

BICUBIC SPLINE ESTIMATOR FOR PROBABILITY DENSITY FUNCTIONS of RAW WATER PROPERTIES

M. Milivojevic¹, S. Obradovic¹, V. Stevanetic², D. Drndarevic¹

¹Technical and Business College, Uzice, Serbia, milovan.milivojevic@vpts.edu.rs,
srdjan.obradovic66@gmail.com, dragoljub.drndarevic@gmail.com

²Institute for Public Health, Uzice, Uzice, Serbia, vlasto.stevanetic@hotmail.rs

Abstract: *Drinking water represents a limited natural resource on the planet Earth, and will, in the time to come, be the focus of scientific research related to sustainable development strategy (SDS). SDS concerning with raw and drinking water as support implies the application of wide array of statistical and mathematical techniques, econometric tools and artificial intelligence heuristics. In this paper, a contribution to one such strategy based on 3D probability density functions (PDF) has been presented. Modeling probability density function was carried out by Bicubic Spline software Estimator-a developed by the authors in Visual Studio 12, the C# programming environment. PDFs have been modeled for raw water properties (physical-chemical, microbiological, and other parameters) for the Case Study in the district of Zlatibor the Republic of Serbia which has the number over 320.000.000 inhabitants. The obtained PDFs of raw water quality, could be essential for the management and planning of the drinking water supply in the future.*

Keywords: *Quality of Raw Water, Probability Density Function, Bicubic Spline Estimator*

1. INTRODUCTION

Providing safe drinking water is a major concern worldwide. Republic of Serbia, according to the SWQI (Serbian Water Quality Index) [1], could be considered a country very rich in water resources [2]. However, international rivers, such as the Danube, Tamiš, Sava..., which constitute 90% of Serbia's water territory, cannot be treated as Serbia's watery wealth, and cannot be used reliably. These lowland rivers, carry with them silt and pollutants, and considering they pass through many countries, they contain industrial and household wastewater. Thus, only 10% of Serbian water resources are domestic, which makes the country water-poor. Therefore, Serbia needs to pay attention to the rational use of existing resources, harmonization of raw and drinking water treatment and distribution systems, and economize in the use of reagents for water purification [3]. Based on the above, strategy of sustainable development (SSD) in the Republic of Serbia implies, among other things, quality management and planning of raw and drinking water resources, and application of a wide array of statistical methods, mathematical techniques, econometric tools and artificial intelligence heuristics (AI).

Although AI techniques are increasingly being applied in modeling quality, processes and properties related to raw and drinking water, the traditional statistical approach is still relevant. The advantages of the statistical models are the simplicity of formulation, the speed of execution and the availability of any type of correlation between independent and response variables [4]. The application of statistical methods often involves water quality stochastic variables based on interpolation by cubic or bicubic splines modeling.

In [5], Jones et al. investigate the ingestion of nitrate and nitrite from drinking water and diet and bladder cancer risk in women among a cohort of 34,708 postmenopausal women in Iowa (1986-2010). The authors used Cox regression to estimate hazard ratios (HR). In drinking water analyses, they compared average nitrate exposure quartiles to the lowest exposure category (Q1). They divided years $> \frac{1}{2}$ -MCL at the median (4 years) and compared to those with no years of exposure at this level. They evaluated the linearity of these relationships by modeling the exposures as continuous variables and by including cubic splines and quadratic exposure terms. Nolz et al. in [6], use a natural cubic spline to smoothing data in determining soil water balance components using an irrigated grass lysimeter in NE Austria. Authors in [7] characterize bivariate short-term temporal relationships among weather, turbidity, and diarrhea ED visits. They first removed the influence of shared trends, seasonal cycles, and day of week patterns from the short-term relationships among the variables by de-trending each time series in a generalized linear model using natural cubic splines with six degrees of freedom per season and a day-of-week indicator variable. In [8] K. Fujinawa studies the future impacts of global climate change, sea-level rise, and adaptation of irrigation practices on groundwater flow, the salinity of groundwater, and salt accumulation on the land surface. He used de Boor's bi-cubic spline function, to simulate a convective-dispersive transfer of heat in porous media. In [9] Holmes examined the relationship between soil erosion and water treatment. He estimated the relationship between water turbidity levels and typical treatment costs using a

cubic spline regression. He used these results to estimate background national turbidity-related water production expenses. Tina M. et al. in [10] use bicubic splines for modeling the Dead Sea depression. The application of statistical methods also involves modeling of probability density functions (PDFs) for stochastic variables related to water quality [11, 12, 13].

