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A Data Mining Approach Based on a Local-Global Fuzzy Modelling for Prediction of Color Change after Tooth Bleaching using Vita Classical Shades

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***Abstract*—Tooth bleaching is receiving an increasing interest by patients and dentists since it is a relatively non-invasive approach for whitening and lightening teeth. Instrument designed for tooth color measurements and visual assessment with commercial shade guides are nowadays used to evaluate the tooth color. However, the degree of color change after tooth bleaching varied substantially among studies and currently, there are no objective guidelines to predict the effectiveness of a tooth bleaching treatment. Fuzzy Logic is a well known paradigm for data modelling; their main advantage is their ability to provide an interpretable set of rules that can be later used by the scientists. However these models have the problem that the global approximation optimization can lead to a deficient rule local modelling. This work proposes a modified fuzzy model that performs a simultaneous global and local modelling. This property is reached thanks to a special partitioning of the input space in the fuzzy system. The proposed approach is used to approximate a set of color measurements taken after a bleaching treatment using the pre-bleaching measurements. The system uses as rule antecedents the colorimetric values of the VITA commercial shade guide. The expected post-bleaching colorimetric values are immediately obtained from the local models (rules) of the system thanks to the proposed modified fuzzy model. Additionally, these post-bleaching CIELAB coordinate values have been associated with VITA shades through the evaluation of their respective membership functions, approximating which VITA shades are expected after the treatment for each pre-bleaching VITA shade.**

***Keywords*-Local-Global Fuzzy Modelling, TSK Fuzzy Systems, Data Mining, Prediction of Color Change, CIELAB Space, Tooth Bleaching**

I. INTRODUCTION

Bleaching of teeth has become an essential component of conservative esthetic dentistry, as it is a non-restorative treatment for whitening of discolored teeth. The current bleaching mechanisms are based on the application of hydrogen-peroxide-releasing agent on external tooth surfaces to penetrate the tooth and produce free radicals that oxidize organic stains.

The most common bleaching technique uses hydrogen peroxide or carbamide as the bleaching agent. It was reported [1] that bleaching with 10%-20% carbamide peroxide is a simple, user-friendly, effective, and inexpensive technique. Numerous clinical studies have documented the effectiveness of bleaching in changing tooth color through whitening and lightening.

The color and appearance of teeth is a complex phenomenon which depends of many factors (scattering, absorption, translucency, etc.). The measurement of tooth color is possible via a number of methods including instruments designed for tooth color measurement and visual assessment with commercial shade guides. These shade guides are the most common method in clinic practice due to its inexpensiveness and ease of use. However, perceptional color evaluation is subjective, and it is often difficult to match a natural tooth with a shade guide. The high frequency of errors associated with the use of commercial shade guide systems has been documented [2] and therefore instrumental measurements are needed for an adequate color specification.

In this context, it is therefore necessary for an adequate clinic practice to have at disposal a direct association among instrumental color measurements and commercial guides. This association will allow us to establish objective guidelines to inform the patients about the expected teeth shades after a bleaching treatment.

In order to carry out this objective, a set of instrumental *in vivo* teeth color measurements were performed on a set of patients before and after a bleaching treatment using CIELAB space [3]. Similarly, a color measurement of the well-known commercial shade guide VITA Classical[1] was carried out.

With the obtained data, a fuzzy logic approach has been

[1]VITA Classical is the most extended guide in dentistry clinics due to its ease of use and to its close relation with dental restoration systems.

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used to design an inference model formed by a rule set whose antecedents correspond to the CIELAB coordinates of the VITA Classical shade guide. The optimized rules establish which post-bleaching color is expectable for each pre-bleaching shade in the VITA guide. This determination of the post-bleaching expectable value for each pre-bleaching VITA shade, as information directly extracted from the designed fuzzy model, is possible thanks to a novel modification of the input space subdivision that allow us to obtain a precise local modelling, apart from the effective global modeling. Finally, the post-bleaching CIELAB coordinates for each pre-bleaching shade have been corresponded with VITA guide shades according to the fuzzy membership functions designed for those shades.

