and

414   Banatska Palanka. The final two clusters contains the final two stations, Dobra (in a shell of

415   its own and dominated only by Radujevac) and Veliko Gradište (dominated only by Dobra,

416   again the sole member of its shell). This is an interesting result, as it shows potential for

417   revealing spatial coherence in the data using PCA even with such small datasets. Figure 8

418   shows examples for other months, and this effect is again seen in October. In that case,

419   Bezdan is the station with the worst quality and is placed far away from the main grouping of

420   stations.

421   Further insight into the data for August is possible using this technique. As can be seen in the

422   average rank case the stations have been arranged such that those with a poor average rank

423   are together and those with a strong average rank are further away. In the extreme, Radujevac

424   is placed away from the main cluster of stations; it has the best average rank for that month

425   and in the Pareto sorting example is Pareto optimal but dominates nothing in the subsequent

426   shell.

427   While it is possible to observe relative quality between individuals using the Pareto shell and

428   PCA visualisations, the actual WQI values of the stations are either not conveyed, in the case

429   of the Pareto shell visualisation, or discarded, in the case of PCA. Having provided this

430   information, we enhance their decision making potential by producing corresponding parallel

431   coordinate plots (Inselberg, 2009). The examples shown in Figure 9 are for February (which

432   corresponds to the results shown in Figure 4) and May. Each line represents a station, and is

433   coloured according to its SWQI score for that month (NB: stations achieving a SWQI score

434   of "excellent" are in this case represented with a dashed line, rather than colouring with

435   white). It can be seen that the station with excellent SWQI is generally at the lowest point of

436   the graph, indicating its superiority. It is, however, difficult to infer the overall quality of a

437   station from these visualisations alone, and thus we recommend that they are used in

438   combination with the Pareto shell or PCA visualisations.

439   As previously mentioned, the station with the best water quality was Radujevac. This was

440   caused by better quality of specific parameters comparing with other stations. The other

441   station with the high water quality was Smederevo, which was caused by high average water

442   quality. At the other hand the station with the worst water quality was Novi Sad, because of

443   low average water quality and Bačka Palanka due to bad quality of specific parameters.

444   Considering the location of these stations, this suggests that downstream stations had a better

445   water quality than upstream ones. This can be explained by high selfpurification of the

446   Danube River, which enabled reduction of organic loading. The other unexpected outcome

447   was the best water quality in the June according to the Pareto sorting visualisation, which was

448   the month with the worst water quality according to the SWQI. The explanation is in the fact

449   that due to the impairment of water quality in all stations and in most parameters, there was

450   no possibility that the stations dominated each other, except in one case. This produced the

451   result that the stations with the worst water quality were in the Rank 1. The parameter which

452   caused the water quality decline was Oxygen saturation with the following values: 34%

453   (Bačka Palanka), 52% (Banatska Palanka), 59% (Čenta) and 64% (Slankamen). Due to this

454   parameter all these stations had poor water quality according to the SWQI as well as III class

455   (Banatska Palanka, Čenta and Slankamen) and IV class (Bačka Palanka). This case is very

456   important in terms of environmental conditions, because low Oxygen saturation values can

457   threaten life of aquatic organisms.

5. Conclusions

458

459 Analysing river quality is an important task for environmental scientists and engineers. Given

460 the range of available criteria according to which river quality can be measured, multi-

461 criterion visualisation is a natural candidate for presenting the information. This work has

462 illustrated the application of such methods to the analysis of water quality in the Serbian

463 stretches of the Danube in 2010.

464 One of the methods employed multi-criterion ranking methods; the first used Pareto sorting,

465 based on the dominance relation, to produce a partial ordering of water quality stations on

466 which a directed graph can be constructed. This graph was shown to produce comparable

467 results to those achieved using SWQI, which is a well-known measure of river quality used in

468 Serbia. Additional information can be included in the visualisation by illustrating the average

469 rank of each station with the colour of its corresponding node in the graph. This also revealed

470 additional information, such as identifying stations with poor quality that had been unduly

471 promoted to a high rank by the Pareto sorting procedure. Examining the average rank of

472 stations provides a useful insight into the overall quality of a station; for example, by

473 inspection it was clear that Radujevac was the station with highest quality in the data used for

474 this study. Principal component analysis provided some additional insight into the data,

475 however it is likely to be more useful in cases where larger numbers of stations are employed.

476 We note that while in some applications using PCA can cause unacceptable levels of

477 information loss, in this case the vast majority of variance in the data was retained in the two

478 principal eigenvalues (89% in the worst case). Using PCA in combination with the Pareto

479 shell visualisations facilitated further insight into the data, as well as the identification of

480 facets of the data that appeared in both visualisations. We plan to extend the use of PCA in

481 this area by considering the criteria as a time series, which we feel will provide further

482 information to the decision maker given the temporal nature of the data.

483   The analyses described in this work have considered each visualisation a description of the

484   river at a specific point in time. Relationships between stations were described in that context,

485   as well as in the context of their results throughout the year. The criteria on which the

486   visualisations are based do not take account of any temporal variation in the parameter values,

487   however the results discussed clearly show that there is a seasonal aspect to them. The rise in

488   temperature and oxygen saturation levels in the summer months demonstrate this. Therefore,

489   beyond the demonstration that the techniques illustrated in this study can provide useful

490   information about river quality, a useful direction of future work would involve incorporating

491   this temporal or seasonal variation into the visualisation. One possibility that is currently

492   under investigation would be to construct additional criteria so that the historical quality of

493   river water can be understood, and issues regarding the sensitivity of the data can be

494   addressed.

495   Water quality has traditionally been assessed in terms of complex variable–by–variable and

496   water body–by–water body summaries. This type of information is of value to water quality

497   experts, but needs to be improved for users who want to know about the state of their local

498   water bodies and for managers and decision makers who require concise information about

499   those water bodies. Water quality index methodologies partially overcome the shortcomings

500   of these methods, and provide the ability to describe water quality with a single value based

501   on arrange of indicators and measurements. This facilitates simple communication of water

502   quality results to interested parties. Disadvantages of such methods include the sensitivity of

503   the results to the formulation of the index and the loss of potentially important interactions

504   between variables. By using the multi-criterion visualisation approaches proposed in this

505   paper, some of these disadvantages can be ameliorated.

506   The Pareto shell visualisation is advantageous in the visualisation of data of this type. It does

507   not require any dimension reduction, presenting the decision maker with a visualisation based

508   on all available data, and does not require the *a priori* selection of importance weights for the

509   criteria (although they can be incorporated into the secondary ranking method used to colour

510   the nodes in the graph if they are available). The method is generally very scalable, and can

511   be combined with well known domain-specific techniques, as was done with SWQI in this

512   paper. That it does not visually represent specific criterion values might be seen as a

513   limitation, however we feel that this is easily addressed by combining it with a separate

514   visualisation, such as the parallel coordinate plots demonstrated in this work. PCA is a

515   suitable choice as it relies on spatial proximity to convey similarity, which decision makers

516   can generally comprehend easily. The obvious limitation with this method is that it discards

517   potentially important information, however it was demonstrated here that the amount of

518   information lost was minimal.

519   Many studies have applied multi criterion decision making to conduct sustainability

520   assessment (Cinelli et al, 2014) in environmental and human health risk assessment (Topuz *et*

521   *al.,* 2011), to assess habitats and wildlife (Cortina and Boggia, 2014), in the case of urban

522   water strategies (Moglia *et al*, 2012) and water supply infrastructure planning and

523   rehabilitation (Scholten *et al.*, 2015; Schoelten *et al.*, 2014) in order to support decision

524   makers, in agricultural systems according to the decision-makers' expectations (Carof *et al.*

525   2012)*,* in the risk assessment of contaminated ground water (Khadam *et al.*, 2003).

526   Techniques presented in this paper could also help decision makers to determine the best and

527   worst quality sites, as well as to determine how these water quality estimation tools relate to

528   land characteristics management choices, urban versus rural designations etc. Ravier et al.,

529   (2015) have used PCA for water quality preservation programme. Pareto optimal set was

530   used in different land uses, crops, pastures, forestry and soil water conservation practices at

531   the basin scale in the Pampas in Argentina (Cisneros *et al.*, 2011), minimising probable flood

532   damages and maximizing water demand supply (Malekmohammadi et al., 2011) as well as

533 Pareto frontier visualisation in support of decision makers in rehabilitation of water quality in

534 Googong Reservoir in Australia (Castelletti *et al.*, 2010). It can be inferred that these water

535 quality estimation techniques have already played important role as support in the process of

536 decision making and their importance will be increase in a future.

6. Acknowledgement

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1   # Multi-criterion Water Quality Analysis of the Danube

2   # River in Serbia: A Visualisation Approach

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Abstract

18 River quality analysis is an important activity which, in Serbia, has been performed using the

19 Serbian Water Quality Index (SWQI). This is a measure based on a weighted aggregation of

20 10 water quality parameters. In this work, alternative methods drawing on visualisation

21 approaches used in multi-criterion decision analysis are applied to the problem of evaluating

22 river quality in the Danube. Two methods are considered: one which constructs a graph using

23 the dominance relation combined with a further multi-criterion ranking method, *average rank*,

24 and the other in which the dimensionality of the data is reduced using PCA for visualisation.

25 Results for data collected in 2010 are analysed and compared with the corresponding SWQI

26 values for the river in that year, and we find that by employing these methods it is possible to

27 reveal more information within the data than is possible by using SWQI alone.

