Desalination and Water Treatment
www.deswater.com

doi: 10.5004/dwt.2017.21525

95 (2017) 45–50
November

Fuzzy logic regression analysis for groundwater quality characteristics

Chris Evangelides[a,*], George Arampatzis[b], Christos Tzimopoulos[a]

[a]*Department of Hydraulics and Transportation Engineering, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece, Tel. +30 2310 996147; Fax: +30 2310 996147; email: evan@vergina.eng.auth.gr (C. Evangelides), Tel. +30 2310 996141; Fax: +30 2310 996049; email: ctzimop@gmail.com (C. Tzimopoulos)*
[b]*Soil and Water Resources Institute, Hellenic Agricultural Organisation-DEMETER, 57400 Sindos, Greece, Tel. +30 2310 798790; Fax: +30 2310 796352; email: arampgeo@gmail.com*

Received 14 July 2017; Accepted 5 October 2017

ABSTRACT

Fuzzy logic is applied in many problems that contain uncertainty. Specifically, fuzzy regression analysis can supply useful information about the validity of measured quantities. This article examines the variation of certain quality characteristics of groundwater in boreholes using fuzzy methodology. Traditionally, classical correlation analysis was used to depict the relation between the dependent variable and the independent variables. Classical regression is considered to be probabilistic and has many uses but can be problematic: (a) if the data set is small, (b) if the error distribution is not normal, (c) if there is uncertainty between dependent and independent variables or if linearity acceptance is not proper. For the previous reasons fuzzy regression analysis is preferable. Water was sampled from these boreholes by Institute of Geology and Mineral Exploration from 2005 to 2008 and the concentration spread of Ca, K and Mg ions was examined. Using fuzzy regression, the range of these concentrations was calculated during the period under consideration with inclusion equations and results are presented in graphic form. All the measured values were taken into account in order to obtain an estimation of future measurement accuracy with a confidence level according to historical values and similar regional conditions.

Keywords: Fuzzy regression; Groundwater quality; Measurement uncertainty; Concentration

1. Introduction

Water is a renewable natural resource, which is necessary for every activity on earth, and also for the ecological balance. It is used not only in covering the needs of urban and tourist areas, agriculture, industry and crafts but also in maintaining a sustainable operation of wetlands.

Traditional methods of water quality assessment, based solely on the comparison of analytical parametric values or calculation of molar ratios [1,2], can be very helpful, but in most cases they do not provide a convenient supervisory correlation between the examined samples. Furthermore, such an analysis requires comprehensive knowledge of water science to understand and may not provide a composite measure of water quality [3]. Therefore appropriate analysis and knowledge translation tools are required to bridge the communication gaps among scientists, policy makers and public [4].

In all physical problems, there is a relationship between precision and uncertainty. The more uncertainty that exists in a problem, the less precise the understanding of that problem is. The more complex a system is, the more imprecise or inexact is the information that is available to characterize that system. It is reasonable to dedicate a certain level of uncertainty within problems, such that an appropriate level of precision can be expressed. Today fuzzy systems are shown to be universal approximators to algebraic functions. Classical correlation analysis was used to depict the relation between the dependent variable and the independent variables. According to this, classical regression is considered to be

* Corresponding author.

probabilistic and has many uses, but can be rendered problematic: (a) if the data set is small, (b) if it is hard to prove that error distribution is normal, (c) if there is fuzziness between dependent and independent variables or if linearity acceptance is not proper [5].

Nowadays, new regression models have been introduced based on fuzzy logic [6–14]. In fuzzy regression, the difference between measurement values and estimated values is attributed to the inherent fuzziness of the system as well as to the fuzziness of input and output data. In contrast with classical regression analysis, fuzzy regression analysis uses fuzzy functions for the regression factors. The above problem [9,15] usually meets one of the three cases, described below: (a) crisp input values x_{ij} and crisp output values y_j, (b) crisp input values x_{ij} and fuzzy output values $\tilde{y}_i$ and (c) fuzzy input values $\tilde{x}_{ij}$ and fuzzy output values $\tilde{y}_i$.

In all the above cases, estimated values $\tilde{Y}_i$ are fuzzy. The adjustment of a fuzzy regression model can be achieved through two general methods:

The possibilistic model [5–7,15]: fuzzy regression is considered possibilistic when the membership function $\mu_{\tilde{F}}$ of a fuzzy number $\tilde{F}$ is considered equal to the possibility distribution function $\pi_x(x)$. The fuzziness of the model is minimized by taking into account the minimum of the spreads around the center of the fuzzy parameters, while considering that the values of every sample are within a specific interval of possible values.

