CLINICAL RESEARCH

Optimization of Tooth Color and Shade Guide Design

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Purpose: One critical prerequisite for dental shade guides is to match the color range and distribution of human teeth. The purpose of this study was to design computer models for dental shade guides and compare them with an existing shade guide. A targeted coverage error for a newly developed shade guide was $\Delta E_{ab} < 2$ with a corresponding CIE2000 value.

Materials and Methods: A total of 1064 teeth were evaluated in vivo using an intra-oral spectrophotometer. Shade guide models were designed using different methods for representation of the data set, hierarchical clustering, and nonlinear constrained optimization. Coverage error was calculated for both CIELAB and CIE2000 values. Recorded values were compared with coverage error of Vitapan Classical (VC) shade guide. Wilcoxon signed-rank test for paired samples and linear regression were used in statistical analysis.

Results: Coverage error of VC was 4.1 (SD 1.8), ranging from 0.5 to 11.5 ΔE_{ab}. Group A shades had the best match for human teeth (43.9%) followed by Groups C (24.1%), B (20.4%), and D (11.7%) shades, respectively. CIELAB coverage error of the newly designed 24-tab shade guide using clustering and optimization was 2.05 (0.95) and 1.96 (0.92), respectively. Corresponding CIE2000 coverage error values were 1.43 (0.68) and 1.40 (0.65), respectively. A significant difference between results obtained using clustering and optimization was determined. CIELAB color differences were greater, but highly correlated as compared with their CIE2000 counterparts ($\Delta E_{00} = 0.64 \times \Delta E_{76} + 0.13, r > 0.99$).

Discussion: This study demonstrated that, compared with existing shade guides, future shade guides can provide either (a) similar coverage of tooth color with fewer tabs, thus simplifying shade matching procedure, or (b) better coverage of tooth color with a similar number of tabs, in both cases increasing the chances of satisfactory matches and, consequently, better esthetics.

Conclusions: Both clustering and optimization enabled better representation of tooth color as compared with an existing dental shade guide. Optimization outperformed clustering and is therefore recommended as a method of choice for representation of tooth color and designing of dental shade guides.

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INDEX WORDS: color, tooth, shade guide, clustering, optimization

TOOTH COLOR encompasses a small part of the visible spectrum. Dealing with subtle color differences makes color matching and reproduction ever challenging tasks in restorative dentistry. These tasks can sometimes be further complicated by the absence of comprehensive education and training of dental professionals in color science, inadequate shade matching conditions and methods, and the suboptimal optical properties of esthetic dental materials and dental shade guides.

Advances related to color in dentistry, including improvements of dental shade guides, are significant and numerous;[1-4] however, all these advances are diminished if shade guides do not adequately cover the color range of natural teeth and do not have proper distribution within this range.[4-6] Therefore, two preliminary steps in establishing adequate principles for shade guide design are to

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determine color range and distribution of human teeth and to choose the most appropriate model of their representation.

Numerous authors have studied color of human teeth in vitro and in vivo. They evaluated the "average" tooth color or color of certain tooth regions of maxillary central incisors solely or on different tooth forms, using either visual or instrumental techniques.[7-15] The use of different measuring devices and techniques in previous studies resulted in variability of results. Edge-loss error (incorrect color readings because a considerable fraction of the light entering the tooth is lost) was frequently listed as a shortcoming of contact-type devices.[1,16,17]

Tooth color can be represented using different methods, such as arbitrary usage of available shades, mechanical division of color coordinate ranges in equal or similar increments (subjective, dimension by dimension approach), or methods based on computer-generated information (objective approach) by means of hierarchical clustering, principal component analysis, optimization, and neural networking.[18-20] The majority of available shade guides were designed using the former two methods, and different tab arrangements were applied or recommended.[21-25] Coverage error, representing the mean value of the minimal color differences among the specimens of one set to each specimen of another set, is a useful parameter for comparison of color ranges and distribution of shade guides and human teeth.[5]

The majority of data from color research in dentistry was obtained using the CIE $L^*a^*b^*$ system (CIE: Commission Interantionale de l'Eclairage; International Commission on Illumination) and is reported in corresponding symbols: L^* (lightness), a^* (green-red coordinate), b^* (blue-yellow coordinate), C^* (chroma), h (hue angle), and ΔE_{ab} (total color difference).[26] Since the new CIE2000 color difference formula has recently been introduced (new symbols: L', a', b', C', h', and ΔE_{00}, respectively) and officially recommended by CIE,[27] new thresholds and standards, similar to ones existing for the CIELAB system, should be provided for the new system.