Based on the above, the goal of research presented in this paper was the development of a bicubic spline software estimator (**bcSSe**) intended for estimation of 2D probability density functions (PDFs) of raw water quality parameters. Performance of *bcSSe* software module is validated in the Case Study and data collected in the district of Zlatibor in the southwest part of Republic of Serbia.

2. THEORETICAL BACKGROUND

The following two sections describe basic theoretical elements (probability density functions and bicubic interpolation) based on which *bcSSe* software module was developed. In addition to the theoretical background, the properties of raw water, which are the focus of this paper, are briefly described.

2.1. Density function

A random variable X has a probability density function (PDF) f_X , where f_X is a non-negative Lebesgue-integrable function, if (eq. 1) [14]:

$$\Pr[a \leq X \leq b] = \int_a^b f_X(x) dx \quad (1)$$

For continuous random variables X_1, \dots, X_n , a probability density function is function of the n variables, such that, for any domain D in the n -dimensional space of the values of the variables X_1, \dots, X_n , the probability that a realization of the set variables falls inside the domain D is (eq. 2):

$$\Pr(X_1, \dots, X_n \in D) = \int_D f_{X_1, \dots, X_n}(x_1, \dots, x_n) dx_1 \dots dx_n \quad (2)$$

2.2. Bicubic interpolation

Bicubic interpolation (Fig.1) is an extension of cubic interpolation for interpolating data points on a two regular dimensional grid [15]. Bicubic interpolation can be accomplished using either Lagrange polynomials, cubic splines, or cubic convolution algorithm [16].

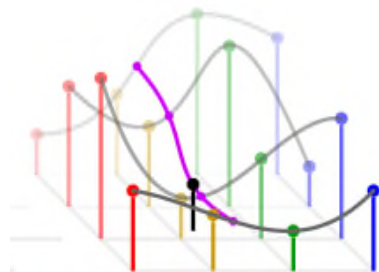


Fig. 1. Bicubic interpolation

For a function f and its derivatives f_x , f_y and f_{xy} , known at the four corners of the unit square $(0,0)$, $(0,1)$, $(1,0)$ and $(1,1)$, the interpolated surface can then be written as (eq. 3):

$$p(x, y) = \sum_{i=0}^3 \sum_{j=1}^3 a_{ij} \cdot x^i \cdot y^j \quad (3)$$

The interpolation problem consists of determining the 16 coefficients a_{ij} . Matching $p(x, y)$ with the function values yields four equations, eight equations for the derivatives in the x -direction and the y -direction

($f_x = \frac{\partial p(x, y)}{\partial x}$), ($f_y = \frac{\partial p(x, y)}{\partial y}$), and four equations for the cross derivative f_{xy} ($f_{xy} = \frac{\partial}{\partial y} \left(\frac{\partial p(x, y)}{\partial x} \right)$):

1. $f(0,0) = p(0,0) = a_{00}$
2. $f(1,0) = p(1,0) = a_{00} + a_{10} + a_{20} + a_{30}$
3. $f(0,1) = p(0,1) = a_{00} + a_{01} + a_{02} + a_{03}$
4. $f(1,1) = p(1,1) = \sum_{i=0}^3 \sum_{j=0}^3 a_{ij}$
5. $f_x(0,0) = p_x(0,0) = a_{10}$
6. $f_x(1,0) = p_x(1,0) = a_{10} + 2a_{20} + 3a_{30}$
7. $f_x(0,1) = p_x(0,1) = a_{10} + a_{11} + a_{12} + a_{13}$
8. $f_x(1,1) = p_x(1,1) = \sum_{i=1}^3 \sum_{j=0}^3 a_{ij} \cdot i$
9. $f_y(0,0) = p_y(0,0) = a_{01}$
10. $f_y(1,0) = p_y(1,0) = a_{01} + a_{11} + a_{21} + a_{31}$
11. $f_y(0,1) = p_y(0,1) = a_{01} + 2a_{02} + 3a_{03}$
12. $f_y(1,1) = p_y(1,1) = \sum_{i=0}^3 \sum_{j=1}^3 a_{ij} \cdot j$
13. $f_{xy}(0,0) = p_{xy}(0,0) = a_{11}$
14. $f_{xy}(1,0) = p_{xy}(1,0) = a_{11} + 2a_{21} + 3a_{31}$
15. $f_{xy}(0,1) = p_{xy}(0,1) = a_{11} + 2a_{12} + 3a_{13}$
16. $f_{xy}(1,1) = p_{xy}(1,1) = \sum_{i=1}^3 \sum_{j=0}^3 a_{ij} \cdot i \cdot j$

structure (6c, Fig. 2) and its potential roles in the system of monitoring the quality of raw water in the Institute for Public Health, Uzice (PHU), are presented on Fig. 2. The presented scheme can be generalized: raw water intakes from the Zlatibor region would be replaced by the specific locations from the other parts of the Republic of Serbia. The appropriate Institute would take the function of the PHU for (Institute of Public Health of Serbia Dr Milan JovanovicBatut et al.).