II. Tooth Color Measurements in the CIELAB color space

A total of 40 subjects, 22 males and 18 females with an average age of 42,8 years, were enrolled in a home-bleaching study at the Stomatology Department in Granada[2]. The volunteers were examined and selected in the clinical facilities of the Stomatology Department attending to a certain set of inclusion criteria adapted to this study. All volunteers used a 20% carbamide peroxide tooth-bleaching agent (Opalescence 20% PF, Ultradent Products Inc., South Jordan, UT, USA) in the custom trays with reservoirs for 2 hours once a dat for 2 weeks.

Subsequently, the color of the patients' teeth was determined objectively using a spectroradiometer (SpectraScan PR-704, Photo Research inc., Chatsworth, USA) with a 4% measurement accuracy. These measurements were repeated three times to each tooth at baseline, on the day before, and 14 days after the initiation of the bleaching procedure. In order to ensure that all measurements were realized in conditions of standard light, we used the lamp Demetron Shade Light (Kerr) as source simulating the spectral relative irradiance of CIE standard illuminant D65. Illuminating and measuring configurations were CIE d/0° and the CIE 1964 10° Supplementary Standard Colorimetric observer.

CIELAB coordinates L*, a* and b* for pre-bleaching (L_i^*, a_i^*, b_i^*) and post-bleaching (L_f^*, a_f^*, b_f^*) were obtained. The L*, a* and b* values were averaged to establish a single set of value for each teeth. In each case, the resulting standard deviations were lower than the instrumental accuracy (4%). Table I shows the ranges of the pre and post bleaching values for coordinates L*, a* and b*.

CIE color coordinates L*, a* and b* for the VITA-Classic shade guide were also obtained under the same measurement conditions. The values for each of the shades is shown in Table II. The Vita-Classical shades present variations in saturation, hue and luminance, showing different shades that teeth color can present in the patients. Figure 1 shows the data distribution in the CIELAB space, together with the VITA-Classical shades distribution within the same space[3].

In [4] it was discussed that the whitening process should in principle provide an approach to (0,0) in the chromatic coordinates a* and b*, and an increase in the L* coordinates increasing the luminance. This was verified as the variations in coordinates L*, a* and b* followed similar-to-normal distributions with mean and deviations equal to (2.9, 7.2), (-1.8, 1.7) and (-3.5, 2.5) respectively. The means of the a* and b* were negative while for the L* it was positive. Those values show the approach of the teeth shade towards the model white (100, 0, 0) after the bleaching treatment. The standard deviation in coordinate L* was strong showing a larger dispersion of the measurements taken in the CIELAB space. This and other studies attempted to establish a colorimetric guideline to predict the effectiveness of tooth bleaching with respect to the original tooth color in order to make tooth bleaching a more reliable dental treatment, obtaining however indeterminate conclusions and sometimes contradictory results [5].

Table I
Ranges of pre-bleaching and post-bleaching for coordinates L*, a* and b*

CIELAB Coord.	Pre-bleaching			Post-bleaching		
	Min	Max	Mean	Min	Max	Mean
L*	32.14	79.85	56.37	33.20	82.16	59.29
a*	4.06	18.50	7.61	1.77	11.02	5.72
b*	7.37	21.78	14.67	4.82	18.04	11.17

Table II
CIELAB coordinates for VITA-Classical shades

VITA-Classical			
shades	L*	a*	b*
C4	34,92	7,23	12,87
A4	43,05	8,34	14,94
C3	46,29	6,78	12,88
B4	50,02	8,17	18,33
A3,5	48,94	8,49	15,7
B3	49,28	7,97	16,83
A3	56,16	7,96	14,58
D3	55,65	7,19	11,69
D4	55,57	6,18	14,4
C2	54,83	6,87	13,4
C1	55,87	5,15	8,81
A2	60,55	6,99	12,46
D2	59,41	5,59	8,59
B2	61,9	6,09	12,55
A1	63,46	5,05	9,11
B1	59,85	4,24	7,34

[2]After the corresponding approval by the Ethical Committee of Human Investigation at the University of Granada