1. Introduction

29 Water quality plays a vital role in all aspects of human and ecosystem survival. All living and

30 industrial activities are controlled by physical, chemical, biological and microbiological

31 activities (Mahapatra *et al.,* 2011; Vasiliev *et al.,* 2014). Anthropogenic influences and

32 natural processes degrade surface waters and impair their use for drinking, industry,

33 agriculture, recreation and other purposes (Sánchez *et al.,* 2007). In aquatic environments

34 organisms are exposed to mixtures of pollutants whose effects are hardly interpreted and

35 predicted exclusively from chemical analyses. Moreover, the analyses of pooled chemicals,

36 present at different compounds, increase uncertainty when evaluating water quality

37 (Monferrán *et al.,* 2011). Hence, analysing the quality of river water requires a range of

38 quality indicators, from which an overall measure of quality can be produced. Evaluation of

39 water quality parameters is necessary to plan and develop better water resource management

40 (Mahapatra *et al.,* 2011). To establish water quality criteria, measures of chemical and

41   physical constituents must be specified, as well as methods for reporting and comparing

42   results of water analysis (Saxena and Gangal, 2010). In order to evaluate water quality

43   synthetically, many techniques have been introduced to monitor and evaluate the effects of

44   pollution: traditional methods, modelling approaches, water quality indices (WQIs, e.g.

45   Armitage *et al.* (1983) and Prati *et al.* (1971)), multivariate statistical techniques, such as

46   principal component analyses (PCA), artificial neural networks, artificial intelligence, fuzzy

47   logic, as well as combinations of some of them (Ma *et al.,* 2013; Othman *et al.* 2012;

48   Monferrán *et al.* 2011; Taner *et al.,* 2011; Saxena and Gangal, 2010; Simões *et al.* 2008;

49   Nasirian, 2007). The work presented in this paper is distinct from these examples in that none

50   of them are based on multi-criterion visualisation techniques constructed in terms of the

51   water quality parameters on which WQIs are based.

52   *Multi-criterion decision making* (MCDM) is a process by which a set of options can be

53   assessed according to a set of criteria. MCDM is often applied in cases where the selection of

54   a single choice from a set of alternatives is required, and provides techniques for drawing

55   together information from all of the criteria so that a *decision maker* can make an appropriate

56   selection. Often the criteria are in conflict with each other, and selecting an option which

57   performs well against one criterion means accepting poor performance on another criterion.

58   A range of MCDM techniques exist, and in this work we are concerned with those in which

59   alternatives are *ranked*, providing an ordering of the alternatives so that the best one can be

60   readily identified through visualisation. Visualisation of alternatives allows the decision

61   maker to observe how they relate to each other, for example, making use of spatial

62   information gleaned from the placement of alternatives in the visualisation, to better

63   understand the nature of the alternatives from which they must choose (e.g., Walker *et al*,

64   2013).

65   In addition to selecting the best alternative, it can also be useful to identify the worst

66   alternatives. Engineers often undertake activities such as constructing maintenance schedules.

67   It is not usually feasible to maintain all of the components of an infrastructure, so those

68   components most urgently in need of maintenance must be identified so that they can be

69   prioritised in the schedule. This too is often formulated as a MCDM task, and one of the

70   visualisation methods used in this study has been applied in this area (for ranking district

71   metered areas in a water distribution network (McClymont *et al.*, 2011) and for analysing the

72   performance of the wireless access points in a mobile telephone network (Walker, 2013) for

73   the purpose of constructing maintenance timetables). MCDM techniques of this variety are

74   particularly well suited to river quality analysis as they allow engineers and scientists to

75   identify regions of the river that have particularly poor quality so that remedial action can be

76   taken.

77   In this work, we examine the quality of water in the Danube in Serbia. Due to its great

78   international importance, the Danube River has been the subject of numerous water quality

79   studies (Živadinović *et al.,* 2012; Micić *et al.,* 2011; Bird *et al.,* 2010; Kirschner *et al.,* 2009;

80   Micić and Hofmann, 2009; Maljević and Balać, 2007; Relić *et al.,* 2005).

81   Data was collected at a range of *stations*; in the MCDM context, these stations are the

82   alternatives, or *individuals*. A range of water quality parameters have been collected for each

83   of the stations at approximately monthly intervals for a year. These parameters are used as

84   criteria in order to compute the Serbian Water Quality Index (SWQI) which ranks stations

85   according to 10 criteria.

86   This paper presents an analysis of the water quality data using the criteria constructed under

87   the scheme. We use multi-criterion visualisation techniques, one based on methods for

88   ranking multi-criterion sets (Walker *et al.*, 2010) and the other employing principal

89   component analysis (Jolliffe, 2002). The visualisations are used to provide new insight into

90   the data, before which we discuss avenues of future work arising from this study.

2. Multi-criterion Visualisation

92   Visualisation is an active area of research within the MCDM community because of the

93   potential for revealing more about the characteristics of a multi-criterion dataset, or

94   *population* of individuals. Visualising a population of multi-criterion individuals is usually a

95   nontrivial task, since it is often the case that a large number of criteria must be incorporated

96   into the visualisation. In the case of a two or three dimensional population the task is

97   relatively straightforward: we must simply construct a scatter plot in two or three dimensions,

98   a visualisation approach with which most people are familiar and able to use. Unfortunately,

99   since most people are not able to comprehend four or more spatial dimensions visually, this is

100   not possible for populations comprising four or more criteria. It is therefore necessary to

101   develop techniques for visualising such populations, and one of two approaches can be taken:

102   either reduce the dimensionality of the population so that it can be visualised with a scatter

103   plot, or find a way of visualising all of the data in an intuitive fashion.

104   A range of methods have been developed for visualising a population in terms of the full set

105   of criteria. A considerable amount of work in visualising populations has been done in the

106   optimisation community; optimisation problems are often formulated in terms of a set of

107   problem objectives.

108   One of the early approaches developed was the *Pareto race* (Korhonen and Wallenius, 1988),

109   which enabled a decision maker to "drive" through the space of possible solutions to an

110   optimisation problem in order to steer an interactive optimisation procedure. More recently,

111   another method developed as part of an interactive optimisation framework was the *Pareto*

112   *navigator* (Eskelinen *et al.*, 2010).

113   Vilfredo Pareto defined the Pareto *dominance* relation; dominance is one of the most

114   frequently used methods for comparing multi-criterion individuals, and is used in MCDM so

115   that the relative quality of individuals can be considered without requiring a weighted

116   summation of their respective criterion values. The dominance relation will be formally

117   introduced shortly. Other techniques for visualising the complete criterion set are *heatmaps*

118   (Pryke *et al.*, 2006; Walker *et al.*, 2013), which represent individuals as the rows in a matrix,

119   criteria as the columns, and criterion values with colour (where "cool" colours indicate low

120   values and "warm" colours indicate high values). The alternative is to use a dimension

121   reduction method to identify a two or three dimensional representation of the individuals that

122   can be visualised with a scatter plot. Two varieties of dimension reduction can be used:

123   *feature selection* and *feature extraction*. In feature selection, the most representative features

124   are retained, and the remainder are discarded. In MCDM, this means finding the two or three

125   most important criteria; methods for doing this have been demonstrated (e.g. Saxena *et al.*,

126   2013). Under feature extraction, a completely new set of coordinates is identified which

127   represent the individuals. Common examples are PCA, which seeks to preserve as much of

128   the variance within the data as possible, and *multidimensional scaling* (MDS) which

129   preserves pairwise distances between individuals. MDS was recently used in combination

130   with a metric defined in terms of dominance to visualise multi-criterion populations (Walker

131   *et al.*, 2013). The application of other feature extraction techniques, *neuroscale* and

132   *generalised topographic mappings*, were examined by Fieldsend and Everson (2005), and

133   Obayashi (2002) demonstrated the use of *self-organising maps* for visualising criterion data.

134   Of particular relevance to this work are *interactive decision maps*, which have been used for

135   analysing river quality (Lotov *et al.*, 2004). Interactive decision maps are used to identify

136   *goal points*, regions of criterion space that are perceived to be of high quality. This is done by

137   allowing the decision maker to experiment with different combinations of criterion values to

138   find the most satisfactory trade-off possible. In their work, Lotov *et al.* (2004) present two

139   relevant analyses using interactive decision maps. The first tackles the problem of designing

140   wastewater treatment strategies that would enhance water quality, while the second optimises

141   the parameters of a water quality decision support system. Another relevant application of

142   multi-criterion visualisation was reported by Udias *et al.*, (2012) in which a watershed

143   management system was presented. Their visualisation was based on a combination of

144   interactive decision maps and 2-dimensional scatter plots. The scatter plots displayed the

145   overall quality in the ordinate axis and the monthly cost for each of four criteria in the

146   abscissa.

147   Each visualisation method has features that make them attractive for specific uses. For

148   example, heatmaps are useful because they incur no information loss and the original

149   criterion values can be recovered from the visualisation. Projection techniques, on the other

150   hand, incur information loss in that the original criterion values are discarded, however are

151   very useful for identifying spatial relationships in the data. In this work, in order to overcome

152   the shortcomings of existing approaches, we employ two methods. The first method uses

153   dominance and rank information to visualise the water quality stations in such a way that no

154   information is discarded. The second uses PCA to project the stations into two dimensions so

155   that they can be visualised using scatter plots, in order to compare the resulting spatial

156   arrangement with the dominance-based approach.

157   ### 2.1 Pareto Sorting Visualisation

158   Ranking is an important component of MCDM framework, as well as in evolutionary

159   algorithms (EAs) used to solve multi-objective optimisation problems. The first method we

160   use draws on ranking methods from multi-objective EAs. One of the most common

161   approaches to ranking a population of multi-criterion individuals is *Pareto* or *non-dominated*

162   *sorting*, particularly well known for its use in the popular non-dominated sorting genetic

163   algorithm (*NSGA*) (Srinivas and Deb, 1994), and its successor *NSGA-II* (Deb *et al.*, 2002).