The least squares model [16–18]: the distance between the estimated output value of the model $\tilde{Y}_i$ and the observed output value $\tilde{y}_i$ is minimized. This method of Diamond [16] is considered to be an extension of the classical linear regression method, based on the notion of model efficiency optimization depending on data.

This article examines the irrigation water quality, derived from surface and groundwater reservoirs. Especially, the variation of certain quality characteristics of groundwater is examined in two boreholes at SE Pinios' basin in Greece. Water was sampled from these boreholes by Institute of Geology and Mineral Exploration (IGME) from 2005 to 2008 [19]. Chemical analyses were taken place at the laboratory of IGME and this article examines the concentrations spread of Ca, K and Mg ions. Using fuzzy correlation, the range of these concentrations was calculated during the period under consideration. Knowing the confidence limits of these ions in a specific period of time and assuming that the management of land and water does not have significant variations then conclusions about the accuracy of future measurements can be obtained utilizing the methodology, which was developed and presented in this article.

2. Mathematical problem

A possibilistic model, where membership functions are trapezoidal, measured input values are crisp and measured output values are triangular fuzzy, is described. The need to use trapezoidal functions is a result of the following reasons [20–22]:

- need to optimize the fuzziness of the model
- need to restrict data inside the estimated value range.

In order to achieve the restriction, a-cuts are used and we aim to restrict for a level of confidence $h = \alpha_0$ that is high enough. However, that could lead to highly inaccurate parameters. According to Moskowitz and Kim [23], the h parameter is referred to as the fitness degree of the estimated fuzzy linear model to the given data. A physical interpretation of h is that an observation $\tilde{y}_i$ is contained in the support interval of the corresponding fuzzy estimate $\tilde{Y}_i$, which has a degree of membership $\geq h_i$. Moreover, solution optimization for level h does not guarantee the same for another level $h' \neq h$. Tanaka and Watada [8] provided the equations for this scenario, but they can only be applied when data is crisp. Thus, restrictions of high confidence levels interfere with model precision. Moreover, constraint for confidence level $h = 1$ and data with triangular membership functions is impossible with the exception of the special case of collinear data.

Using trapezoidal membership functions for estimated values [20–22] allows us to achieve inclusion for output measured data with triangular membership functions $\tilde{y}_i$ (x) and estimated values with trapezoidal membership functions $\tilde{Y}_i$ (x), for confidence level $h = 1$, for which the kernel is not minimized in a point: $[\tilde{y}_i]_{h=1} \subseteq [\tilde{Y}_i]_{h=1}$. In addition, for a level of confidence $h = 0$, inclusion is achieved: $[\tilde{y}_i]_{h=0} \subseteq [\tilde{Y}_i]_{h=0}$. Due to the linearity of the membership function, inclusion for those levels of confidence allows us to ensure that inclusion is possible for every level of confidence: $[\tilde{y}_i]_h \subseteq [\tilde{Y}_i]_h, \forall h \in [0,1]$.

In this article, a possibilistic model is described [14] different from Bisserier model, where membership functions are trapezoidal, measured input values are crisp and measured output values are fuzzy and triangular, divided in two steps. In the general case of trapezoidal membership functions, the estimated value is given as follows:

$$\tilde{Y}_i = \tilde{A}_0 + \tilde{A}_1 x_{1j} + \tilde{A}_2 x_{2j} + \ldots + \tilde{A}_n x_{nj} = \sum_{i=0}^{n} \tilde{A}_i x_{ij}, \quad x_{0j}=1 \tag{1}$$

where

$\tilde{A} = ([K_A^-, K_A^+], [S_A^-, S_A^+])$,

$K_{\tilde{A}} = \text{kernel}(\tilde{A}) = [K_A^-, K_A^+]$

$S_{\tilde{A}} = \text{supp}(\tilde{A}) = [S_A^-, S_A^+]$

Based on the above, median (M) and radius (R) are:

Kernel:

$$M_{K_{\tilde{A}}} = (K_A^- + K_A^+)/2, \; R_{K_{\tilde{A}}} = (K_A^+ - K_A^-)/2$$

Supports:

$$M_{S_{\tilde{A}}} = (S_A^- + S_A^+)/2, \quad R_{S_{\tilde{A}}} = (S_A^+ - S_A^-)/2$$

In the case of triangular membership function, the following apply:

Kernel: k. In case of symmetry $k = k_A$

Supports:

$$M_{S_{\tilde{A}}} = (S_A^- + S_A^+)/2 = k_A, \; R_{S_{\tilde{A}}} = (S_A^+ - S_A^-)/2$$

The problem can now be divided into the following two steps:

Step 1: Kernel inclusion:

$$k_{\tilde{y}_j} \in \left[K^-_{\tilde{y}_j}, K^+_{\tilde{y}_j} \right] \tag{2}$$

Namely the kernel of measured values is included in the kernel of estimated values. According to Shapiro et al. [24], for the case of crisp output values only measured values are included in the kernel. According to Tanaka's method [7], the range $\left[Y^-, Y^+\right]^{h=0}$ encircles the kernels of measured values. In this stage, only triangular functions $\tilde{A}_0\left(r_0, c_0\right), \tilde{A}_1\left(r_1, c_1\right)$ are applied for the method of Tanaka and the possibilistic model is: $\tilde{Y}_i = \tilde{A}_0 + \tilde{A}_1 x_{1j}$ The elements r,c are the mean and the spread of the parameter $\tilde{A}$, respectively. Thus, the problem of determining the estimated values becomes:

$$\min(c) = mc_0 + c_1 \sum_{j=1}^{m} x_{1j}, \text{ where } c_0 \text{ and } c_1 \geq 0 \tag{3}$$

s.t.

$$\begin{aligned} (a) \quad & Y_j^+ = \sum_{i=0}^{1} r_i x_{ij} + \sum_{i=0}^{1} c_i x_{ij} \geq y_j \\ (b) \quad & Y_j^- = \sum_{i=0}^{1} r_i x_{ij} - \sum_{i=0}^{1} c_i x_{ij} \leq y_j,\ x_{0j} = 1 \end{aligned} \tag{4}$$

where i is the number of variables 0,1 and j is the number of measured values 1,2,….,m.

Through the solution of this system the surroundings $\left[\tilde{Y}\right]_{\pm} = \left[Y^-, Y^+\right]^{h=0}$ is as follows:

$$\begin{aligned} (a) \quad & Y^+ = (r_0 + c_0) + (r_1 + c_1)x \\ (b) \quad & Y^- = (r_0 - c_0) + (r_1 - c_1)x \end{aligned} \tag{5}$$

As long as they meet the same constraint, these surroundings coincide with the kernel of trapezoidal functions, resulting to the relations below:

$$\begin{aligned} Y^- &= K^-_{\tilde{Y}_j} = K^-_{\tilde{A}_0} + K^-_{\tilde{A}_1} x_{1j}, \quad j = 1, \text{ .... } m \\ Y^+ &= K^+_{\tilde{Y}_j} = K^+_{\tilde{A}_0} + K^+_{\tilde{A}_1} x_{1j}, \quad j = 1, \text{ .... } m \end{aligned} \tag{6}$$

Step 2: Support inclusion is applied:

$$[S^-_{\tilde{y}_j}, S^+_{\tilde{y}_j}] \subseteq [S^-_{\tilde{Y}_j}, S^+_{\tilde{Y}_j}], \tag{7}$$

where space $S^-_{\tilde{y}_j}, S^+_{\tilde{y}_j}$ is given as follows:

$$[S^-_{\tilde{y}_j} = y_j - e_j = y_j^-, S^+_{\tilde{y}_j} = y_j + e_j = y_j^+] \tag{8}$$

Based on relations (4) and (8):

$$K^-_{\tilde{Y}_j} - \sum_{i=0}^{1} c_i^- x_{ij} \leq y_j - e_j, \qquad x_{0j} = 1, \tag{9}$$

$$K^+_{\tilde{Y}_j} + \sum_{i=0}^{1} c_i^+ x_{ij} \geq y_j + e_j, \quad x_{0j} = 1, \quad j = 1,2,\text{....} m \tag{10}$$

where $K^+_{\tilde{Y}_j}$ and $K^-_{\tilde{Y}_j}$ are known since they have been calculated during step 1.