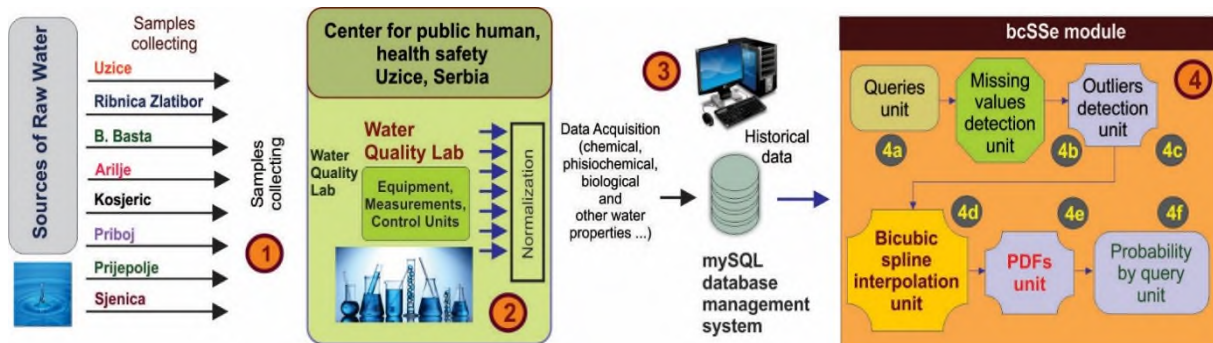


Figure 2: Schematic view of bcSSe module's structure

From the appropriate water intakes (1), according to the prescribed standards, methods, and sampling dynamics, raw water samples are collected and analyzed in public health institutions (2). By means of measuring equipment, the measured values of chemical, physicochemical, physical, biological and other properties of raw water are stored in the database (3). MySQL DBMS was used to manage data. The *bcSSe* software module consists of several units. *Queries unit* (4a) based on pre-defined queries or queries requested by the user will return the appropriate records. For data pre-processing, the *Missing values detection unit* (4b) and *Outliers detection unit* (4b) are employed. Component (4d, *Bicubic spline interpolation unit*) for selected stochastic input variables and data points on a two-dimensional grid realizes bicubic interpolation in accordance with the theoretical framework described in Section 2.2. Graphical representations and estimation of 2D PDFs are entrusted to the *PDFs unit module* (4e), and the estimation of the probability of the existence of raw water, characteristics specified in an interval, *Probability by Query Unit* (4f).

4. CASE STUDY

The following section presents the validation of the developed *bcSSe* software module.

4.1. Location description

The historical data set was collected in the region of Zlatibor in the western part of Republic of Serbia, which together have over 320.000 inhabitants (Fig. 3). Samples were collected from 8 water intakes (Fig. 3): Uzice (Source: Sušičkavrela, Susica river), Zlatibor (Reservoir on Ribnica River, Ribnica lake), Arilje (Rzav river), Kosjeric (Sources: Taorskavrela, Despotovica), Bajina Bašta (Source: by the river Drina), Priboj (Reservoir on the river Uvac - Radoinjskolake), Prijepolje (Source: Seljašnica) and Sjenica (Source: Vrelo). The waters of the Zlatibor district, which are the subject of research in this paper, can be divided into two groups: *surface waters* (Arilje, Priboj, Zlatibor) and *spring (underground) waters* (Uzice, Bajina Bašta, Kosjeric, Prijepolje, Sjenica). Rivers Rzav, Uvac (middle watercourses) and Ribnica (small watercourse) are above 500 AMSL, have good ecological status and do not contain polluting substances. All the mentioned water sources have good chemical properties, i.e. they do not contain contaminating substances that would significantly impair the use for human use.