164   Non-dominated, or *Pareto* sorting is a technique that is based on the *dominance* relation.

165   Under dominance, an individual $\boldsymbol{u}$ *dominates* individual $\boldsymbol{v}$ if its criterion values u_m are no

166   worse than those of $\boldsymbol{v}$, and are better than $\boldsymbol{v}$ on at least one criterion. More formally:

167    $$u \prec v \Leftrightarrow \forall m(u_m \leq v_m) \land \exists m(u_m < v_m) \qquad (1)$$

168   If an individual exists such that it is dominated by no other individuals within the population,

169   it is called *non-dominating*. A pair of individuals where neither dominates the other are called

170   *mutually non-dominating*. Pareto sorting follows a simple procedure by which a partial

171   ordering of solutions is constructed. This begins by identifying all of the individuals in the

172   population that are non-dominated. Those individuals are the strongest, and are assigned to

173   the first Pareto *shell* before being temporarily discarded. The removal of shell 1 individuals

174   means that a new subset of the individuals in the population are non-dominated (those

175   previously dominated only by shell 1 individuals). These become the second Pareto shell, and

176   are themselves discarded from the population, leaving a third subset of non-dominated

177   individuals. This procedure continues until the entire population has been assigned to a Pareto

178   shell.

179   A visualisation method was presented in Walker *et al.* (2010) that uses dominance

180   information and the partial ordering resulting from Pareto sorting to construct a visualisation

181   of a population. The population is cast as a directed graph, such that individuals are nodes

182   arranged into columns according to their Pareto shell (each column represents a shell) and

183   edges are used to show dominance relations between individuals in adjacent shells.

184 *2.2 Average Rank*

185 The Pareto sorting visualisation furnishes us with a way of discriminating between

186 individuals in different Pareto shells, however it provides limited information about the

187 difference between individuals in the same shell. We therefore enhance the visualisation with

188 a complementary ranking method. Additionally, while dominance is capable of distinguishing

189 between individuals comprising a small number of criteria, it is known that individuals

190 comprising a large number of criteria (often called "many-objective" or "many-criterion"

191 individuals) are likely to be mutually non-dominating (Farina and Amato, 2003). As such,

192 various alternative schemes for ranking multi-criterion populations have been developed; one

193 of these methods is *average rank* (Bentley and Wakefield, 1998). In order to calculate the

194 average rank $\bar{r}_i$ of an individual $\boldsymbol{y_i}$ the population is ranked M times, once for each criterion.

195 This converts the population to *rank-coordinates*, such that each criterion is on the scale 1 to

196 N; the best individual has a score of 1, and the worst has a score of N. Then, an average of the

197 rank-coordinate values for the individual is taken:

198
$$\bar{r}_i = \frac{1}{M} \sum_{m=1}^{M} r_{im} \tag{2}$$

199 Other multi-criterion ranking methods can be employed instead of average rank; several were

200 demonstrated in Walker *et al.*, (2010), and were found to provide complementary rankings to

201 the partial ordering resulting from Pareto sorting. In fact, any colour scheme can be used. In

202 the next section, we also colour the nodes according to the classification of the stations under

203 SWQI.

204 *2.3 Principal Component Analysis*

205 A widely used visualisation method is Principal Component Analysis (PCA) (Jolliffe, 2002),

206 and we use it here to perform multi-criterion analyses. PCA is well suited to reducing the

207 dimensionality of multi-criterion individuals. It has, for example, been used to reduce the

208 dimensionality of populations of solutions in evolutionary algorithms (e.g., Deb and Saxena,

209 2005). In terms of water quality analysis, Astel *et al.* (2007), Kowalkowski *et al.* (1971) and

210 Vega *et al.* (1998) presented visualisations of water quality using PCA. Other studies have

211 used PCA for reasons other than visualisation, such as data clustering. Examples include

212 Koklu *et al.* (2010), Simeonov *et al.* (2003), Singh *et al.* (2004), Alberto *et al.* (2001) and

213 Zhang *et al.* (2010).

214 PCA projects data points into a low-dimensional space such that their new low-dimensional

215 representation retains as much of the variance contained within the original, high-dimensional,

216 data as possible. The low-dimensional space does not comprise any of the original criteria. In

217 the context of MCDM, each individual is a data point, and the original dimensions are the

218 criteria. Projecting the individuals into a low-dimensional space should therefore preserve as

219 much of the original variance within in the criteria, so that the most important information is

220 preserved. The principal components are identified by first computing the covariance matrix

221 of the data. Given the covariance matrix, the principal components are the eigenvectors

222 corresponding to the eigenvalues, which correspond to the original criteria, with largest

223 magnitude. In this study, as the goal is to produce a visualisation, the first two principal

224 components are retained. Having projected the individuals onto the first two principal

225 components, they can be visualised with a two-dimensional scatter plot.

226 ## 3. Case Study

227 We apply the methods described above to the analysis of water quality in the Serbian

228 stretches of the Danube; this region of the river is 588km long and constitutes 20.6% of the

229 total 2857km river (Fig 2a). Data is collected for eleven monitoring stations along the river,

230 shown in Fig. 2b. The available data is for 2010, and was collected at monthly intervals with

231   some exceptions. Number of measurements for each constituent was following: 1) Bezdan

232   station: 11 measurements for 8 constituents, 10 for Oxygen Saturation and BOD; 2) Bogojevo

233   station: 9 measurements for all constituents; 3) Bačka Palanka station: 8 measurements for all

234   constituents except 7 for BOD; 4) Novi Sad station: 12 measurements for all constituents; 5)

235   Slankamen station: 11 measurements for all constituents; 6) Čenta station: 11 measurements

236   for all constituents; 7) Smederevo station: 12 measurements for all constituents; 8) Banatska

237   Palanka station: 10 measurements for all constituents; 9) Veliko Gradište station: 12

238   measurements for all constituents; 10) Dobra station: 12 measurements for all constituents

239   except 11 for BOD; 11) Radujevac station; 12 measurements for all constituents. E. Coli

240   criterion is omitted from this study, because of small number of measurements in all stations.

241   Where a station was omitted from data collection, it is omitted from the results presented

242   herein. No attempt was made to impute missing values.

243   The parameters collected in the study (Jakovljević, 2012) are used to calculate the Serbian

244   Water Quality Index (SWQI). SWQI is an environmental indicator, developed by Serbian

245   Environmental Protection Agency and based on the Water Quality Index method (Scottish

246   Development Dept., 1976). SWQI uses ten quality parameters: oxygen saturation,

247   biochemical oxygen demand (BOD_5), ammonium, pH, total nitrogen oxides, orthophosphate,

248   suspended solids, temperature, conductivity and most probable number of coliform bacteria

249   (E. Coli/MPN). Each of these parameters has value q_i (the water quality of the i-th parameter)

250   and weight unit w_i (the weight attributed to the i-th parameter). Parameters have varying

251   degrees of importance on the overall water quality, specified by an appropriate weight (w_i)

252   where the sum of all weights is 1. By summarizing the products of all quality parameters (q_i)

253   and all weights (w_i) an index is created representing a weight sum of all parameters (q_i).

254   (Veljković, 2013; Veljković et $al.,$ 2010; Veljković et $al.$, 2008). SWQI is then calculated as

255   the sum of $q_i \times w_i$. The maximum value of each parameter is shown in Table 1.

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263 **Table 1: SWQI parameters and their corresponding maximum $q_i \times w_i$ value (Veljković et al., 2010).**

Parameter (unit)	Maximum $q_i \times w_i$ value
Oxygen Saturation (%)	18
BOD$_5$ (mg/l)	15
Ammonium (mg/l)	12
pH	9
Total Nitrogen oxides (mg/l)	8
Orthophosphates (mg/l)	8
Suspended solids (mg/l)	7
Temperature (°C)	5
Conductivity (µS/cm)	6
E. Coli (MNP/100 ml)	12
$SWQI = \sum (q_i \times w_i)$	100

264

265   For each SWQI range a descriptive quality indicator has been defined ranging from very poor

266   (0–38), poor (39–71), good (72–83), very good (84–89), and excellent (90–100) (Veljković et

267   al., 2008). Parameter values are shown in Table 2.

268

269   **Table 2: Parameters concentration corresponding to** $q_i \times w_i$ (*Scottish Development Department, 1976*)

Water quality (q_i x w_i)	Oxygen saturation (%)		BOD (mg/l)		Ammonium (mg/l,)		E.coli (coli/100ml)		Suspended solids (mg/l)
18	93-109		-		-		-		-
17	88-92	110-119	-	-	-		-		-
16	85-87	120-129	-	-	-		-		-
15	81-84	130-134	0	0.9	-		-		-
14	78-80	135-139	1.0	1.9	-		-		-
13	75-77	140-144	2.0	2.4	-		-		-
12	72-74	145-154	2.5	2.9	0	0.09	0	249	-
11	69-71	155-164	3.0	3.4	0.10	0.14	250	999	-
10	66-68	165-179	3.5	3.9	0.15	0.19	1000	3999	-
9	63-65	180 +	4.0	4.4	0.20	0.24	4000	7999	-
8	59-62	-	4.5	4.9	0.25	0.29	8000	14999	-
7	55-58	-	5.0	5.4	0.30	0.39	15000	24999	0-9
6	50-54	-	5.5	6.1	0.40	0.49	25000	44999	10-14
5	45-49	-	6.2	6.9	0.50	0.59	45000	79999	15-19
4	40-44	-	7.0	7.9	0.60	0.99	80000	139999	20-29
3	35-39	-	8.0	8.9	1.00	1.99	140000	249999	30-44
2	25-34	-	9.0	9.9	2.00	3.99	250000	429999	45-64
1	10-24	-	10.0	14.9	4.00	9.99	430000	749999	65-119
0	0-9		15.0+		10.00+		750000+		120+