The purpose of this study was to design computer models for a dental shade guide and compare them with an existing shade guide. Research hypotheses of this study were that there would be no differences in coverage error between commercial shade guides and newly developed models of dental shade guides, regardless of the method of the design or colorimetric system used (clustering or optimization, CIELAB, or CIE2000), and that a shade guide with coverage error of $\Delta E_{ab} < 2$ could be achieved with a reasonable number of samples.

Materials and Methods

Approval was obtained from the institutional review board and informed consent was obtained from each patient. A total of 133 patients (60.9% female, 39.1% male) were evaluated.

Color of nonrestored, nondiscolored, vital, right maxillary central incisor, canine, first premolar, and first molar teeth and their counterparts in the mandible was determined in vivo, for a total of 1064 teeth. If any of the right teeth were absent or not suitable for use, the corresponding left tooth was used; patients with nonrepresented teeth were excluded from the study. Tooth color was evaluated in the middle third, both incisocervically and mesiodistally, using a Vita Easyshade spectrophotometer (Vident, Brea, CA). After placement of an infection control polyurethane barrier over the probe tip, the Vita Easyshade was calibrated using a ceramic block provided by the manufacturer.

Tooth color coordinates (D65 illuminant, 2° standard observer) and color difference metric values between each tooth and the closest tab from Vitapan Classical (VC) shade guide, determined by the measuring device, were recorded.

The CIELAB color difference (ΔE_{ab}) was calculated as follows:[26]

$$\Delta E_{ab} = \left[(\Delta L^*)^2 + (\Delta a^*)^2 \, (\Delta b^*)^2 \right]^{1/2} \quad (1)$$

Coverage error was calculated as the color difference representing the mean value of the minimal color differences among each tooth and VC (data provided by measuring device) as follows:[5]

$$\Delta E_{\text{cov}} = \sum \Delta E_{\text{Min}} / n \quad (2)$$

For practical interpretation of color differences, the following thresholds were used: (a) $\Delta E_{ab} = 1$ as 50:50% detectable point for normal observers,[28] (b) $\Delta E_{ab} \leq 2$ as clinically acceptable match,[29] (c) $\Delta E_{ab} = 2.7$ as 50:50% replacement point of esthetic dental materials,[30] and (d) $\Delta E_{ab} = 3.7$ as the largest color difference with no mismatches observed.[31] In addition, the CIE2000 color coordinate values and color differences (ΔE_{00}) were calculated for all data using the following equation:[27]

$$\Delta E_{00} = \sqrt{\left(\frac{\Delta L'}{k_L S_L}\right)^2 + \left(\frac{\Delta C'_{ab}}{k_C S_C}\right)^2 + \left(\frac{\Delta H'_{ab}}{k_H S_H}\right)^2 + R_T \left(\frac{\Delta C'_{ab}}{k_C S_C}\right)\left(\frac{\Delta H'_{ab}}{k_H S_H}\right)} \quad (3)$$

Shade guide models were designed using agglomerative hierarchical clustering and nonlinear constrained optimization, with numerical calculations performed in Matlab (MathWorks, Natick, MA). Representation of tooth color for both CIELAB and CIE2000 was first preformed using hierarchal clustering.[19] Cluster color representatives were calculated as mean $L^*a^*b^*$ values of teeth belonging to the respective clusters. Ward's criterion of minimum variance was used for clustering, as it yielded minimum coverage error values relative to other linkage criteria.