[3]For plane b*L*, a fictitious line joins the VITA Shades from C4 to B1 according to Table II

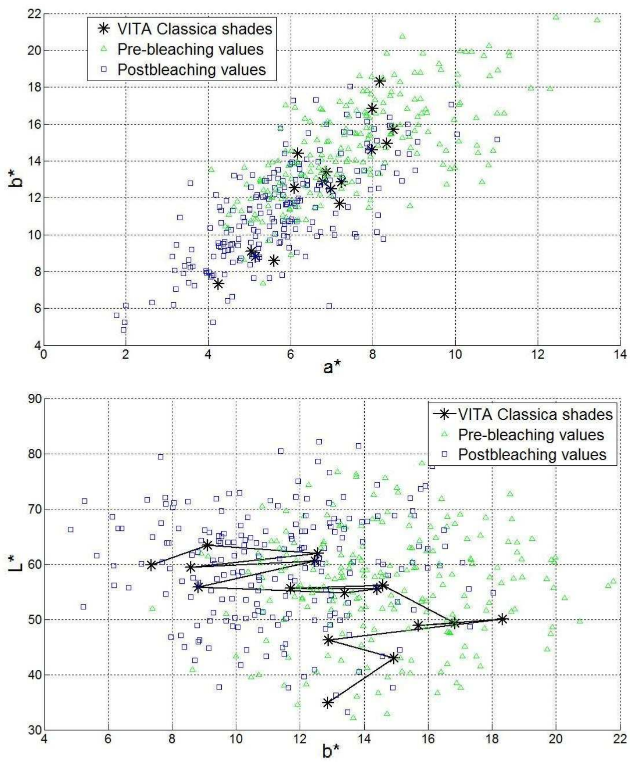


Figure 1. Data and VITA-Classical shade distribution in the CIELAB space in planes a*b* and b*L*

III. Fuzzy Logic Approach for VITA identification of Tooth Color Measurements and Fuzzy Inference for Color Change Prediction

The use of fuzzy logic for color representation has been traditionally employed for the color naming problem and for control tasks [6] [7]. Specifically in the dentistry field, some works have dealt with the characterization of tooth surface in parodontological practice and the soft removal of dental calculus [8], or to detection and quantification of dental plaque [9].

This work proposes the use of a fuzzy inference process as a way to perform data mining to extract information about the behavior of a bleaching treatment using VITA shade guides. On that purpose, a rule-based fuzzy model will be designed with antecedents corresponding to VITA shades, and will be optimized through least-squares to obtain the optimal consequents in the CIELAB coordinates L*, a* and b* for those initial shades. Since it is a Multiple-Input Multiple-Output model, three separated optimizations for each rule output coordinate will be performed.

Scatter-partitioning fuzzy models however present the problem that, due to the possible overlapping of the rules at their centres, their consequents might not appropriately be associated with the effective area they are covering and representing. In order to obtain rule consequents that effectively model the area represented by their corresponding antecedents, apart from performing the desired global modelling, a modified novel fuzzy model obtained from previous approaches for grid-based fuzzy systems will be applied. Thanks to this characteristic, the rule system built will be able to describe the CIELAB post-bleaching values for each VITA pre-bleaching shade. The correspondence of the CIELAB post-bleaching expected values with VITA post-bleaching shades will be obtained through the same fuzzy membership functions designed for the VITA-based rules.

A. Rules shape using VITA values in the antecedents

Each possible pre-bleaching shade s will define a Takagi-Sugeno-Kang (TSK) rule with the following shape:

$$\begin{array}{l} \text{IF } L_i^* \text{ is } \widehat{\text{VITAC}}_{L*}^{s} \text{ AND } a_i^* \text{ is } \widehat{\text{VITAC}}_{a*}^{s} \\ \text{AND } b_i^* \text{ is } \widehat{\text{VITAC}}_{b*}^{s} \text{ THEN} \\ L_f^* = expected^s L_f^* \quad \text{AND} \\ a_f^* = expected^s a_f^* \quad \text{AND} \\ b_f^* = expected^s b_f^* \end{array} \tag{1}$$