270

Water quality (q_i x w_i)	pH	Total nitrogen oxides (mg/l)	Orthophosphate (mg/l)	Conductivity (µS/cm)	Temperature (°C)
18	-	-	-	-	-
17	-	-	-	-	-
16	-	-	-	-	-
15	-	-	-	-	-

14	-		-		-		-		-
13	-		-		-		-		-
12	-		-		-		-		-
11	-		-		-		-		-
10	-		-		-		-		-
9	6.5-7.9		-		-		-		-
8	6.0-6.4	8.0-8.4	0	0.49	0	0.029	-		-
7	5.8-5.9	8.5-8.7	0.50	1.49	0.030	0.059	-		-
6	5.6-5.7	8.8-8.9	1.50	2.49	1.060	0.099	0-49	50-188	
5	5.4-5.5	9.0-9.1	2.50	3.49	0.100	0.129	189	190-239	0-17.4
4	5.2-5.3	9.2-9.4	3.50	4.49	0.130	0.179	240	289	17.5-19.4
3	5.0-5.1	9.5-9.9	4.50	5.49	0.180	0.219	290	379	19.5-21.4
2	4.5-4.9	10.0-10.4	5.50	6.99	0.220	0.279	380	539	21.5-22.9
1	3.5-4.4	10.5-11.4	7.00	9.99	0.280	0.369	540	839	23.0-24.9
0	0-34	11.5-14	10.00+		0.370+		810+		25+

271

According to the Regulation – Official Gazette 1978, all surface waters in Serbia are categorized in four classes (class I – best water quality). Parameters from Regulation were used as input parameters for SWQI calculation. Maximum Concentration Level (MCL) is defined for each of these classes; this is shown in Table 3. MCL values have been established by the Regulation 1978 and they have been constant. There were no their changes, as well as maximum $q_i \times w_i$ values have not changed during the time. This is an important for calculation of long term trends by SWQI method.

279

280　**Table 3: Correlation between SWQI and Maximum Concentration Level (MCL), *(Veljković et al., 2010).***

281　**Temperature and conductivity are omitted as they are not used in water quality characterisation using MCL.**

Parameter (unit)	Max $q_i \times w_i$ value	MCL Class I	MCL Class II	MCL Class III	MCL Class IV
Oxygen saturation (%)	18	90-105	70-90	50-75	30-50
			105-115	115-125	125-130
BOD (mg/l)	15	2	4	7	20
Ammonium (mg/l)	12	0.1	0.1	0.5	0.5
pH	9	6.8–8.5	6.8–8.5	6–9	6–9
Total Nitrogen Oxides (mg/l)	8	10	10	15	15
Orthophosphate (mg/l)	8	0.005	0.005	0.01	0.01
Suspended solids (mg/l)	7	10	30	80	100
Temperature (°C)	5	-	-	-	-
Conductivity (µS/cm)	6	-	-	-	-
E.coli (coli/100ml)	12	200	10000	20000	20000
$\sum(q_i \times w_i)$=WQI	100	85–84	69–71 74–71	44–48 56–52	35–36 51–46

282　# 4. Results

283　The two visualisation methods described above are now applied to the case study data. Due to

284　its absence in many cases, the E. Coli criterion is omitted from these results. The results

285 presented herein are based on the remaining 9 SWQI parameters. In all cases, the criteria

286 were arranged for minimisation, such that small criterion values are preferred to large ones

287 when stations are ranked. This is in some ways an arbitrary choice, but was made because in

288 a ranking of N items 1 is generally the best rank and N is the worst. The methods were

289 applied to all of the populations (one for each month that data was collected), and we begin

290 by illustrating the features of each visualisation.

4.1   Rank-based Visualisation

292 Figure 3 illustrates the population describing the water quality stations in February 2010. The

293 left-hand plot shows the data visualised as a Pareto shell graph. The stations sort into four

294 Pareto shells; the most powerful (best) station is Smederevo, which is in shell 1 and has the

295 best average rank (light colours indicates a good average rank; dark colours indicates a poor

296 average rank). Generally, the ordering of individuals according to Pareto sorting corresponds

297 to that average ranking; stronger individuals are on the left-hand side of the visualisation and

298 weaker individuals are on the right-hand side. This corresponds to the findings presented in

299 Walker *et al.*, (2010). That said, according to the Pareto sorting Veliko Gradište is the

300 weakest station, Bezdan (shell 2) has the worst average rank of any in the population. This

301 highlights a useful feature of the method first observed in Walker *et al.*, (2010), whereby it is

302 possible for an individual with an extremely poor average rank to be placed in a high Pareto

303 shell. In order for this to happen, the individual must have a very strong score on one of the

304 criteria, making it very hard for other individuals to dominate it; this means that the

305 individual is likely to be placed into a strong Pareto shell. If the remainder (and majority) of

306 the criterion values are extremely poor, the overall average rank for the individual will be

307 very poor. In fact, Bezdan has a very strong score on the BOD criterion, and poor scores on

308 the other eight criteria. By combining the two ranking methods we prevent stations from

311   Figure 4 presents the visualisations shown in Figure 3, this time coloured according to the

312   quality rating assigned to each station using SWQI. With the exception of three stations

313   (Smederevo, Čenta and Radujevac) all are "good". Of the three that are not, two are "very

314   good" and one (Smederevo) is "excellent". This corresponds with the ranking induced by

315   average rank, under which the strongest station was Smederevo, followed by Radujevac and

316   Čenta. This is a useful result, as it shows that the average rank procedure allows for

317   comparison between individuals that were incomparable under the SWQI scheme without

318   conflicting with the partial ordering produced under SWQI. Average rank scores for the

319   stations throughout the year are shown in Table 4. Note, that these scores do not take account

320   of the absence of some stations from the data in some months, which causes artificially low

321   average rank scores (this is particularly prevalent in December, where the measurement of

322   just five stations results in a maximum average rank of 5). Figure 6 presents the distribution

323   of average ranks graphically; in order to facilitate comparison of stations, the average rank

324   values shown in Table 4 have been ranked, placing them on the scale 1, ..., N (for N stations

325   in a given month) and then normalised to the range (0, 1).

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329

330   **Table 4: Monthly average rank scores for water quality stations.**

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Bačka Palanka	-	-	11	9	8	11	3	4	6.5	10	-	-
Banatska Palanka	7.5	5	10	5	6	7	-	10	8	8	10	1
Bezdan	4.5	9	3	10	10	5	6	7	6.5	11	2	-
Bogojevo	-	-	5	3	7	4	2	6	1	7	8	-
Čenta	7.5	3.5	5	8	9	10	5	3	3	5	5.5	-
Dobra	4.5	7	1	4	4	3	8	8	10	1	3.5	2.5
Novi Sad	9	6	5	11	11	6	8	9	5	3	3.5	5
Radujevac	2	2	9	2	3	2	8	1	2	9	1	4
Slankamen	3	3.5	8	6.5	5	8.5	10	2	4	5	5.5	-
Smederevo	1	1	7	1	1	8.5	1	5	11	5	7	-
Veliko Gradište	6	8	2	6.5	2	1	4	11	9	2	9	2.5

331

332 Radujevac had the highest quality according to Pareto sorting. It achieved rank 1 on nine

333 occasions and rank 2 twice. One of these two occasions was February, in which it was

334 dominated by Smederevo. Radujevac in turn dominated Dobra and Veliko Gradište. The

335 SWQI values for these four stations agree with the ordering according to dominance:

336 Smederevo is rated excellent, Radujevac is very good, while Dobra and Veliko Gradište are

337 rated good. The parameter that causes this relationship is BOD. In the case of Smederevo, the

338 BOD result was 2mg/l (14 according to SWQI and class I according to the maximum

339 concentration level (MCL)). Radujevac had BOD of 2.8mg/l (12 according to SWQI, class II

340 MCL), while Dobra and Veliko Gradište measured 4.8mg/l (8 under SWQI and class III

341 MCL) and 5.3 mg/l (7 under SWQI, class III MCL). The average rank results support this

342 ordering too: Smederevo and Radujevac are the best two individuals in the population, while

343 Dobra and Veliko Gradište are two of the worst. This agreement between the Pareto sorting

344 method and well understood measures such as SWQI and MCL is reassuring, as it provides a

345 simple approach to visualising the relationship between stations in a context with which

346 engineers and scientists are familiar. This, when combined with its ability to compare stations

347 without requiring WQIs to be weighted, illustrates the potential of the visualisation method

348 for analysing multi-criterion water quality data. That said, if weights are available, as is the

349 case here, then they can be incorporated via the colouring approach taken (e.g., there is an

350 optional provision for incorporating weights into average rank).

351 The other occasion in which Radujevac was dominated was October, when it was dominated

352 by Veliko Gradište. Both stations were rated very good under SWQI, however Veliko

353 Gradište's Ammonium value was better than that of Radujevac (0.05mg/l, or 12 according to

354 SWQI and MCL class I-II, in the case of Veliko Gradište; 0.19mg/l, or 10 under SWQI and

355 MCL class III-IV in the case of Radujevac). Interestingly, however, Radujevac has a poor

356 average rank. This, in concert with the fact that Radujevac does not dominate anything in the

357 next shell, indicates overall poor quality. By observing the average rank results for the rest of

358 the year we can see that its performance according to average rank was poor in five months.

359 In three of these cases, March, July and December, its SWQI rating is good, the worst

360 classification assigned to a station in those months. That said, when considering the

361   distribution of normalised ranks in Figure 6, Radujevac has the best overall quality according

362   to average rank. While it might be tempting to interpret Smederevo as the best station (it

363   achieves rank 1 in five months, more than any other station) its ranking in some months is

364   particularly poor. Radujevac, on the other hand, has more consistent performance. It appears

365   in the top three positions in the ranking in all but four months of the year.