The problem now becomes:

$$\min(c) = m(c_0^- + c_0^+) + (c_1^- + c_1^+) \sum_{j=1}^{m} x_{1j}, \quad c_0^-, c_0^+, c_1^-, c_1^+ \geq 0 \tag{11}$$

s.t.

$$\begin{aligned} & K^-_{\tilde{Y}_j} - \sum_{i=0}^{1} c_i^- x_{ij} \leq y_j - e_j, \quad x_{0j} = 1 \\ & K^+_{\tilde{Y}_j} + \sum_{i=0}^{1} c_i^+ x_{ij} \geq y_j + e_j, \quad x_{0j} = 1 \end{aligned} \qquad j = 1,2, \text{....} m \tag{12}$$

3. Materials and methods

Water samples were selected from two boreholes (ϒΓ3 and ϒΓ6) at SE Pinios' basin in Greece during the period 2005–2008. Both boreholes belong to the same aquifer. The samples were analyzed for concentrations of Ca, K and Mg ions in the laboratory. Representative values of the specific ions from both boreholes were recorded for the above time period. The collection of the samples was not carried out at the same time intervals and samples for K were collected more times, but were representative. The exact location of the boreholes is given by their coordinates, where ϒΓ3 has longitude 22°41′10.8588″E and latitude 39°14′26.7138″N and ϒΓ6 has longitude 22°44′15.6793″E and latitude 39°12′33.3763″N. The transport of water samples and the conservation at the laboratory were done under special conditions in order to preserve sample validity. The concentrations of Ca, K and Mg for ϒΓ3 and ϒΓ6 are presented in Table 1.

In this application measurements were available for two boreholes that belonged to the same aquifer and so the values from one borehole are considered as input values (x) and the values of the other borehole as output values (y). Triangular membership functions are used in order to convert crisp measured values to fuzzy values. An assumption is made that measurements of (y) output values contain a 20% error, since this contains the total error of the whole procedure from sampling to final laboratory results, as shown in Table 1. Furthermore fuzzy regression analysis was carried out using trapezoidal membership functions. All the sample values were taken into account in order to obtain an estimation of future measurement accuracy with a confidence level according to historical values and similar conditions.

4. Results and discussion

Fuzzy logic regression analysis was carried out using the available data of the two boreholes, as described above. Input data is converted into fuzzy using triangular membership functions. Afterwards assuming a percentage error (e), output values are calculated utilizing trapezoidal membership functions. The equations and the results for all three element concentration are presented.

Utilizing the measured values from Table 1, the process described previously was applied to the elements of the table and the application with the results is shown with the corresponding figures below.

Application 1 for Ca

Step 1

According to Tanaka's model, considering that output data is crisp and for h = 0, the model is described by the following equations:

Table 1
Concentrations of Ca (mg/L), K (mg/L) and Mg (mg/L) for the boreholes ϒΓ3 and ϒΓ6

Ca (mg/L)			K (mg/L)			Mg (mg/L)		
ϒΓ3	ϒΓ6	e = 0.2*ϒΓ6	ϒΓ3	ϒΓ6	e = 0.2*ϒΓ6	ϒΓ6	ϒΓ3	e = 0.2*ϒΓ3
$x_{1,j}$	y_j	e_j	$x_{1,j}$	y_j	e_j	$x_{1,j}$	y_j	e_j
105.81	96.19	19.2	0.78	1.56	0.31	13.25	14.95	3.0
101.00	109.00	21.8	0.78	1.56	0.31	25.29	16.54	3.3
59.32	70.54	14.1	0.80	0.80	0.16	28.70	23.10	4.6
64.13	64.13	12.8	0.78	1.56	0.31	14.59	16.54	3.3
84.97	80.16	16.0	0.43	0.87	0.17	24.32	16.54	3.3
74.63	67.74	13.5	0.87	1.30	0.26	17.51	13.13	2.6
56.91	73.35	14.7	0.43	0.87	0.17	20.43	15.08	3.0
83.37	94.59	18.9	0.87	1.74	0.35	21.40	17.30	3.5
52.90	76.20	15.2	1.74	2.61	0.52	15.10	13.10	2.6
69.70	83.40	16.7	1.00	1.30	0.26	30.60	30.60	6.1
69.70	69.70	13.9	0.40	1.30	0.26	9.20	13.60	2.7
			0.90	0.90	0.18			
			0.90	1.30	0.26			
			0.90	1.30	0.26			

$$\begin{aligned}
&\min(11c_0 + 822.44c_1)\\
&\text{s.t.}\\
&r_0 - c_0 + 105.8r_1 - 105.8c_1 \le 96.2\\
&\ldots\ldots\ldots\ldots\ldots\ldots\\
&r_0 - c_0 + 69.7r_1 - 69.7c_1 \le 69.7\\
&r_0 + c_0 + 105.8r_1 + 105.8c_1 \ge 96.2\\
&\ldots\ldots\ldots\ldots\ldots\ldots\\
&r_0 + c_0 + 69.7r_1 + 69.7c_1 \ge 69.7
\end{aligned} \tag{13}$$