where $\widehat{VITAC}_{L*}^{s}$, $\widehat{VITAC}_{a*}^{s}$ and $\widehat{VITAC}_{b*}^{s}$ are fuzzy sets centered in the corresponding values of shade s for coordinates L*, a* and b* given in Table II. The fuzzy sets were considered gaussian and for a fair partitioning of the input space, the radius was calculated for each center according to the distance to the nearest center in the three dimensional space [10]. The optimally obtained $expected^s L_f^*$, $expected^s a_f^*$ and $expected^s b_f^*$, will correspond to the expected CIELAB value for those teeth with shade equal or around VITA shade s.

B. A Local-Global modelling approach for fuzzy systems

When dealing with the optimization of a TSK fuzzy system, global accuracy is usually the single objective to optimize, and the problem of local model optimization is barely addressed [11]. Some works have studied multiobjective optimization formulations of TSK fuzzy systems, that deal with both local and global modelling [12]. On the other hand, some approaches have been presented for grid-based TSK fuzzy systems that allow us to directly keep the interpretation of the local models whereas they are globally trained from a set of input/output data [13] [14]. However in this work a scatter-partitioning fuzzy system is needed; i.e., the rules and the local models to be extracted are placed in specific points in the n-dimensional space.

In order to obtain a simultaneous global-local modelling, it is needed that the overlapping degree of all the rules activations vanish at each rule centre, without loosing the approximation and interpolation properties of the set of fuzzy rules and of the fuzzy inference process. This way, every point of the n-dimensional space $\vec{c}^k$ identified by the centre of a rule k, is only affected by its respective rule in the global system output function, which is calculated as shown in equation 2:

$$\hat{F}(\vec{x}) = \frac{\sum_{k=1}^{K} \mu^k(\vec{x}) y^k}{\sum_{k=1}^{K} \mu^k(\vec{x})} \tag{2}$$

where K is the number of rules of the system, y^k (considering a single-output system) are their consequents, and the $\mu^k(\vec{x}) = \prod_{i=1}^{n} \mu_i^k(x_i)$ are the activations of the rules for an n-dimensional problem, that when using Gaussian kernels can be expressed in each dimension as :

$$\mu_i^k(x_i) = e^{-\frac{(x_i - c_i^k)^2}{2\sigma_i^{k\,2}}}, \tag{3}$$

being c_i^k and σ_i^k the center and radius of the Gaussian function of rule k at dimension i.

For the sake of simplicity, we first explain how the special partitioning of the input space with the overlapping properties needed will be performed for a one-dimensional case. As it will be shown, it can be easily extrapolated to a general case. Let us assume the simple case of a one-dimensional space with domain [0,1] with two rules with gaussian membership functions (MF) centred for example in $c^1 = 0.2$ and $c^2 = 0.8$ with $\sigma = 0.3$ (see Figure 2.(a)). In this case, there is a moderated overlapping between the two rule activations. In order to comply with the afore-mentioned overlapping conditions we will allow the domain of the first rule activation $\mu^1(x)$ to be limited by the function $1-\mu^2(x)$. That is, when the activation value of the opposite rule is 1, the first rule activation will be forced to take the value 0. That is, the final activation value for any point in the system using normalization would be

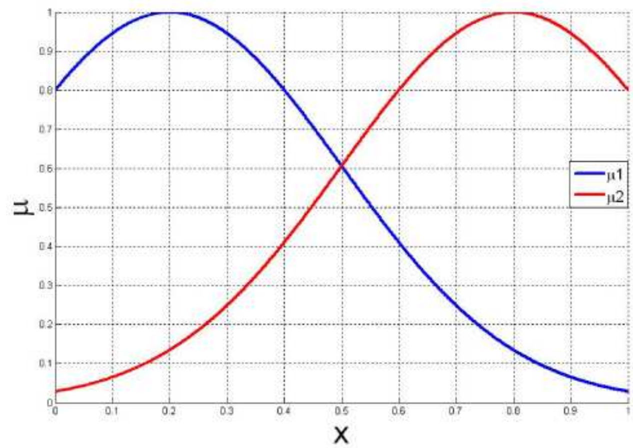
$$\begin{array}{c} \mu^{1*}(x) = \mu^1(x)\left(1-\mu^2(x)\right), \\ \hat{\mu}^{1*}(x) = \frac{\mu^{1*}(x)}{\mu^{1*}(x)+\mu^{2*}(x)} \end{array} \tag{4}$$