366   One of the important utilities of this type of analysis is that hydrologists can use them to

367   observe stations with low quality, so that efforts can be made to improve river quality at those

368   locations. Two stations with poor performance under Pareto sorting were Veliko Gradište and

369   Bogojevo. Veliko Gradište was in rank 1 on 8 occasions, rank 2 twice, and on one occasion

370   was the sole member of rank 4. Though it achieved a good rank in some of the months, its

371   lower rank on other occasions reduced its overall quality. On the occasion it appeared in rank

372   4, it had one of the lowest average ranks for that month (February). Bogojevo was in rank 1

373   on 7 occasions, rank 2 twice and rank 4 once. Bačka Palanka also achieved poor results.

374   Though it was in rank 1 on 5 occasions, there was also a month in which it appeared in ranks

375   2, 3 and 4, respectively. This corresponds to relatively low quality SWQI results. It was

376   predominantly classified "good" under SWQI, and was classified "very good" just once; most

377   of the other stations achieved a "very good" classification multiple times. In June it was

378   classified "poor", the worst possible classification under SWQI. Novi Sad was the worst

379   station according to Pareto sorting. It appeared in rank 1 only once, and was mainly placed

380   into rank 2. It was also placed into ranks 3 and 4 on one occasion each.

381   Beyond analysing the relative performance of individual months, considering the

382   visualisations for the year as a whole also offers useful insight. Under SWQI, the months

383   with lowest water quality are the summer months, June to September, inclusive. June is the

384   only month in which stations were classified "poor", and both July and August are entirely

385   comprised of "good" classifications, with no station achieving "very good" or "excellent".

386   Examining the Pareto shell visualisations for these months shows that they are also the

387   months in which the overall structure of the dominance graph is flattest. Figure 7 shows the

388   distribution of values throughout the year for the temperature and oxygen saturation

389   parameters. As can be seen, there is a significant peak in the values for the summer months,

390   which implies that these parameters have significant influence on the overall structure of the

391   population; we can infer a large degree of conflict between these parameters and one of the

392   other parameters, as the increased temperature appears to cause the stations in the data to

393   become mutually non-dominating. In order to properly evaluate this result it would be

394   necessary to collect data over a number of years, and currently this data is unavailable.

4.2   *PCA Visualisation*

395

396   We also applied PCA to the data, in order to produce two dimensional scatterplots of the data.

397   In this work we did not consider the data a time series; rather, each month was treated as its

398   own case, unrelated to the other data. One of the potential difficulties with using PCA is that

399   a loss of information is incurred. The data was projected onto the first two principal

400   components, which, as explained earlier, represent the stations in a new coordinate space that

401   may be, but is not necessarily, correlated with the original criterion values. Inspection of the

402   eigenvalues indicates in all cases between 89 and 99% of the variance in the data was

403   contained in the first two eigenvectors. This means that the majority of the information in the

404   data has been retained for all 12 months.

405   As with the Pareto sorting visualisations, the data is presented in terms of both average rank

406   and SWQI classification. The lower panel of Figure 3 illustrates the PCA projection of the

407   data for February, and examining the clustering reveals an interesting result. The data can be

408   broadly grouped into four clusters. The first cluster contains four stations: Čenta, Slankamen,

409   Bezdan and Novi Sad. Examining the Pareto shell visualisation of February (Figure 2) shows

410   that these four stations form a cluster in terms of their dominance relations too. Slankamen

411   and Čenta are Pareto optimal, and both Bezdan and Novi Sad are dominated by Čenta.

412   Bezdan is also dominated by Čenta. The second cluster includes Radujevac, Banatska

413   Palanka and Smederevo. Smederevo is Pareto optimal, and dominates both Radujevac and

414   Banatska Palanka. The final two clusters contains the final two stations, Dobra (in a shell of

415   its own and dominated only by Radujevac) and Veliko Gradište (dominated only by Dobra,

416   again the sole member of its shell). This is an interesting result, as it shows potential for

417   revealing spatial coherence in the data using PCA even with such small datasets. Figure 8

418   shows examples for other months, and this effect is again seen in October. In that case,

419   Bezdan is the station with the worst quality and is placed far away from the main grouping of

420   stations.

421   Further insight into the data for August is possible using this technique. As can be seen in the

422   average rank case the stations have been arranged such that those with a poor average rank

423   are together and those with a strong average rank are further away. In the extreme, Radujevac

424   is placed away from the main cluster of stations; it has the best average rank for that month

425   and in the Pareto sorting example is Pareto optimal but dominates nothing in the subsequent

426   shell.

427   While it is possible to observe relative quality between individuals using the Pareto shell and

428   PCA visualisations, the actual WQI values of the stations are either not conveyed, in the case

429   of the Pareto shell visualisation, or discarded, in the case of PCA. Having provided this

430   information, we enhance their decision making potential by producing corresponding parallel

431   coordinate plots (Inselberg, 2009). The examples shown in Figure 9 are for February (which

432   corresponds to the results shown in Figure 4) and May. Each line represents a station, and is

433   coloured according to its SWQI score for that month (NB: stations achieving a SWQI score

434   of "excellent" are in this case represented with a dashed line, rather than colouring with

435 white). It can be seen that the station with excellent SWQI is generally at the lowest point of

436 the graph, indicating its superiority. It is, however, difficult to infer the overall quality of a

437 station from these visualisations alone, and thus we recommend that they are used in

438 combination with the Pareto shell or PCA visualisations.

439 As previously mentioned, the station with the best water quality was Radujevac. This was

440 caused by better quality of specific parameters comparing with other stations. The other

441 station with the high water quality was Smederevo, which was caused by high average water

442 quality. At the other hand the station with the worst water quality was Novi Sad, because of

443 low average water quality and Bačka Palanka due to bad quality of specific parameters.

444 Considering the location of these stations, this suggests that downstream stations had a better

445 water quality than upstream ones. This can be explained by high selfpurification of the

446 Danube River, which enabled reduction of organic loading. The other unexpected outcome

447 was the best water quality in the June according to the Pareto sorting visualisation, which was

448 the month with the worst water quality according to the SWQI. The explanation is in the fact

449 that due to the impairment of water quality in all stations and in most parameters, there was

450 no possibility that the stations dominated each other, except in one case. This produced the

451 result that the stations with the worst water quality were in the Rank 1. The parameter which

452 caused the water quality decline was Oxygen saturation with the following values: 34%

453 (Bačka Palanka), 52% (Banatska Palanka), 59% (Čenta) and 64% (Slankamen). Due to this

454 parameter all these stations had poor water quality according to the SWQI as well as III class

455 (Banatska Palanka, Čenta and Slankamen) and IV class (Bačka Palanka). This case is very

456 important in terms of environmental conditions, because low Oxygen saturation values can

457 threaten life of aquatic organisms.

5. Conclusions

458

459 Analysing river quality is an important task for environmental scientists and engineers. Given

460 the range of available criteria according to which river quality can be measured, multi-

461 criterion visualisation is a natural candidate for presenting the information. This work has

462 illustrated the application of such methods to the analysis of water quality in the Serbian

463 stretches of the Danube in 2010.

464 One of the methods employed multi-criterion ranking methods; the first used Pareto sorting,

465 based on the dominance relation, to produce a partial ordering of water quality stations on

466 which a directed graph can be constructed. This graph was shown to produce comparable

467 results to those achieved using SWQI, which is a well-known measure of river quality used in

468 Serbia. Additional information can be included in the visualisation by illustrating the average

469 rank of each station with the colour of its corresponding node in the graph. This also revealed

470 additional information, such as identifying stations with poor quality that had been unduly

471 promoted to a high rank by the Pareto sorting procedure. Examining the average rank of

472 stations provides a useful insight into the overall quality of a station; for example, by

473 inspection it was clear that Radujevac was the station with highest quality in the data used for

474 this study. Principal component analysis provided some additional insight into the data,

475 however it is likely to be more useful in cases where larger numbers of stations are employed.

476 We note that while in some applications using PCA can cause unacceptable levels of

477 information loss, in this case the vast majority of variance in the data was retained in the two

478 principal eigenvalues (89% in the worst case). Using PCA in combination with the Pareto

479 shell visualisations facilitated further insight into the data, as well as the identification of

480 facets of the data that appeared in both visualisations. We plan to extend the use of PCA in

481 this area by considering the criteria as a time series, which we feel will provide further

482 information to the decision maker given the temporal nature of the data.

483   The analyses described in this work have considered each visualisation a description of the

484   river at a specific point in time. Relationships between stations were described in that context,

485   as well as in the context of their results throughout the year. The criteria on which the

486   visualisations are based do not take account of any temporal variation in the parameter values,

487   however the results discussed clearly show that there is a seasonal aspect to them. The rise in

488   temperature and oxygen saturation levels in the summer months demonstrate this. Therefore,

489   beyond the demonstration that the techniques illustrated in this study can provide useful

490   information about river quality, a useful direction of future work would involve incorporating

491   this temporal or seasonal variation into the visualisation. One possibility that is currently

492   under investigation would be to construct additional criteria so that the historical quality of

493   river water can be understood, and issues regarding the sensitivity of the data can be

494   addressed.

495   Water quality has traditionally been assessed in terms of complex variable–by–variable and

496   water body–by–water body summaries. This type of information is of value to water quality

497   experts, but needs to be improved for users who want to know about the state of their local

498   water bodies and for managers and decision makers who require concise information about

499   those water bodies. Water quality index methodologies partially overcome the shortcomings

500   of these methods, and provide the ability to describe water quality with a single value based

501   on arrange of indicators and measurements. This facilitates simple communication of water

502   quality results to interested parties. Disadvantages of such methods include the sensitivity of

503   the results to the formulation of the index and the loss of potentially important interactions

504   between variables. By using the multi-criterion visualisation approaches proposed in this

505   paper, some of these disadvantages can be ameliorated.