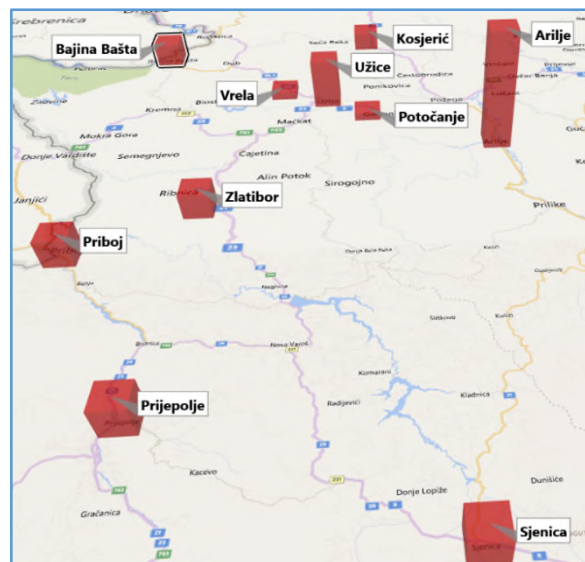


Figure 3: Locations of raw water intakes in the Zlatibor district, in the south-west part of Republic of Serbia.

4.2. Dataset. Variables, acquisition and equipment

The historical data set ((3), Fig.2) was collected at the 8 locations in Zlatibor region, for the period of 01.01.2015. to 31.12.2016 (*dd.mm.yydate* formatting was applied). The database contained 814 records with values of attributes that define primary quality of raw water.

The *bcSSe* module ((4), Fig. 2) has an input vector which contains 6 variables from which the quality of the primary characteristics of the raw water can be evaluated. The primary characteristics of raw water are indicated with the following variables: *T*, *Turbidity*, *pH*, *Ec*, *Oxid*, and *Chlor*, which represent: temperature, turbidity, pH value, electrical conductivity (20⁰C), oxidizability - potassium permanganate consumption (KMnO₄) and chlorides (Cl), respectively. The historical data set was collected in *The Laboratory for quality control of water*, in the *Institute for Public Health, Uzice, Serbia* (Fig.4).



Figure 4: Institute for Public Health, Uzice, Serbia

Measuring of raw water properties was achieved by using the following laboratory equipment: the *pH* value were measured using the *Hach USApH* Meter, type:*Sension 3*, range: 0-14/method: P-IV- 6/A, C3333, 1990;*turbidity* was measured using the *HACH 2100N-ISTurbidimeter*, range: 0-1000 FNU/method: EN ISO 7027;*electrical conductivity* were measured on the ((Hach USAConductometer, type: *Sension 7*, ranges: 0-19.99μS/cm, 20-199.9μS/cm, 200-1999 μS/cm))/method: EN27888:1993. Determination of KMnO₄ consumption(*oxidizability*): glass burette, 50 mL, lab hotplate, /method: P-IV-9a, C3333, 1990. The remaining parameters were measured and determined by applying the appropriate analytical methods. Table 1 lists the elements of descriptive statistic for the input data for all water intakes, separately.

Table 1. Historical dataset of raw water quality - descriptive statistics

Locat.		Chl.	Oxid.	Ec	pH	Turb.	T	Locat.	Chl.	Oxid.	Ec	pH	Turb.	T
		[mg/l]	[mg/l]	[μS/cm]		[NTU]	[°C]		[mg/l]	[mg/l]	[μS/cm]		[NTU]	[°C]
Zlatibor	Min	4	14.8	123	7	0.6	2.5	Uzice	5	3.8	309	6.7	0.5	7.5
	Max	12	31.1	217	8.2	3.7	20.5	Samples	22	24.2	555	7.5	25.2	14.8
	Aver.	7.361	23.26	169.16	7.649	1.62	10.26	137	13.255	9.57	440.36	7.169	2.77	11.47
	StD	1.906	3.85	24.17	0.266	0.72	5.52		2.547	4.25	44.63	0.130	3.71	1.98
Prijepolje	Min	5	1.6	300	7.1	0.2	7	Priboj	5	2.8	248	7.2	0.3	6
	Max	15	6.6	403	7.9	4.8	12	Samples	11	20.8	380	7.9	9.5	16
	Aver.	6.833	3.36	354.06	7.590	0.93	10.00	69	7.406	5.92	296.00	7.575	0.85	11.00
	StD	1.547	1.14	24.44	0.157	0.82	1.03		1.565	2.18	30.94	0.131	1.12	2.43
B. Basta	Min	5	1.5	239	6.7	0.1	7	Sjenica	4	1.6	237	7.2	0.2	4
	Max	13	5.4	326	7.4	0.9	14	Samples	12	5.7	375	7.8	1	14
	Aver.	9.475	2.92	276.42	7.025	0.38	10.51	70	7.143	2.81	328.73	7.466	0.49	10.61
	StDev	1.633	0.83	18.78	0.142	0.16	1.65		1.627	0.83	23.78	0.144	0.17	1.56
Kosjeric	Min	6	1.9	401	6.9	0.3	6	Arilje	4	2.2	239	7.1	0.2	1
	Max	14.3	6.6	522	7.5	9	16	Samples	12	33	355	8.2	90.4	21
	Aver.	9.581	3.16	452.79	7.211	0.95	11.02	297	6.044	6.38	296.77	7.923	3.93	9.94
	StD	1.758	0.99	32.19	0.149	1.36	2.35		1.178	3.26	27.85	0.149	9.79	5.65

