

17 **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.

28 **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.

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 \mathbf{u} *dominates* individual \mathbf{v} if its criterion values u_m are no
 166 worse than those of \mathbf{v} , and are better than \mathbf{v} on at least one criterion. More formally:

$$167 \quad \mathbf{u} < \mathbf{v} \Leftrightarrow \forall m (u_m \leq v_m) \wedge \exists m (u_m < v_m) \quad (1)$$

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 \mathbf{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:

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

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 SWQL.

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

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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.

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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+

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Water quality ($q_i \times w_i$)	pH	Total nitrogen oxides (mg/l)	Orthophosphate (mg/l)	Conductivity (μ S/cm)	Temperature ($^{\circ}$ 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+

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

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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	$\frac{69-71}{74-71}$	$\frac{44-48}{56-52}$	$\frac{35-36}{51-46}$

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.

291 **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, Bezdán (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, Bezdán 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.

458 **5. Conclusions**

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.

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

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16 indicators

17 **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.

28 **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.

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 \mathbf{u} *dominates* individual \mathbf{v} if its criterion values u_m are no
 166 worse than those of \mathbf{v} , and are better than \mathbf{v} on at least one criterion. More formally:

$$167 \quad \mathbf{u} < \mathbf{v} \Leftrightarrow \forall m (u_m \leq v_m) \wedge \exists m (u_m < v_m) \quad (1)$$

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 \mathbf{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:

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

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 SWQL.

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) Beždan
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 (BOD₅), 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 (μ S/cm)	Temperature ($^{\circ}$ 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

272 According to the Regulation – Official Gazette 1978, all surface waters in Serbia are
273 categorized in four classes (class I – best water quality). Parameters from Regulation were
274 used as input parameters for SWQI calculation. Maximum Concentration Level (MCL) is
275 defined for each of these classes; this is shown in Table 3. MCL values have been established
276 by the Regulation 1978 and they have been constant. There were no their changes, as well as
277 maximum $q_i \times w_i$ values have not changed during the time. This is an important for
278 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	<u>69–71</u> 74–71	<u>44–48</u> 56–52	<u>35–36</u> 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.

291 **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, Bezdán (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, Bezdán 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 Bezdán 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.

458 **5. Conclusions**

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.

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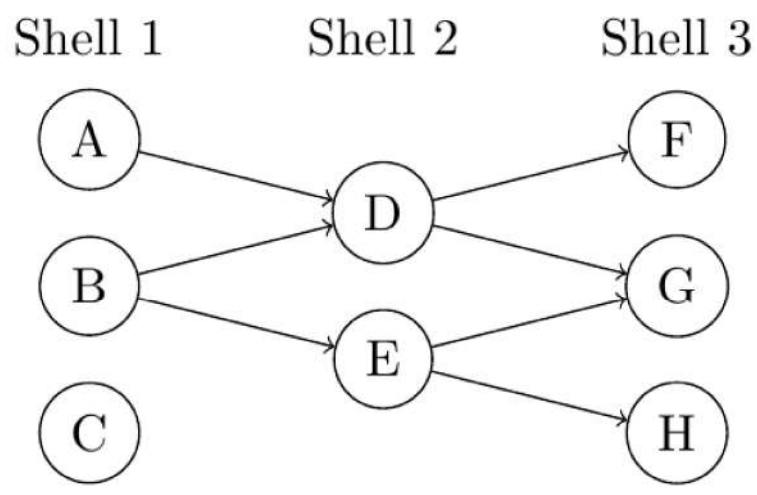


Figure 1: A simple Pareto shell visualisation of a population comprising eight individuals. Edges represent dominance relations, e.g., individual B (shell 1) dominates individuals D and E (shell 2). Although B may also dominate individuals in later shells (e.g., individual F in shell 3) this relationship is omitted to preserve the clarity of the visualisation.