506   The Pareto shell visualisation is advantageous in the visualisation of data of this type. It does

507   not require any dimension reduction, presenting the decision maker with a visualisation based

508   on all available data, and does not require the *a priori* selection of importance weights for the

509   criteria (although they can be incorporated into the secondary ranking method used to colour

510   the nodes in the graph if they are available). The method is generally very scalable, and can

511   be combined with well known domain-specific techniques, as was done with SWQI in this

512   paper. That it does not visually represent specific criterion values might be seen as a

513   limitation, however we feel that this is easily addressed by combining it with a separate

514   visualisation, such as the parallel coordinate plots demonstrated in this work. PCA is a

515   suitable choice as it relies on spatial proximity to convey similarity, which decision makers

516   can generally comprehend easily. The obvious limitation with this method is that it discards

517   potentially important information, however it was demonstrated here that the amount of

518   information lost was minimal.

519   Many studies have applied multi criterion decision making to conduct sustainability

520   assessment (Cinelli et al, 2014) in environmental and human health risk assessment (Topuz *et*

521   *al.,* 2011), to assess habitats and wildlife (Cortina and Boggia, 2014), in the case of urban

522   water strategies (Moglia *et al*, 2012) and water supply infrastructure planning and

523   rehabilitation (Scholten *et al*., 2015; Schoelten *et al*., 2014) in order to support decision

524   makers, in agricultural systems according to the decision-makers' expectations (Carof *et al.*

525   2012)*,* in the risk assessment of contaminated ground water (Khadam *et al*., 2003).

526   Techniques presented in this paper could also help decision makers to determine the best and

527   worst quality sites, as well as to determine how these water quality estimation tools relate to

528   land characteristics management choices, urban versus rural designations etc. Ravier et al.,

529   (2015) have used PCA for water quality preservation programme. Pareto optimal set was

530   used in different land uses, crops, pastures, forestry and soil water conservation practices at

531   the basin scale in the Pampas in Argentina (Cisneros *et al*., 2011), minimising probable flood

532   damages and maximizing water demand supply (Malekmohammadi et al., 2011) as well as

533 Pareto frontier visualisation in support of decision makers in rehabilitation of water quality in
534 Googong Reservoir in Australia (Castelletti *et al.*, 2010). It can be inferred that these water
535 quality estimation techniques have already played important role as support in the process of
536 decision making and their importance will be increase in a future.

537 ## 6. Acknowledgement

541 ## 7. References

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Figure

Figure 1: A simple Pareto shell visualisation of a population comprising eight individuals. Edges represent dominance relations, e.g., individual B (shell 1) dominates individuals D and E (shell 2). Although B may also dominate individuals in later shells (e.g., individual F in shell 3) this relationship is omitted to preserve the clarity of the visualisation.
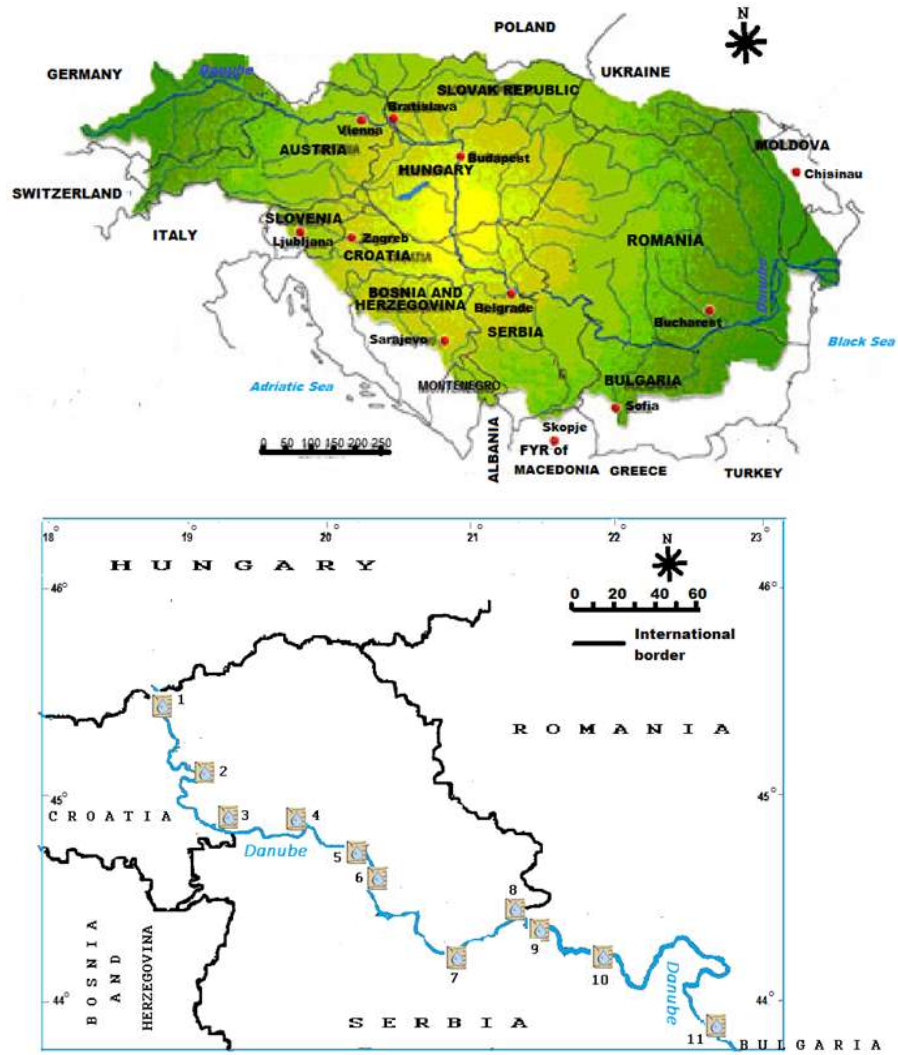
Figure