To further reduce the coverage error, constrained nonlinear optimization was used, with minimization calculated by the line search method and constraints implemented via Lagrange multipliers.[20] In the following formulae, the set of measured $[L^*a^*b^*]^T$ values was denoted x_i, $i = 1, m$, where m was the size of the tooth set. The set of $[L\ a\ b]^T$ of calculated $L^*a^*b^*$ values was denoted X_j, $j = 1, n$, where n was the size of the set of tooth shades represented, and T denoted matrix transpose. The main criterion of optimality was defined as follows:

$$\min\left(f\left(X_j\right)\right),\ j = 1, m \quad \text{subject to} \quad (4a)$$

$$X_j \le B_U,\ j = 1, m \quad (4b)$$

$$X_j \ge B_L,\ j = 1, m \quad (4c)$$

$$f\left(X_j\right) = \frac{1}{m}\sum_i \min_j\left(\left\|x_i - X_j\right\|\right),\ j = 1, m \quad (4d)$$

where $\|x_i - X_j\|$ is either ΔE_{ab} or ΔE_{00}, depending on the method. The lower and upper bounds, B_L and B_U, for each X_j were chosen as the maximum and minimum L^*, a^*, and b^* from the x_i set.

One hundred twenty shade guides were designed, 30 each within the CIELAB system using clustering ($RG_{ab} - C_n$), CIELAB using optimization ($RG_{ab} - O_n$), CIE2000 using clustering ($RG_{00} - C_n$), and CIE2000 using optimization ($RG_{00} - O_n$), where subscripted n represented the number of samples ranging from 1 to 30. The data were compared with corresponding values for VC. Means and standard deviations were determined. Wilcoxon signed-rank test for paired samples and linear regression were performed using SPSS (SPSS, Chicago, IL).

Table 1. Mean Color Differences, ΔE_{ab} (SD) among Chosen Shade Tabs and Corresponding Teeth, and Shade Frequency (%) of VC Shades

Shade	ΔE_{ab} *(SD)*	*Shade Frequency (%)*
A1	4.4 (1.6)	12.1
A2	4.6 (1.5)	10.6
A3	4.1 (1.4)	10.8
A3.5	3.6 (1.4)	5.3
A4	4.1 (1.8)	5.1
B1	4.6 (1.5)	5.1
B2	4.0 (1.9)	6.4
B3	3.5 (1.6)	5.3
B4	3.6 (2.4)	3.7
C1	2.9 (1.0)	4.1
C2	3.4 (1.7)	5.2
C3	3.9 (2.0)	7.0
C4	5.2 (1.8)	7.8
D2	5.1 (2.2)	4.4
D3	3.9 (1.5)	4.5
D4	2.4 (0.9)	2.7

Results

Coverage error of VC was 4.1 (SD 1.8). Color differences (ΔE_{ab}) among chosen VC tabs and corresponding teeth ranged from 0.5 to 11.5. Means (SD) for these differences for each VC shade and shade frequency for VC are listed in Table 1. Group A shades were the most frequently chosen as the best match for human teeth (43.9%), followed by groups C (24.1%), B (20.4%), and D (11.7%). The same shade of all four teeth in the same jaw was registered in only 1.1%; the same shade was determined for three of four teeth in 9.0%, for two of four teeth in 44.7%, and four different shades were determined in 45.1%.

Coverage errors for all shade guides designed within both CIELAB and CIE2000 after optimization were smaller and had more uniform group composition as compared with the ones designed using clustering (Table 2). These differences were statistically significant ($z = -4.78$, $p < 0.001$). High correlation ($r > 0.99$) was found between clustering and optimization for both CIELAB and CIE2000 and between these two systems for both clustering and optimization ($\Delta E_{00} = 0.64 \times \Delta E_{76} + 0.13$).

Color coordinates and possible arrangement of independently developed $RG_{ab} - C_{24}$ and $RG_{ab} - O_{24}$ shade guides are listed in Table 3, while the percentage of human teeth fitting into one of color