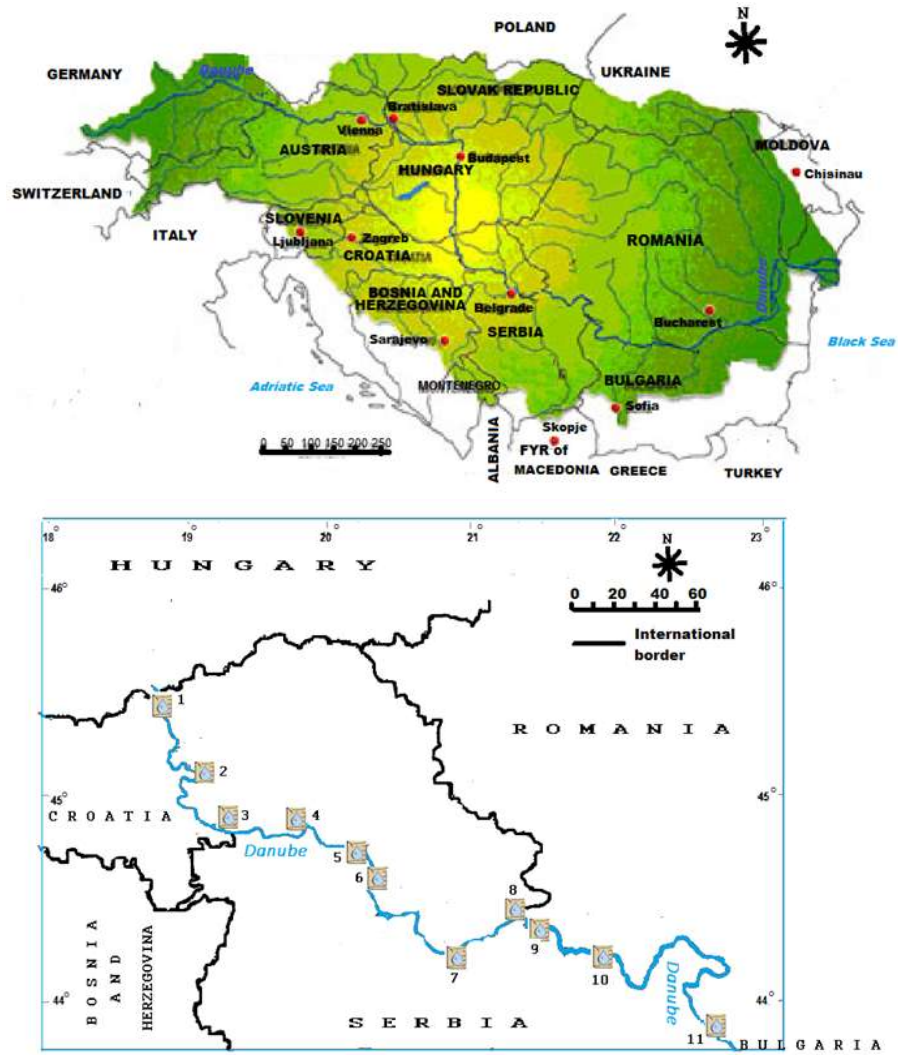


Figure 2: (top) Danube River Basin (Relić et al, 2011); (bottom) A map showing the locations of the 11 monitoring stations used in this study. The stations are as follows: 1 - Bezdán, 2 - Bogojevo, 3 - Baka Palanka, 4 - Novi Sad, 5 - Slankamen, 6 - Čenta, 7 - Smederevo, 8 - Banatska Palanka, 9 - Veliko Gradište, 10 - Dobra, 11 - Radujevac.