4.3. Methods

For each location, bicubic spline interpolation modeling is carried out for the following pairs: Turbidity/Oxidizability, Turbidity/Electrical conductivity and Electrical conductivity/Oxidizability. The remaining variables were not modeled by PDFs, because their values were significantly lower than the permissible ones. A total of 24 PDFs were modeled (3 models x 8 locations).

4.4. Results and discussion

In the course of the case study all modeling, experiments and simulations were performed on an Microsoft Windows 10 based PC with the following features: Intel i5-4670 CPU, Intel Z87 chipset, 8GB of DDR3. The proposed bicubic spline estimation, by its nature, does not provide the generation of PDFs in analytical form, so

two-dimensional models of PDFs for features of raw drinking water in the Zlatibor region, are shown graphically in Fig. 5a to Fig. 7b.

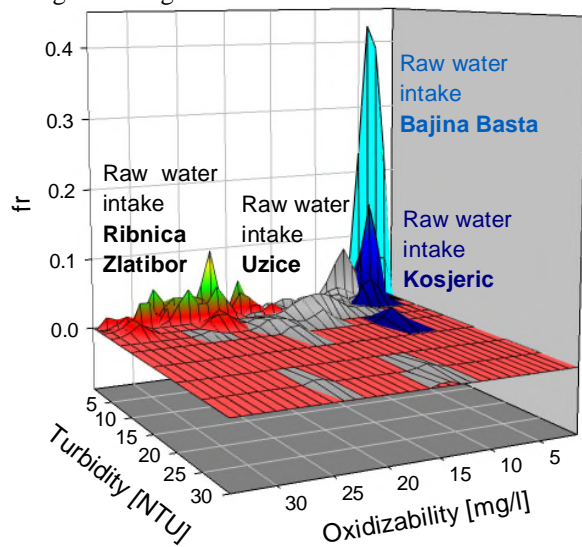


Figure 5a: PDFs(turbidity, oxidizability) 2015/16 of raw water in Zlatibor region for 2015/16

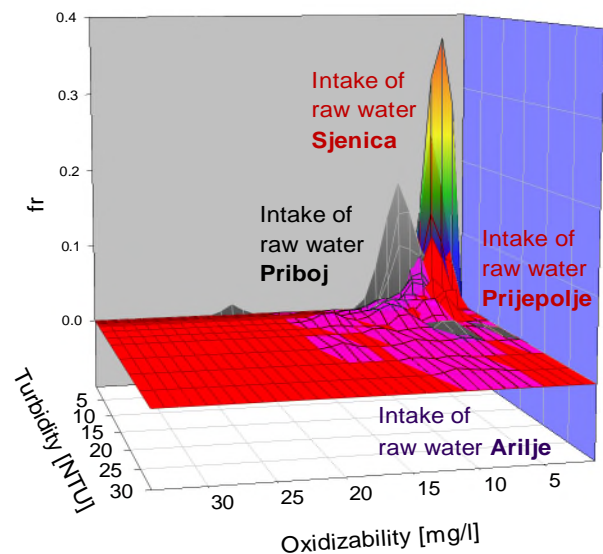


Figure 5b: PDFs(turbidity,oxidizability) 2015/16 of raw water in Zlatibor region for 2015/16

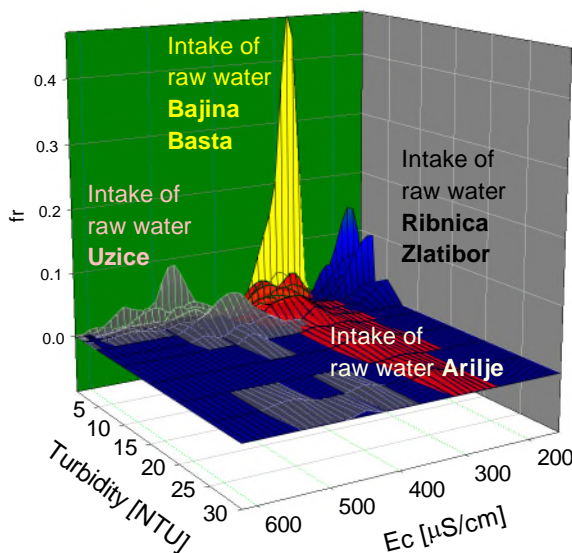


Figure 6a: PDFs(conductivity,turbidity) of raw water in Zlatibor region for 2015/16