Solving the above system of equations, kernel equations are obtained (Fig. 1):

$$\begin{aligned}
y^- &= 16.8448 + 0.6819x,\\
y^+ &= 40.1268 + 0.6819x
\end{aligned} \tag{14}$$

Step 2

In step 2, the kernel is considered to be known from the previous step and the model takes the form:

$$\begin{aligned}
&\min\{11(c_0^- + c_0^+) + 822.44(c_1^- + c_1^+)\}\\
&\text{s.t.}\\
&-c_0^- - 105.81c_1^- \le -12.04\\
&\ldots\ldots\ldots\ldots\ldots\ldots\\
&-c_0^- - 69.70c_1^- \le -8.61\\
&c_0^+ + 105.81c_1^+ \ge 3.15\\
&\ldots\ldots\ldots\ldots\ldots\ldots\\
&c_0^+ + 69.70c_1^+ \ge -4.02
\end{aligned} \tag{15}$$

Finally, solving the above system of equations, support equations are obtained (Fig. 1):

$$\begin{aligned}
y^- &= 16.8448 + 0.5004x,\\
y^+ &= 40.1268 + 0.9700x
\end{aligned} \tag{16}$$

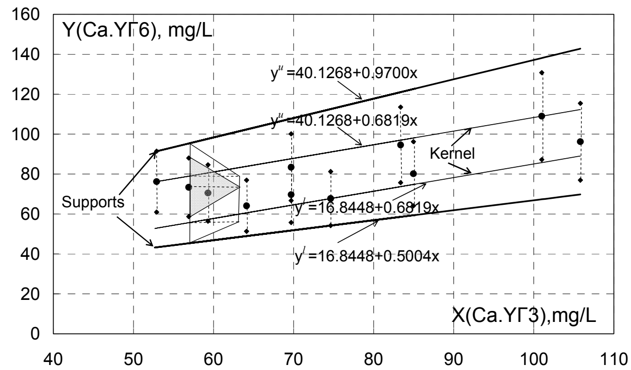

Fig. 1. Kernel and support for Ca. Input data is on x axis and output data on y axis.

Fig. 1 shows the measured data as x axis, output data as y axis, the kernel and also the support. In Fig. 2, the triangular fuzzy number for the crisp value Ca = 56.91 mg/L of is shown for the range of the confidence interval (h = 0–1) and also the output value interval using trapezoidal membership function.

Application 2 for K

Step 1

Kernel equations:

$$\begin{aligned}
y^- &= 0.0186 + 0.9767x,\\
y^+ &= 0.9093 + 0.9767x
\end{aligned} \tag{17}$$

Step 2

Support equations:

$$\begin{aligned}
y^- &= 0.799x,\\
y^+ &= 1.09 + 1.171x
\end{aligned} \tag{18}$$

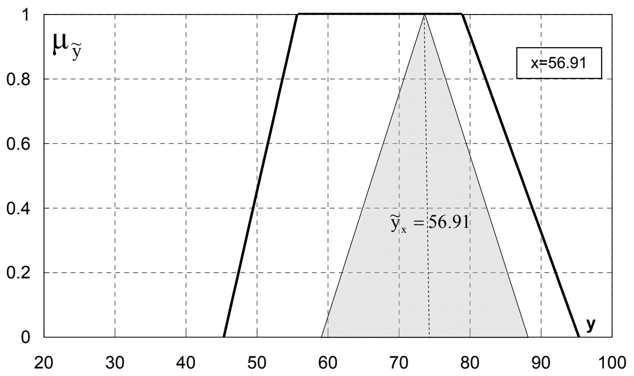

Fig. 2. Kernel and support for Ca = 59.91 mg/L.

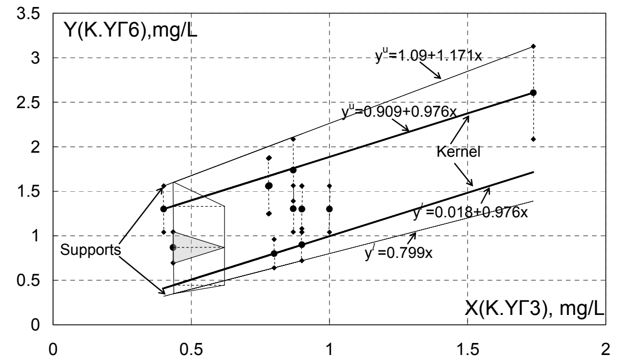

Fig. 3. Kernel and support for K. Input data is on x axis and output data on y axis.