Table 2. Coverage Error in Each of 120 Shade Guides (Containing 1 to 30 tabs)*

Number of Samples	$RG_{76} - C_{1\text{-}30}$	$RG_{76} - O_{1\text{-}30}$	$RG_{00} - C_{1\text{-}30}$	$RG_{00} - O_{1\text{-}30}$
1	7.90 (3.82)	7.89 (3.76)	5.30 (2.77)	5.29 (2.74)
2	6.13 (2.87)	6.10 (2.76)	4.00 (2.00)	3.94 (2.03)
3	5.16 (2.46)	5.00 (2.14)	3.49 (1.61)	3.31 (1.67)
4	4.57 (2.19)	4.44 (2.08)	3.08 (1.43)	2.94 (1.35)
5	4.17 (1.97)	**4.11** (1.89)	2.72 (1.24)	2.65 (1.22)
6	3.87 (1.73)	3.70 (1.79)	2.52 (1.17)	2.46 (1.20)
7	3.56 (1.60)	**3.47** (1.62)	2.34 (1.06)	2.30 (1.08)
8	3.37 (1.50)	3.23 (1.46)	2.24 (0.96)	2.20 (0.87)
9	3.19 (1.41)	3.12 (1.29)	2.14 (0.92)	2.09 (0.96)
10	3.07 (1.30)	2.94 (1.34)	2.05 (0.92)	2.02 (0.91)
11	2.88 (1.27)	2.82 (1.32)	1.98 (0.88)	1.94 (0.89)
12	2.74 (1.21)	2.70 (1.29)	1.92 (0.87)	1.87 (0.88)
13	2.67 (1.23)	2.62 (1.27)	1.85 (0.85)	1.81 (0.86)
14	2.59 (1.21)	2.54 (1.22)	1.80 (0.85)	1.75 (0.83)
15	2.52 (1.11)	2.45 (1.22)	1.74 (0.80)	1.70 (0.78)
16	2.46 (1.13)	2.40 (1.18)	1.70 (0.78)	1.65 (0.77)
17	2.41 (1.07)	2.35 (1.11)	1.66 (0.76)	1.60 (0.74)
18	2.36 (1.03)	2.26 (1.07)	1.62 (0.72)	1.58 (0.71)
19	2.29 (1.02)	2.22 (1.04)	1.58 (0.71)	1.54 (0.70)
20	2.23 (1.02)	2.16 (1.00)	1.55 (0.70)	1.52 (0.71)
21	2.18 (1.00)	2.10 (0.98)	1.51 (0.70)	1.48 (0.69)
22	2.13 (0.98)	2.05 (0.97)	1.47 (0.68)	1.45 (0.67)
23	2.09 (0.98)	2.00 (0.95)	1.44 (0.68)	1.42 (0.66)
24	**2.05** (0.95)	**1.96** (0.92)	**1.43** (0.68)	**1.40** (0.65)
25	2.01 (0.93)	1.93 (0.90)	1.41 (0.67)	1.38 (0.65)
26	1.98 (0.94)	1.90 (0.90)	1.40 (0.67)	1.37 (0.64)
27	1.94 (0.93)	1.86 (0.88)	1.38 (0.66)	1.34 (0.63)
28	1.91 (0.91)	1.84 (0.87)	1.36 (0.65)	1.32 (0.62)
29	1.87 (0.90)	1.82 (0.85)	1.35 (0.64)	1.30 (0.62)
30	1.84 (0.88)	1.78 (0.83)	1.34 (0.62)	1.29 (0.60)

*Thirty each within CIELAB using clustering ($RG_{ab} - C_{1\text{-}30}$), CIELAB using optimization ($RG_{ab} - O_{1\text{-}30}$), CIE2000 using clustering ($RG_{00} - C_{1\text{-}30}$), and CIE2000 using optimization ($RG_{00} - O_{1\text{-}30}$).
Numbers in bold represent $RG_{ab} - O$ that matched measured coverage error of Vitapan Classical (4.11), approximated coverage error of Vitapan 3D Master (3.5), and coverage errors of $RG_{ab} - C_{24}$, $RG_{ab} - O_{24}$, $RG_{00} - C_{24}$, and $RG_{00} - O_{24}$. CIELAB and CIE2000 values were independently calculated.

difference thresholds in VC and $RG_{ab} - O_{24}$ is given in Table 4. Beside statistically significant reduction of coverage error, optimization enabled better distribution of natural teeth within a shade guide (Fig 1).