$$\begin{array}{c} \mu^{2*}(x) = \mu^2(x)\left(1-\mu^1(x)\right), \\ \hat{\mu}^{2*}(x) = \frac{\mu^{2*}(x)}{\mu^{1*}(x)+\mu^{2*}(x)} \end{array} \tag{5}$$

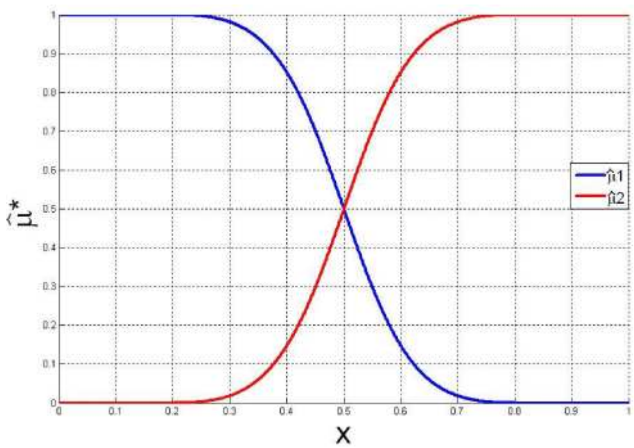
Generalizing to the n-dimensional case, the activation value of the k-th rule is obtained by the following equation

$$\mu^{k*}(\vec{x}) = \mu^k(\vec{x}) \prod_{\substack{j=1;\\ j\neq k}}^{K} \left(1-\mu^j(\vec{x})\right) \tag{6}$$

Therefore, for any given number of rules K, the general expression for the TSK fuzzy system output, using normalization (which forces the activation value of the rules to sum up to one in every point) can be calculated as



(a)



(b)

Figure 2. a) Original μ^1 and μ^2 MFs for the one-dimensional example. b) Normalized final MFs activations using the modified calculation $\hat{\mu}^{1*}$ and $\hat{\mu}^{2*}$.

$$\begin{array}{l} \hat{F}(\vec{x}) = \sum_{k=1}^{K} \hat{\mu}^{k*}(\vec{x}) y^k = \\ = \frac{\sum_{k=1}^{K}\left(\mu^k(\vec{x}) \prod_{\substack{j=1;\\ j\neq k}}^{K}\left(1-\mu^j(\vec{x})\right)\right) y^k}{\sum_{k=1}^{K}\left(\mu^k(\vec{x}) \prod_{\substack{j=1;\\ j\neq k}}^{K}\left(1-\mu^j(\vec{x})\right)\right)} \end{array} \tag{7}$$

where $\hat{\mu}^{k*}(\vec{x}) = \mu^{k*}(\vec{x}) / \sum_{j=1}^{K} \mu^{j*}(\vec{x})$ is the normalized activation value for rule k.

With this new formulation of the system's output given in equation 7, the final normalized rules activations are modified so that they consider the relative positioning of each rule with respect to the others. Moreover, the output function of the proposed model is continuous and differentiable, since it is a linear composition of continuous and differentiable functions. It is furthermore immediate to deduce that the following properties hold, due to the continuity of the gaussian function:

$$\begin{array}{l}\hat{\mu}^{2*}(c^1) = 0; \hat{\mu}^{1*}(c^1) = 1; \Rightarrow \hat{F}(c^1) = y^1(c^1) = a^1 \\ \hat{\mu}^{1*}(c^2) = 0; \hat{\mu}^{2*}(c^2) = 1; \Rightarrow \hat{F}(c^2) = y^2(c^2) = a^2\end{array} \tag{8}$$

Note that those properties are hold thanks to the use of the designed partitioning. Thus, according to equation 8, it holds that the consequents y^k of the rules are exactly the values of the fuzzy system output around the respective rule centre. Those results can directly be extrapolated to the n-dimensional case, thanks to the continuity of the compounded functions.