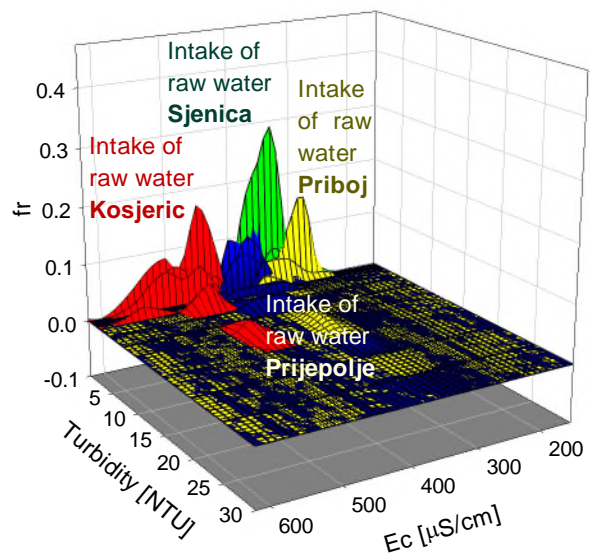


Figure 6b: PDFs(conductivity,turbidity) 2015/16 of raw water in Zlatibor region for 2015/16

With Fig. 5a and Fig. 5b, showing the density of distribution of probability of turbidity and oxidizability, it can be seen that the raw waters of the Zlatibor region can be classified into four groups / categories: I) RibnicaZlatibor (low level of turbidity and high oxidizability), II) Uzice (a wide range of oxidizability), III) Arilje (lower level of oxidizability and turbidity in a wide range) and IV) BajinaBašta, Kosjerić, Priboj, Prijepolje and Sjenica with the lowest values of turbidity and oxidizability.

High oxidizability value in the first category, Ribnica - Zlatibor is a consequence of specific biogeochemical processes in the drainage area of the Ribnica river / Zlatibor mountain, which lead to the increased values of humic matter in the water.Changes in water turbidity ofRibnicaare depreciated by the accumulation lake and depend on the erosive characteristics of the drainage area of the Ribnica River. The wide range of oxidizabilityvalues in the second group is due to the high dependence of the Sušica springs from precipitation, i.e. a large share of atmospheric water in rainy periods or periods of melting snow.The third category is the river Rzav, the water intake is on the river itself, whose drainage basinlies in a mountainous area (Čemernica, Mučanj, Zlatibor), the amount of water and features are very dependent on precipitation, which by the erosion of different terrains causes changes in turbidity and oxidizability.The fourth category, with the exception of Priboj, are groundwaters (springs), therefore protected from acute impacts of precipitation. Pribojgets water from

Radoinjsko Lake on the river Uvac, where there are three accumulating lakes on the river, and Radoinjsko is the last one. Practically, the river Uvac almost has no free flow, large water masses amortize changes in turbidity and oxidizability and stabilize their values. The lakes are located at altitudes from 800 to 1000 meters.

Fig. 6a and Fig. 6b, PDFs for turbidity and electrical conductivity are displayed. Four groups of water categories can be spotted again: I) Ribnica Zlatibor (low level of turbidity and electrical conductivity), II) Uzice and Kosjeric (wide range of turbidity and increased value of conductivity), III) Arilje (lower level of electrical conductivity and turbidity in a wide range) And IV) Bajina Bašta, Priboj, Prijepolje and Sjenica with the lowest values of turbidity and electrical conductivity in the lower range.

In the level of electroconductivity- oxidizability, each of the sites has a significant separation, except for the raw drinking water of Sjenica, Prijepolje and Priboj, which are characterized by the lower to medium level of electrical conductivity and very small oxidizability.

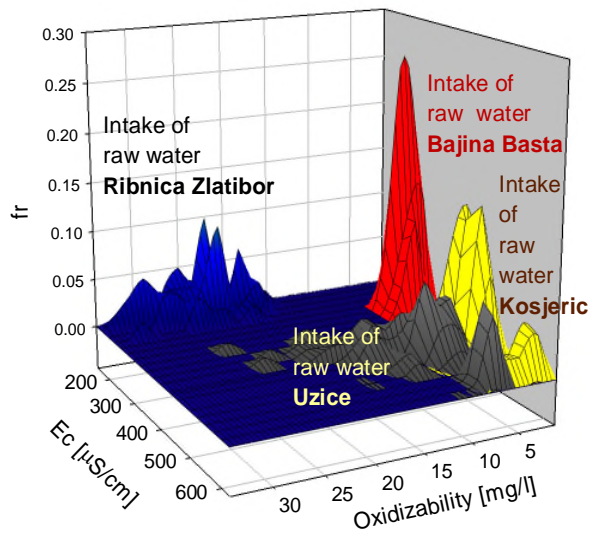


Figure 7a: PDFs (oxidizability, electroconductivity) of raw water in Zlatibor region for 2015/16