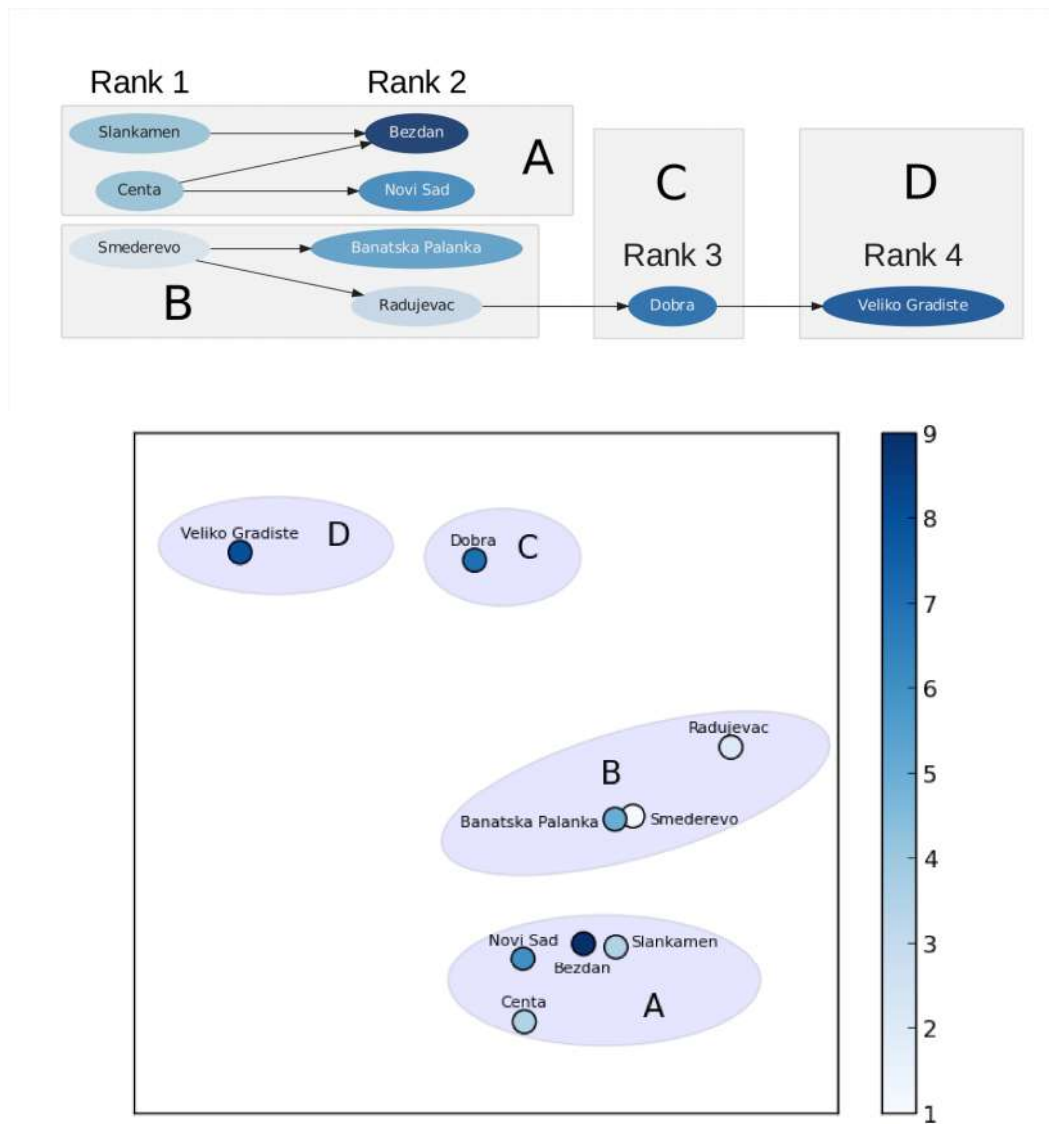


Figure 3: Visualisations of the water quality stations for February 2010. The upper plot shows a Pareto shell visualisation of the population in which the nodes are coloured according to average rank. The lower plot shows the corresponding PCA embedding of the individuals, again, coloured according to average rank.

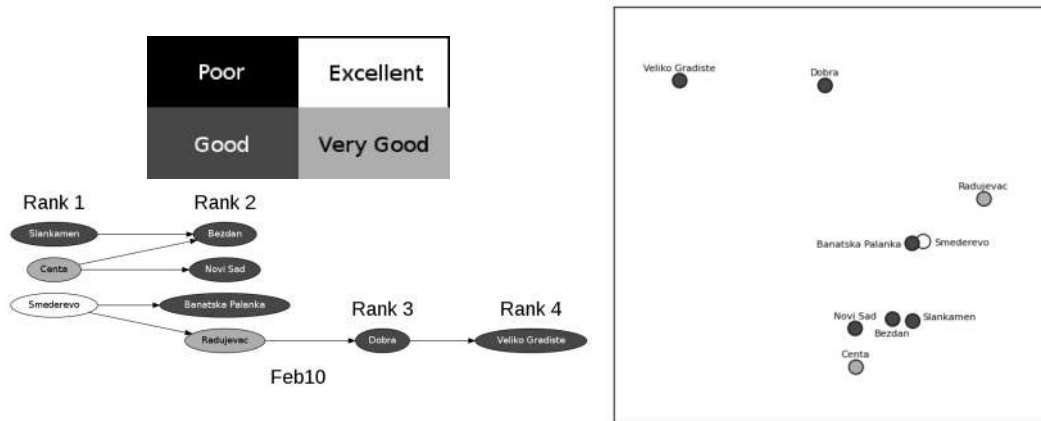


Figure 4: The visualisations of the February 2010 population shown in Figure 3. Rather than the colour scale used in the earlier average rank visualisations (Figure 3) these stations are coloured according to the class indicated by their SWQI scores.