C. Optimization of the VITA-based fuzzy system

A fuzzy system has been designed with K = 16 rules corresponding to the values of the VITA Classical shades in the $n = 3$ dimensional CIELAB space. The data were normalized to be inside the range [0,1] in the three dimensions L*, a* and b*, in order to provide the same importance to the three dimensions; note that dimension L* has a wider range of values but with a higher dispersion [4]. The rule centres have been initialized according to the VITA Classical CIELAB values as a way to cluster the possible values for pre-bleaching shades, so the rules have the shape shown in equation 1. Since the model output function (Eq. 2) is linear with respect to all the rules consequents, given a set of M input/output data $D = ((\{L_i^*, a_i^*, b_i^*\}^1, \{L_f^*, a_f^*, b_f^*\}^1), \ldots, (\{L_i^*, a_i^*, b_i^*\}^M, \{L_f^*, a_f^*, b_f^*\}^M))$, it is possible to optimally obtain these parameters through the use of a wide range of mathematical methods. In this work we will use the Least Square Error (LSE) approach for the optimization of the consequents. Singular Value Decomposition (SVD) was used to solve the three linear equation system constructed, obtaining the L*, a* and b* output consequents. The objective in each case is to minimize the mean square error function $J = \sum_{m \in D} \left(\hat{F}^m \left(\{L_i^*, a_i^*, b_i^*\}^m \right) - y^m \right)^2$, where for each sample m, $\hat{F}$ represents $\hat{L}_f^*$, $\hat{a}_f^*$ and $\hat{b}_f^*$ and y^m represents L_f^*, a_f^* and b_f^* in each case.

IV. Data Mining from the Fuzzy System

From the 16 rules, four of them were eliminated from the optimization process since they do not present a sufficient data coverage; i.e. there were no teeth found with pre-bleaching shade similar to VITA shades B1, A1, D2 and C1. The 12 remaining rules with optimal consequents are the following

$$\begin{array}{l}
\text{IF } L_i^* \text{ is } \widehat{\text{B2}}_{L*} \text{ AND } a_i^* \text{ is } \widehat{\text{B2}}_{a*} \\
\text{AND } b_i^* \text{ is } \widehat{\text{B2}}_{b*} \text{ THEN} \\
L_f^* = 67.43 \ \text{ AND } a_f^* = 4.69 \ \text{ AND } b_f^* = 9.51 \\
\text{IF } L_i^* \text{ is } \widehat{\text{A2}}_{L*} \text{ AND } a_i^* \text{ is } \widehat{\text{A2}}_{a*} \\
\text{AND } b_i^* \text{ is } \widehat{\text{A2}}_{b*} \text{ THEN} \\
L_f^* = 64.02 \ \text{ AND } a_f^* = 4.73 \ \text{ AND } b_f^* = 8.78 \\
\text{IF } L_i^* \text{ is } \widehat{\text{C2}}_{L*} \text{ AND } a_i^* \text{ is } \widehat{\text{C2}}_{a*} \\
\text{AND } b_i^* \text{ is } \widehat{\text{C2}}_{b*} \text{ THEN} \\
L_f^* = 55.30 \ \text{ AND } a_f^* = 6.58 \ \text{ AND } b_f^* = 11.90 \\
\text{IF } L_i^* \text{ is } \widehat{\text{D4}}_{L*} \text{ AND } a_i^* \text{ is } \widehat{\text{D4}}_{a*} \\
\text{AND } b_i^* \text{ is } \widehat{\text{D4}}_{b*} \text{ THEN} \\
L_f^* = 59.40 \ \text{ AND } a_f^* = 4.16 \ \text{ AND } b_f^* = 11.27 \\
\text{IF } L_i^* \text{ is } \widehat{\text{D3}}_{L*} \text{ AND } a_i^* \text{ is } \widehat{\text{D3}}_{a*} \\
\text{AND } b_i^* \text{ is } \widehat{\text{D3}}_{b*} \text{ THEN} \\
L_f^* = 57.77 \ \text{ AND } a_f^* = 3.83 \ \text{ AND } b_f^* = 5.38 \\
\ldots
\end{array} \tag{9}$$