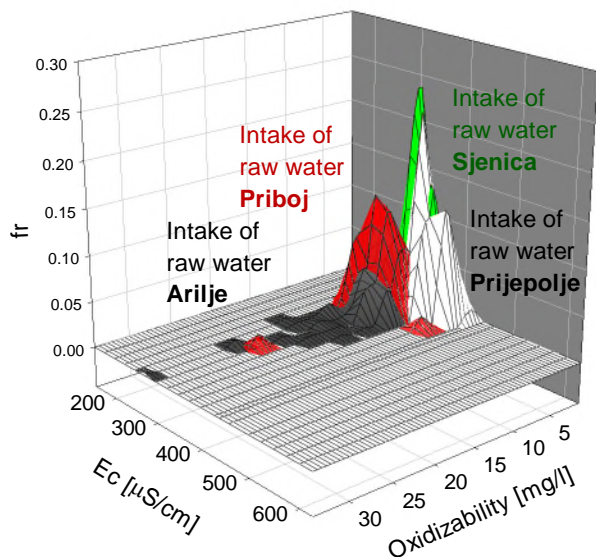


Figure 7b: PDFs (oxidizability, electroconductivity) of raw water in Zlatibor region for 2015/16 to 2015/16

In addition to the obtained PDFs for the raw drinking water of the Zlatibor district, for creating PDFs in the domain of quality management and planning of raw and drinking water resources in the Republic of Serbia (SDS), it is also important to assess the probability that the water properties of a water intake will be in a given 2D range.

Raw drinking Water properties:
Oxidizability: [20-25 mg/l]
Turbidity: [5-15 NTU]
probability: 11.23%

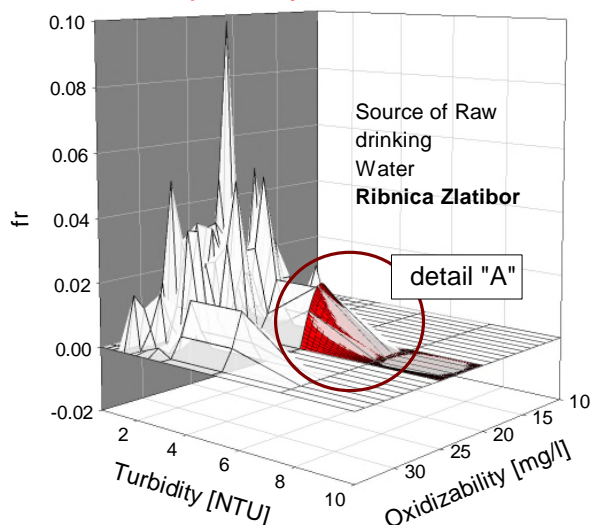


Figure 8: Estimated probability for turbidity-oxidizability to be in a given range for the Ribnica-Zlatibor water intake.

Raw drinking Water properties:
Oxidizability: [7-10 mg/l]
Ec: [400-525 µS/cm]
probability: 28.01%

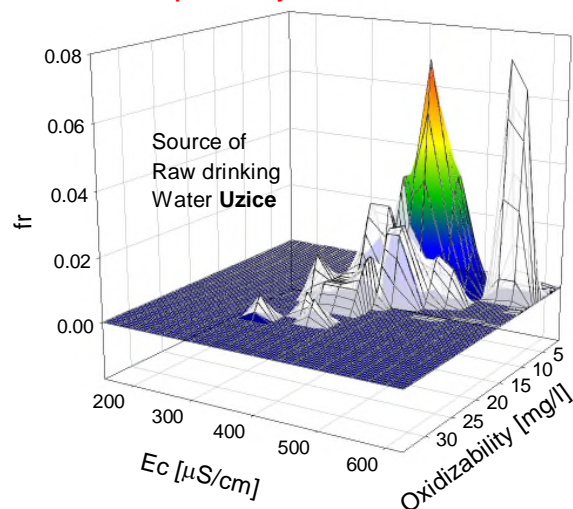


Figure 9: Estimated probability for conductivity-oxidizability to be in a given range for the Uzice-Susica water intake.