Figure

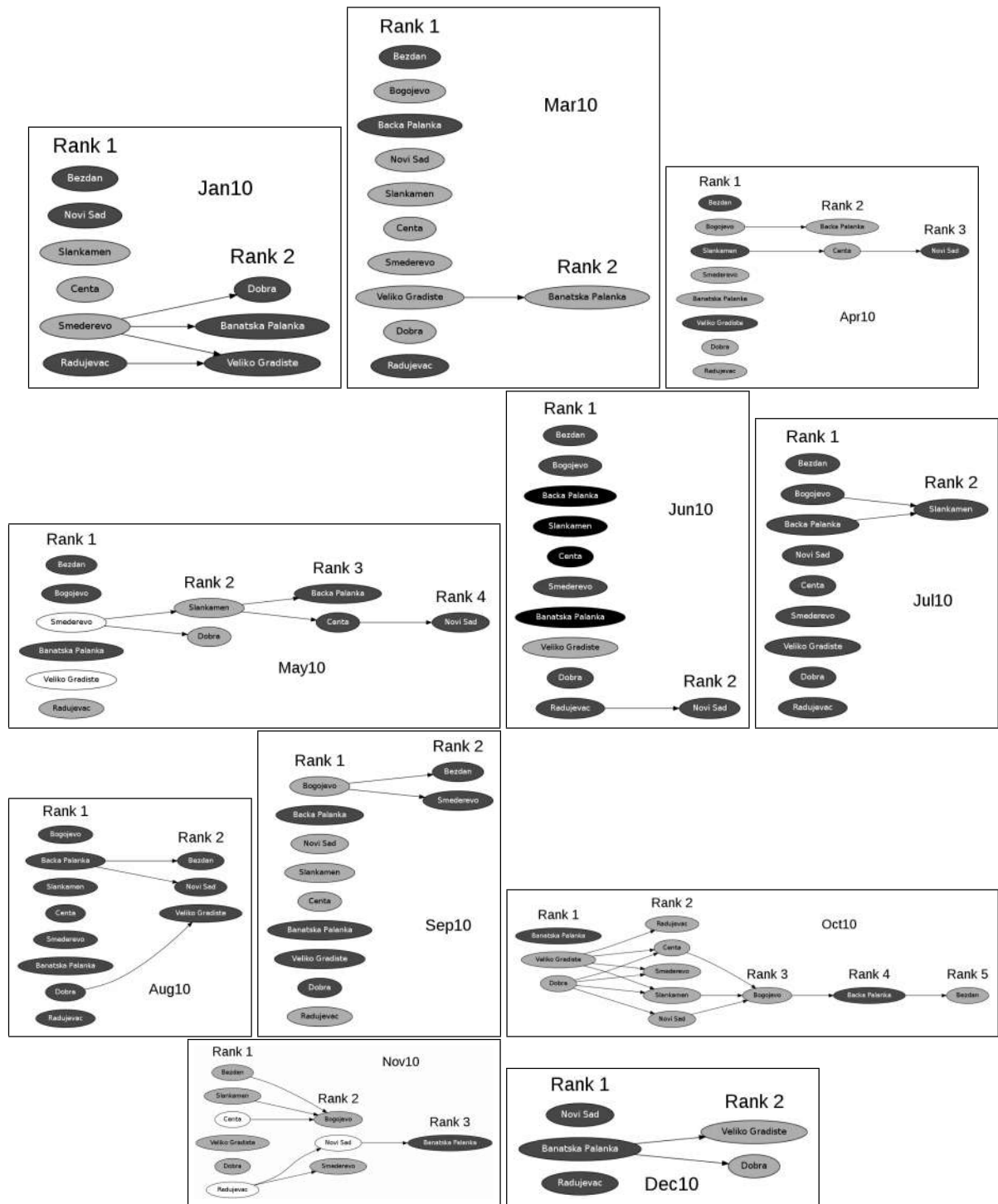


Figure 5: The complete set of Pareto shell visualisations for 2010 (for February, see Figure 3), coloured according to SWQI scores.