Figure 2: (top) Danube River Basin (Relić et al, 2011); (bottom) A map showing the locations of the 11 monitoring stations used in this study. The stations are as follows: 1 - Bezdan, 2 - Bogojevo, 3 - Baka Palanka, 4 - Novi Sad, 5 - Slankamen, 6 - Čenta, 7 - Smederevo, 8 - Banatska Palanka, 9 - Veliko Gradište, 10 - Dobra, 11 - Radujevac.
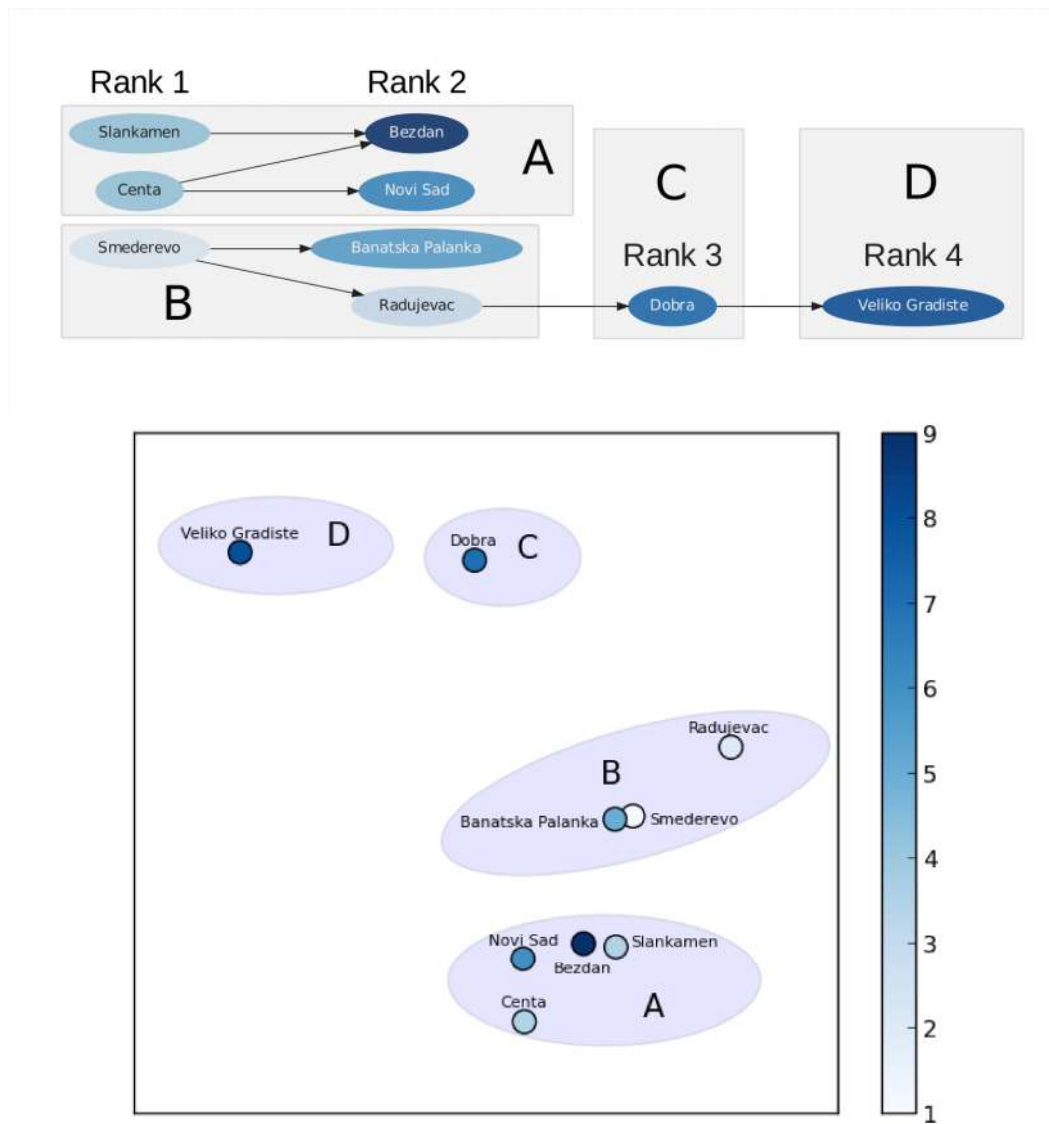
Figure 3: Visualisations of the water quality stations for February 2010. The upper plot shows a Pareto shell visualisation of the population in which the nodes are coloured according to average rank. The lower plot shows the corresponding PCA embedding of the individuals, again, coloured according to average rank.
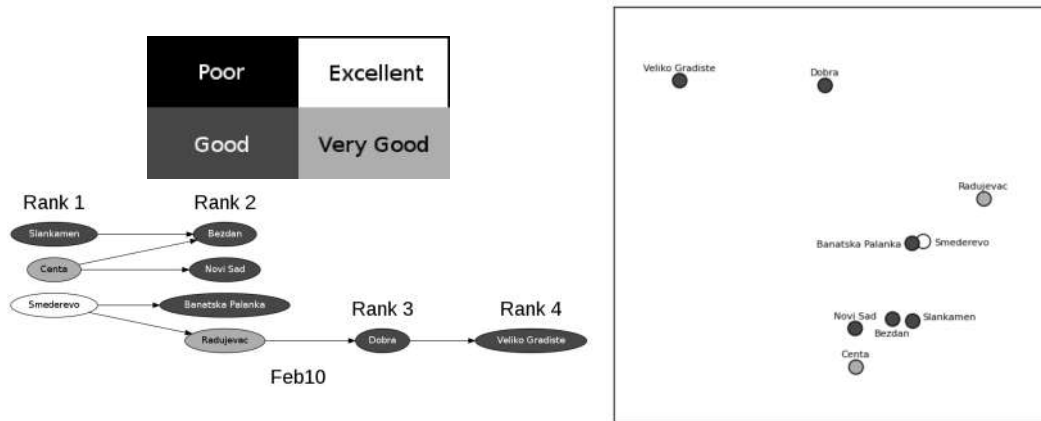
Figure 4: The visualisations of the February 2010 population shown in Figure 3. Rather than the colour scale used in the earlier average rank visualisations (Figure 3) these stations are coloured according to the class indicated by their SWQI scores.
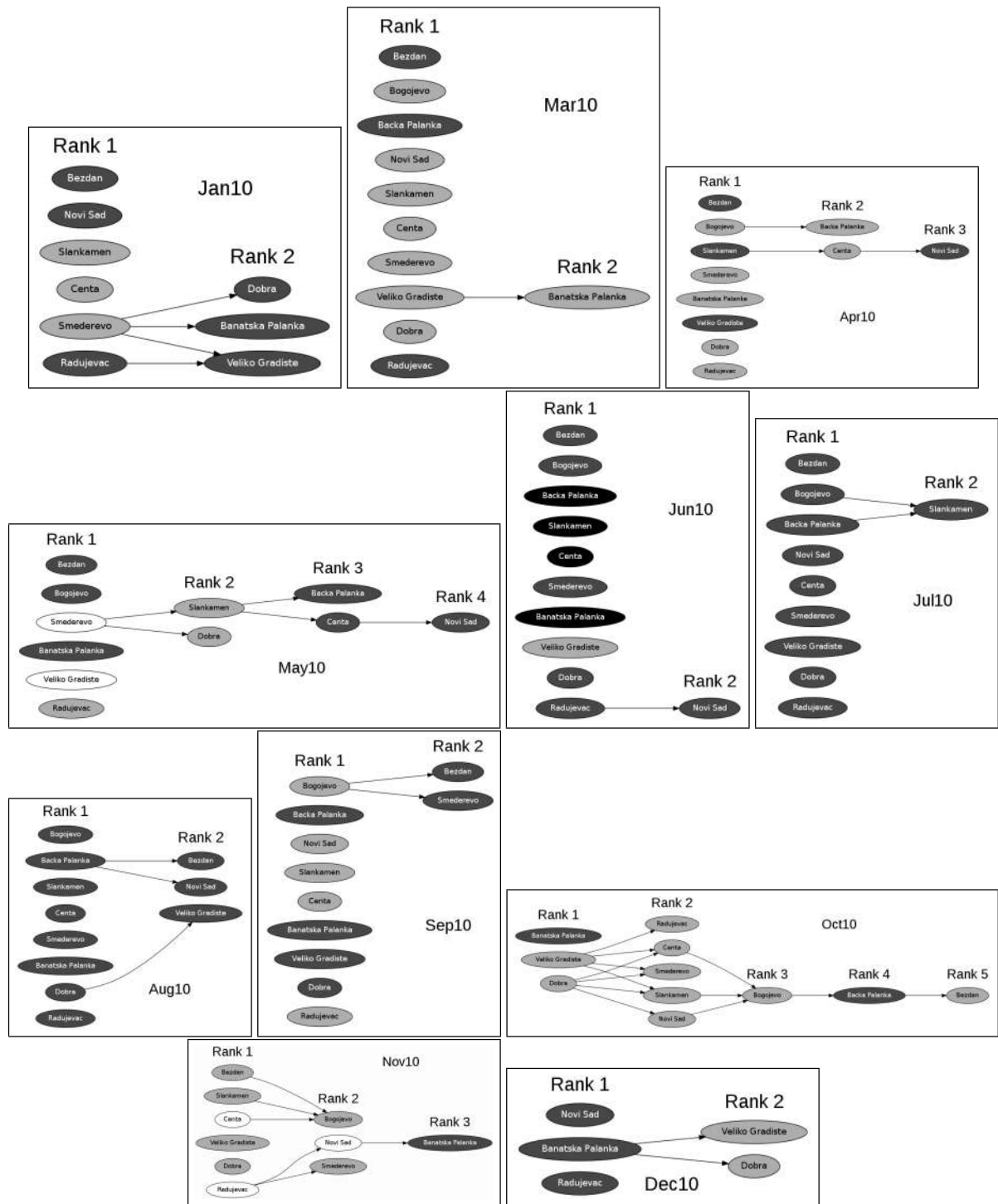
Figure 5: The complete set of Pareto shell visualisations for 2010 (for February, see Figure 3), coloured according to SWQI scores.
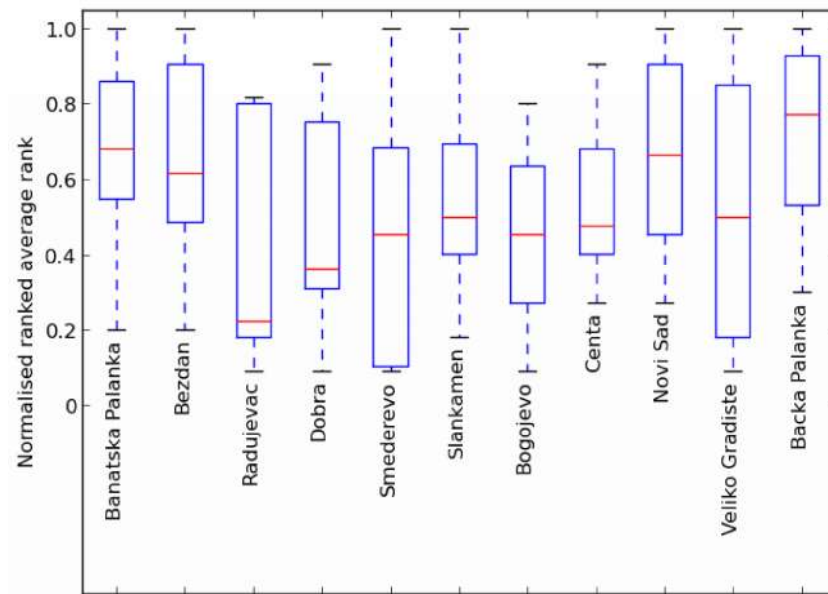
Figure