This optimal set of rules provides a standard error of 7.17 in coordinate L*, 1.39 in coordinate a* and 2.28 in coordinate b*, similar to those obtained using multivariate linear models in the previous work [4] (standard errors equal to 6.72, 1.41 and 2.15 in coordinates L*, a* and b* respectively). A confidence value for each fuzzy rule was calculated as the mean standard error contributed by the rule to the error committed in the CIELAB tridimensional space, according to the following formula:

$$\text{confid.value}_k = \sum_{m \in D} \|\hat{\vec{F}}^m - \vec{y}^m\| \cdot \hat{\mu}^{k*}(\vec{x}^m) \tag{10}$$

where $\hat{\vec{F}}^m = \{\hat{a}_f^*, \hat{b}_f^*, \hat{L}_f^*\}^m$ are the estimated post-bleaching CIELAB coordinate values for sample m, $\vec{y}^m = \{L_f^*, a_f^*, b_f^*\}^m$ its post-bleaching coordinate values (of sample m), and $\hat{\mu}^{k*}(\vec{x}^m)$ the activation value of rule k for its pre-bleaching coordinate values, $\vec{x}^m = \{L_i^*, a_i^*, b_i^*\}^m$. Last column of Table III shows the confidence values for the rules (the mean error for the whole set of samples in the tridimensional space is 6.5).

Once the post-bleaching CIELAB coordinate values are obtained for each pre-bleaching VITA shade, they were fuzzified in order to identify which VITA shades correspond to those post-bleaching values. Table III show the three VITA shades with a higher correspondence with each post-bleaching CIELAB coordinate values, i.e. the post-bleaching VITA shades expectable for each possible VITA pre-bleaching shade after the treatment. These VITA shades are obtained through evaluating their membership function for each post-bleaching CIELAB values, and taking those VITA shades that were most activated (the membership value for each instance is also shown in Table III).

Table III
POST-BLEACHING VITA SHADES EXPECTED FOR EACH PRE-BLEACHING VITA SHADE

VITA-Classical				
pre-bl.	post-bleaching			confid.
shade	shade 1	shade 2	shade 3	value
C4	C3 (0.71)	C4 (0.29)		7.98
A4	C3 (0.77)	C4 (0.22)		5.35
C3	C1 (0.52)	B1 (0.23)	A1 (0.09)	7.10
B4	C2 (0.34)	A3 (0.28)	D4 (0.18)	6.87
A3,5	D3 (0.57)	C2 (0.12)	A2 (0.10)	4.72
B3	C2 (0.47)	D4 (0.15)	A3 (0.15)	6.62
A3	B2 (0.78)	A2 (0.19)		7.34
D3	B1 (1.00)			6.33
D4	B1 (0.72)	A1(0.24)		5.84
C2	A2 (0.55)	B2(0.38)		5.05
A2	A1 (0.65)	B1(0.31)		4.18
B2	A1 (0.79)	B1(0.21)		5.20

V. CONCLUSIONS AND FUTURE WORK

This work has proposed a fuzzy-logic based approach in order to model a set of pre- and post-bleaching tooth colorimetric values through a set of rules whose antecedents correspond to the chromatic coordinate values of a VITA guide. A novel proposed fuzzy model allows to obtain a global and local efficient modelling that obtains the exact colorimetric expected values for each possible pre-bleaching shade. Additionally, an association between the expected post-bleaching values and VITA shades was performed, and a confidence value was obtained for the rules extracted. This work has showed that it is possible to establish a correspondence between colorimetric measurements and a well-known guide commonly used in dentistry clinics. As future work, we plan to corroborate the results obtained in this work with a clinic study of the subjective estimations of post-bleaching shades performed by dentistry practitioners. Additionally, this study should be extended to consider commercial guides recently appeared and appointed to the evaluation of bleaching treatments.

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