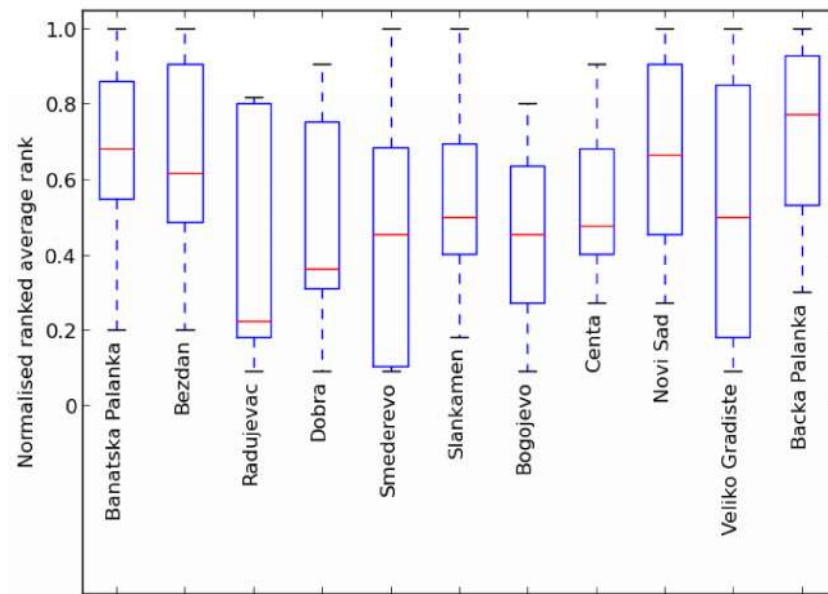


Figure 6: The distribution of ranks for the stations throughout the year. This type of visualisation makes it possible to begin identifying the best and worst stations throughout the year according to average rank; Radujevac is the best station, with the joint lowest normalised rank and the lowest median rank of any of the stations.