Figure 6: The distribution of ranks for the stations throughout the year. This type of visualisation makes it possible to begin identifying the best and worst stations throughout the year according to average rank; Radujevac is the best station, with the joint lowest normalised rank and the lowest median rank of any of the stations.
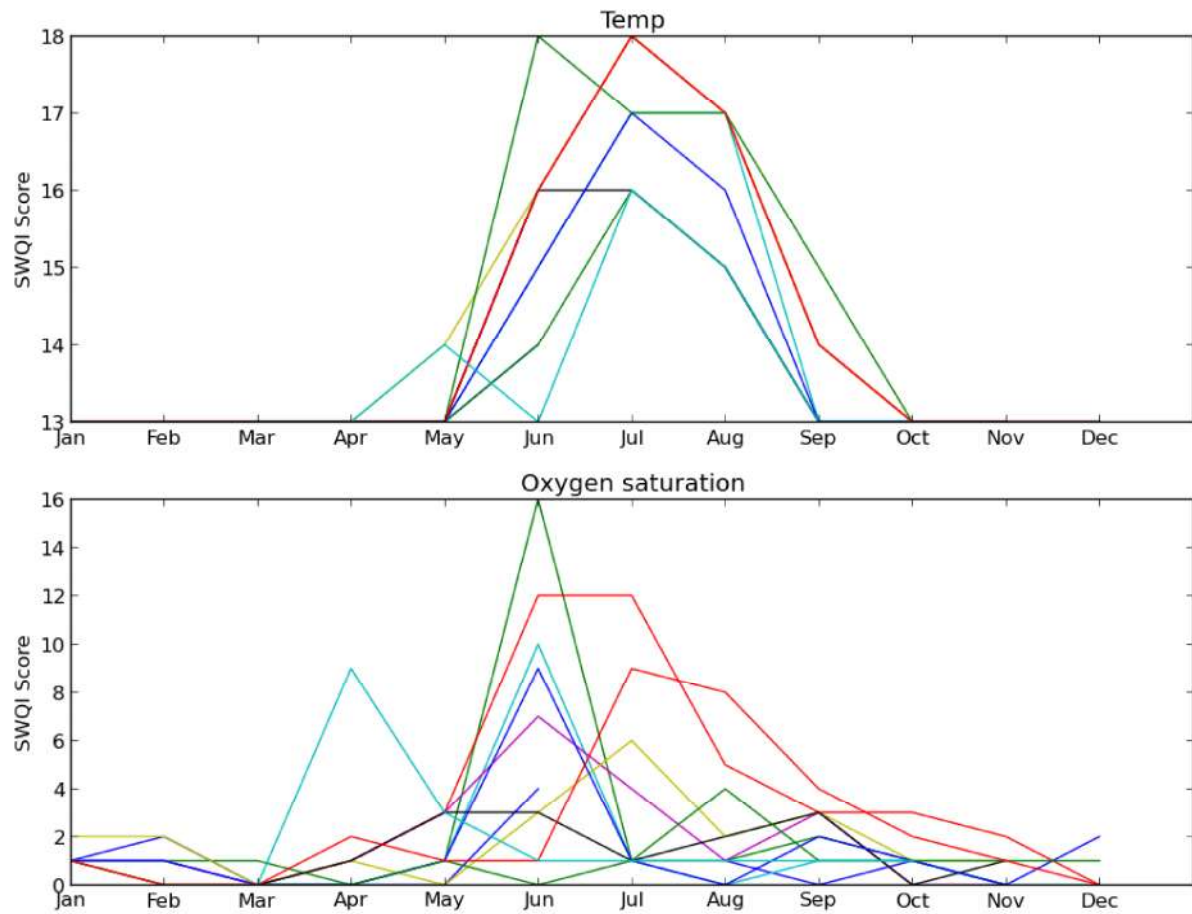
Figure

Figure 7: The distribution of temperature (top) and oxygen saturation (bottom) values throughout the year; each line represents a station. The peak corresponds to the months in which the Pareto shell visualisations are flattest, indicating that this parameter has a strong structural influence on the data.
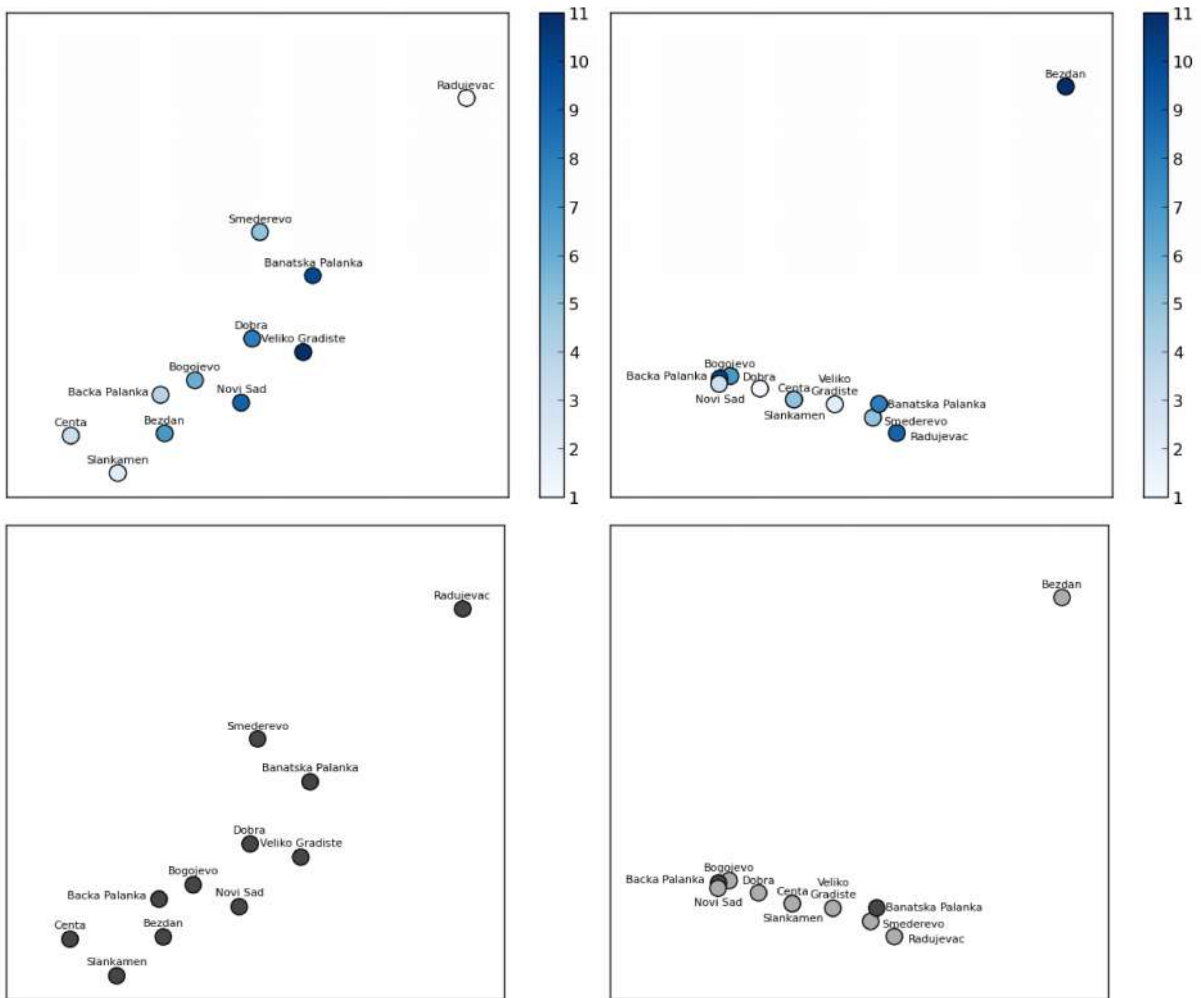
Figure

Figure 8: PCA projections for August (left-hand column) and October (right-hand column). The visualisations in the top row are coloured according to average rank while those in the bottom row are coloured according to the stations' SWQI classification.
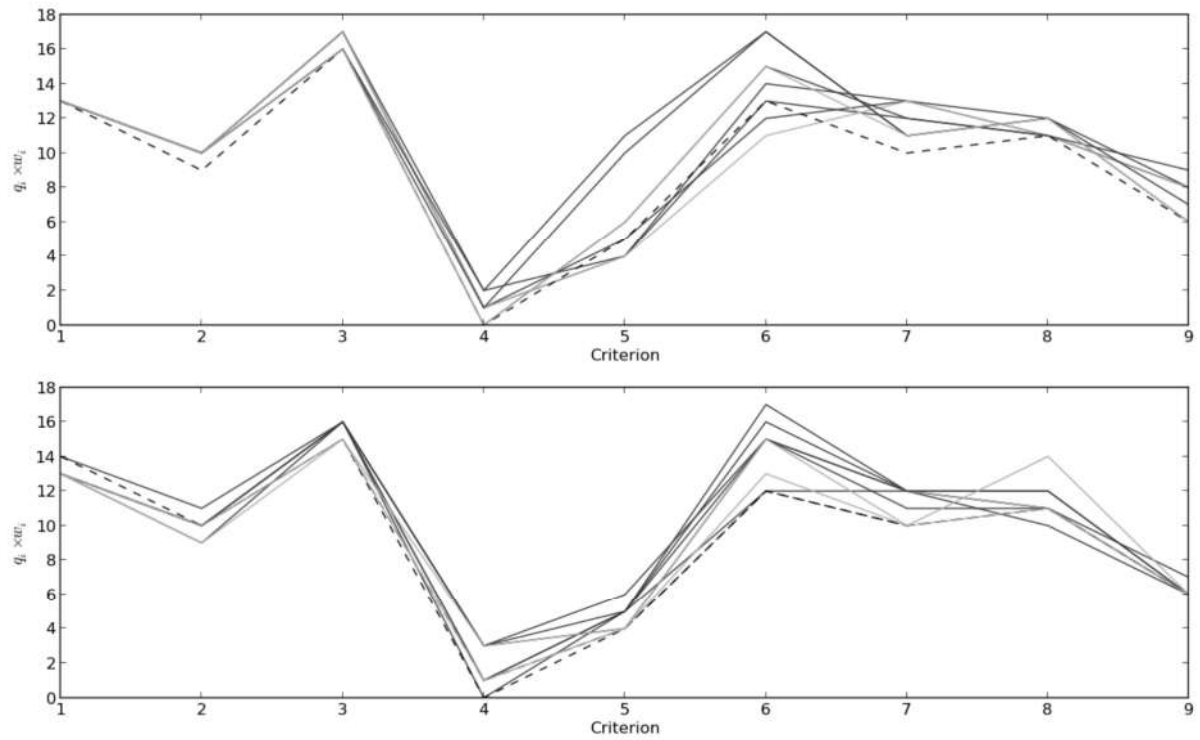
Figure

Figure 9: Parallel coordinate plots of the populations for February (top) and May (bottom). The colours correspond with that used for the SWQI scheme in earlier figures; white stations are now shown with a dashed line. With these plots it is possible to observe the individual criterion values of an individual, however it is more difficult to compare the overall quality of two stations.