An example is the estimate of the probability that the raw water on the Ribnica-Zlatibor water intake will have the following characteristics: Oxidizability: [20-25 mg / l], Turbidity: [5-15 NTU]. The estimated probability of such an event is 11.23% and is calculated as a quotient of the volume below the PDF and the level of turbidity-oxidizability constrained by the given domain (Figure 8, detail "A") and the volume below the PDF surfaces for the entire research domain.

Similarly, the probability of raw water at the water intake Uzice (Susica) having the following values of properties: Ec: [400-525 μ S/cm], Oxid: [7-10] is 28.01% (Fig. 9, volume of PDF undercolored surface), while the probability of raw water from the Arilje (Rzav) water intake having the values of properties: Ec[230-275 μ S/cm], Turbidity: [5-15 NTU] is 7.29% (Fig. 10, detail "A" and Fig. 11)

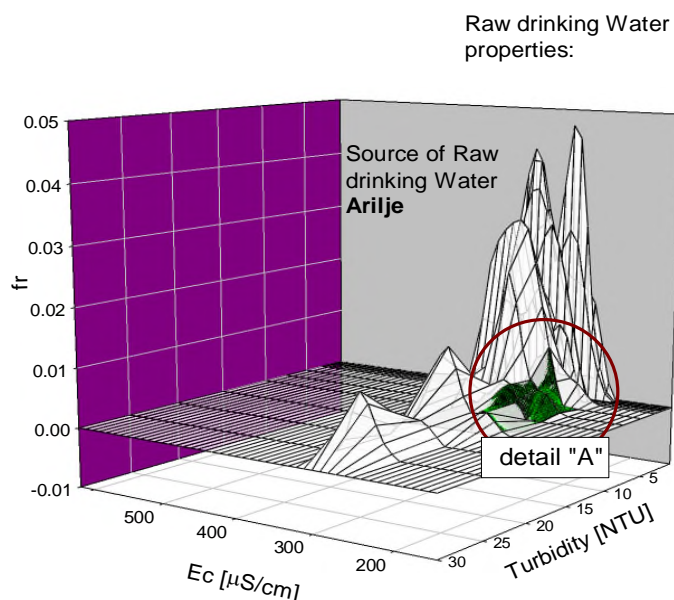


Figure 10: Estimated probability for turbidity-conductivity to be in a given range for the Arilje-Rzav water intake.

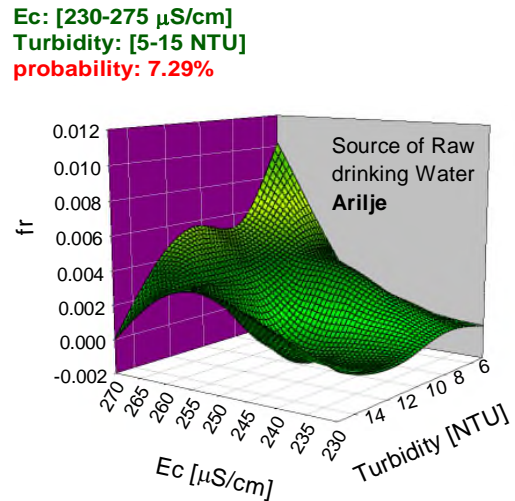


Figure 11: Event probability as the quotient of volume under PDF and volume under Ec-turbidity surface constrained by the given domain: detail "A" -enlarged-

5. CONCLUSION

Providing safe drinking water is a major concern worldwide. SSD in the Republic of Serbia in accordance with these trends implies quality management and planning of raw and drinking water resources and application of a wide array of statistical, mathematical, econometric tools and also artificial intelligence heuristics (AI), in this field. Although the application of AI techniques is on the rise, the traditional statistical approach, is still relevant. The application of statistical methods often involves water quality stochastic variables based on interpolation by cubic or bicubic splines modeling and modeling of its probability density functions (PDFs).

This paper presents a bicubic spline software estimator (*bcSSe*), developed by authors, intended for estimation of 2D probability density functions (PDFs) of raw water quality parameters. Performance of *bcSSe* software module is validated in the Case Study and data collected from eight raw water intakes in the Zlatibor region in the southwest part of Republic of Serbia. More than twenty PDFs 2D models were created for *turbidity-electroconductivity*, *turbidity-oxidizability* or *electroconductivity-oxidizability* planes. The performance of *bcSSe* was additionally tested by estimating the probability for a chosen pair of raw water properties to be in a given range. Examples are given for the water intakes Uzice, Arilje and Ribnica-Zlatibor, which represent water sources for most of the population of the Zlatibor district and surrounding regions. The obtained PDFs of raw water features quality, could be essential for the management and planning of the drinking water supply in the future.

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