Figure

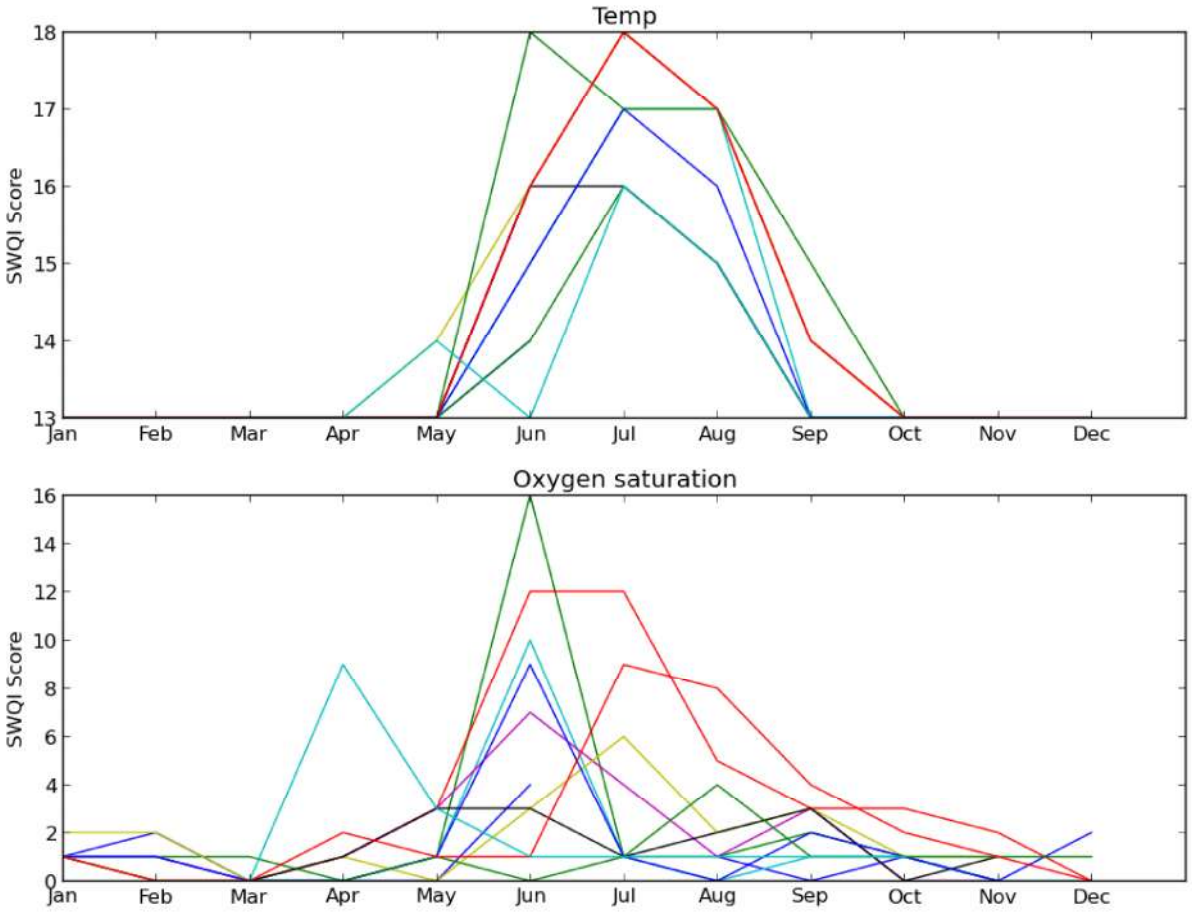


Figure 7: The distribution of temperature (top) and oxygen saturation (bottom) values throughout the year; each line represents a station. The peak corresponds to the months in which the Pareto shell visualisations are flattest, indicating that this parameter has a strong structural influence on the data.