Fig. 3 shows the measured data as x axis, output data as y axis, the kernel and also the support. In Fig. 4, the triangular fuzzy number for the crisp value K = 0.434 mg/L is shown for the range of the confidence interval (h = 0–1) and also the output value interval using trapezoidal membership function.

Application 3 for Mg

Step 1

Kernel equations:

$$y^{-} = 5.472 + 0.4375x, \quad y^{+} = 6.2916 + 0.7944x \tag{19}$$

Step 2

Support equations:

$$y^{-} = 5.4720 + 0.2875x, \quad y^{+} = 7.5499 + 0.9532x \tag{20}$$

Fig. 5 shows the measured data as x axis, output data as y axis, the kernel and also the support. In Fig. 6, the triangular fuzzy number for the crisp value Mg = 14.6 mg/L is shown for the range of the confidence interval (h = 0–1) and also the output value interval using trapezoidal membership function.

5. Conclusions

Knowledge of the underground water quality is very important for agricultural and human activities. The spread

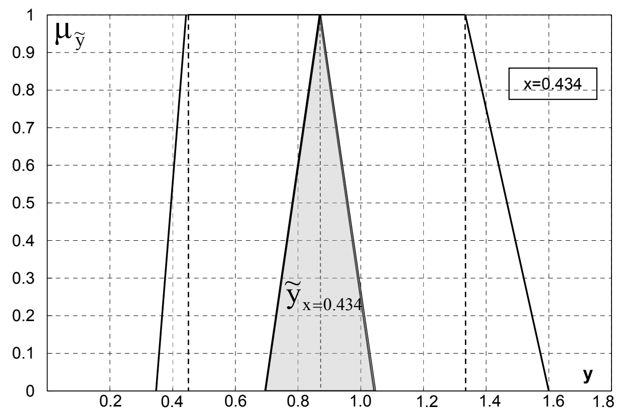

Fig. 4. Kernel and support for K = 0.434 mg/L.

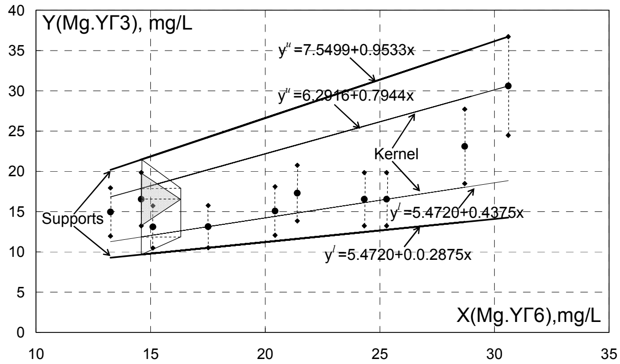

Fig. 5. Kernel and support for Mg. Input data is on x axis and output data on y axis.

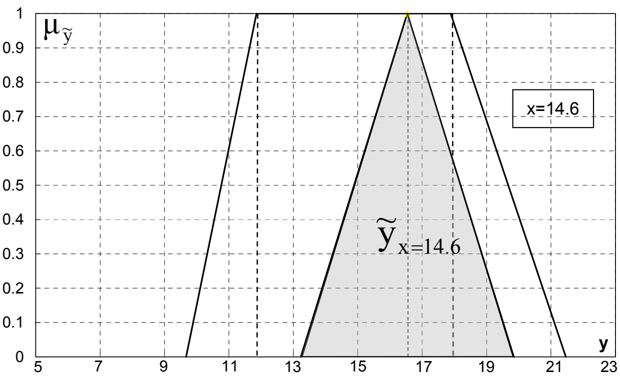

Fig. 6. Kernel and support for Mg = 14.6 mg/L.

of the measured irrigation water ions due to inherent measurements errors is significant in evaluating water quality. Introducing uncertainty and fuzzy logic analysis to the measured values can supply results with certain confidence level.

The trapezoidal model has the advantage of inclusion of measured data for every level of confidence and has the following property: data kernels are included into estimated kernels and data supports are also included into estimated supports. Besides, the new two-phase model has the advantage of using only four unknown quantities during each phase, in contrast with Bisserier model that uses eight. Arithmetic results of the Bisserier and the suggested model converge and the difference between quantitative error indicators is close to 0.0002. In the case of measurement observations, station association is achieved, even for small samples and it can be extended for the shorter time series, due to fuzzy correlation of the two measurement points.

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