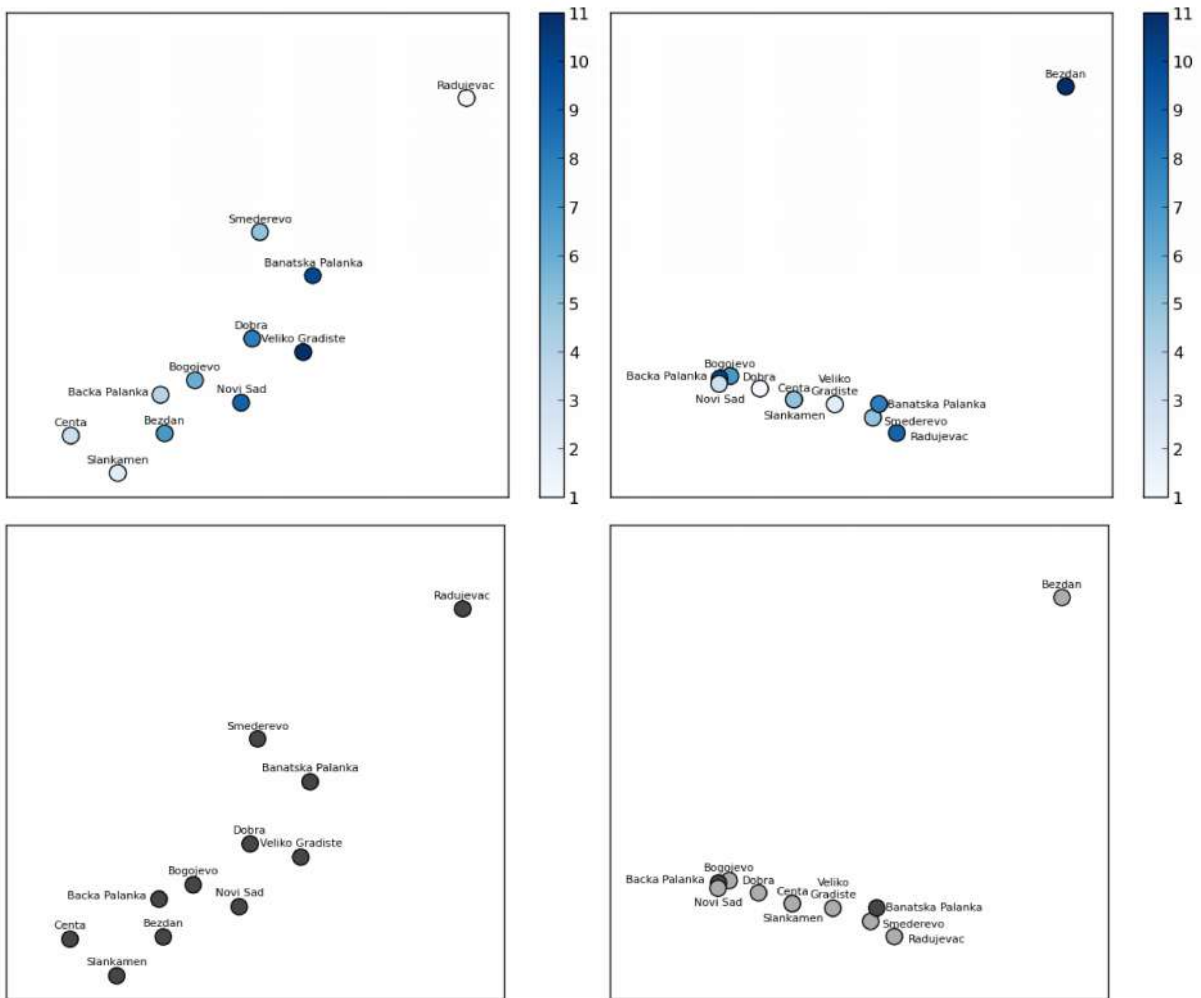


Figure 8: PCA projections for August (left-hand column) and October (right-hand column). The visualisations in the top row are coloured according to average rank while those in the bottom row are coloured according to the stations' SWQI classification.

Figure

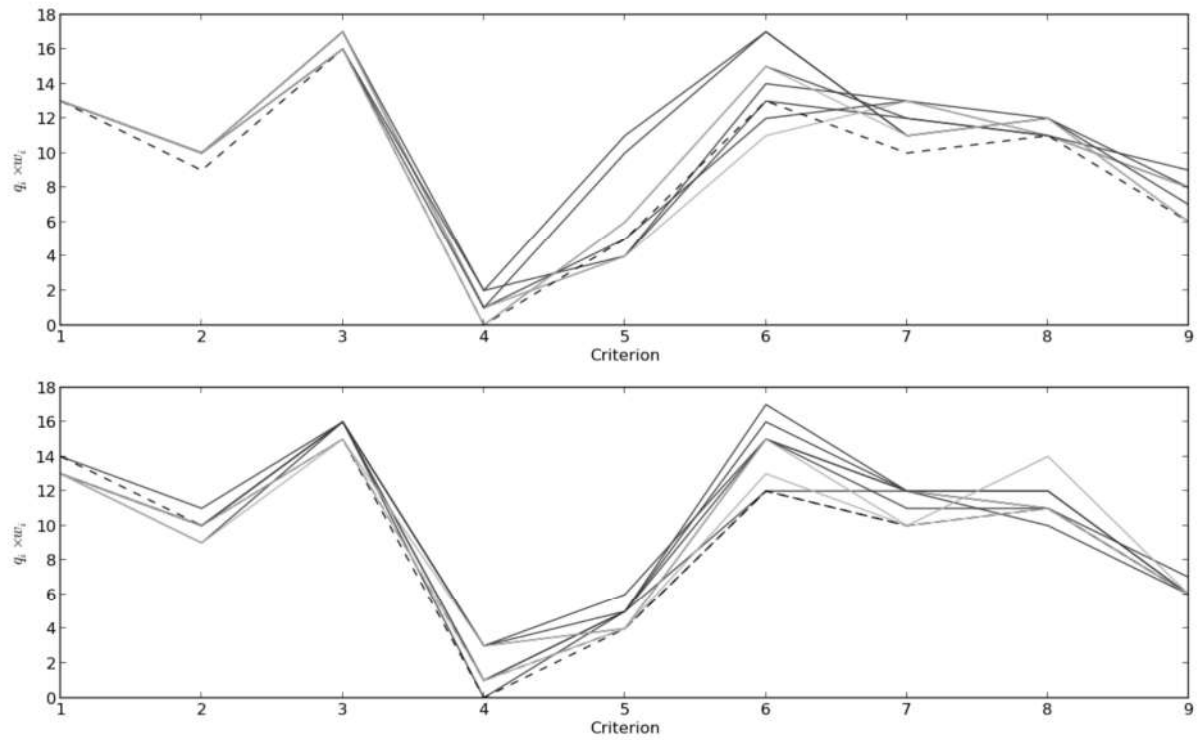


Figure 9: Parallel coordinate plots of the populations for February (top) and May (bottom). The colours correspond with that used for the SWQI scheme in earlier figures; white stations are now shown with a dashed line. With these plots it is possible to observe the individual criterion values of an individual, however it is more difficult to compare the overall quality of two stations.