Discussion

The maxillary central incisor has frequently been used in evaluations of tooth color.[12-14] Since color differences have been recorded among different maxillary and mandibular teeth of the same patients,[15] it appears that maxillary central incisors do not represent overall tooth color. Therefore, one tooth form from each group in both jaws was chosen for this study. The total number of evaluated teeth in this study is higher than the number of teeth used in other similar studies.[8-14] Two studies used higher numbers of teeth.[7,15] Determination of the sample size for statistically significant results for this observational study on color range and distribution of human teeth is not simple, since the data are actually distributed throughout the whole population. The outcome was represented by color coordinates where numerous combinations contributed to color differences (presented by a single number) to various extents. Even if the values for each of the coordinates were normally distributed, there would still be the matters of the range and relative contributions of each coordinate to the actual colors found in each individual. Furthermore, there was

Table 3. Shade Guides with 24 Tabs Obtained after Optimization in CIELAB System ($RG_{ab} - O_{24}$) and after Optimization in CIE2000 System ($RG_{00} - O_{24}$)*

Sample	$RG_{ab} - O_{24}$			$RG_{00} - O_{24}$		
	L^*	a^*	b^*	L'	C'	h'
1	84.9	−2.5	12.6	85.3	13.0	103.5
2	84.3	−1.3	22.5	84.3	23.0	93.8
3	82.5	−2.0	17.0	82.6	18.8	96.9
4	80.2	−1.2	20.9	81.8	15.3	101.7
5	79.9	−2.5	8.7	79.9	8.9	112.3
6	79.8	−0.6	25.2	79.9	22.5	93.1
7	79.4	−1.9	13.0	79.2	10.5	102.4
8	78.0	0.0	27.9	79.2	12.5	102.9
9	76.8	−0.4	24.1	78.8	26.8	90.5
10	76.1	−1.6	15.7	76.3	20.9	92.9
11	74.8	−0.5	21.5	76.2	15.7	98.5
12	73.8	1.6	30.0	75.8	24.8	90.0
13	73.2	0.2	24.6	74.1	29.9	86.0
14	72.9	−0.9	18.2	72.8	18.9	94.3
15	72.3	−1.9	10.2	72.8	24.1	89.4
16	70.2	−0.2	21.5	70.0	27.8	86.6
17	69.8	1.2	27.0	69.9	15.1	96.6
18	69.7	−1.2	15.0	69.8	20.9	89.5
19	68.5	3.0	30.9	67.9	17.8	93.5
20	67.9	−0.3	18.6	66.9	28.7	83.5
21	65.3	0.9	22.7	65.6	21.9	88.6
22	64.2	3.4	28.0	63.2	27.5	81.7
23	61.5	0.5	19.5	61.4	19.8	87.3
24	56.8	2.9	25.4	56.6	25.7	82.0

*Arranged by decreasing lightness.
Although CIELAB values were used as initial guess for CIE2000 coordinates, $L'C'h'$ values are not converted $L^*a^*b^*$ values—they were independently calculated.

no intervention that would enable comparison to predefined values or before/after result comparisons.

Based on the uneven influence of hue, value, and chroma differences on total color difference and the fact that visual thresholds for lightness, chroma, and hue differences are not identical, it should be emphasized that the conventionally accepted thresholds used in this article are arbitrary. However, they do provide orientation—when VC and $RG_{ab} - O_{24}$ were compared, 74.7% versus 18.3% of teeth were beyond the 50:50% clinical replacement point, while 55.6% versus 4.7% of teeth were above the limit of $\Delta E_{ab} = 3.7$.

Table 4. Percentage of Human Teeth Fitting into One of the Color Difference Thresholds for VC and $RG_{ab} - O_{24}$: A*

ΔE_{ab}	VC (%)	$RG_{ab} - O_{24}$ (%)
A	1.1	14.0
B	10.7	43.6
C	13.5	24.1
D	19.1	13.6
E	55.6	4.7

*Perceptibility limit ($\Delta E_{ab} \leq 1.0$); B) between perceptibility limit and clinical acceptability limit ($\Delta E_{ab} > 1.0$ and ≤ 2.0); C) between clinical acceptability limit and 50:50% replacement point ($\Delta E_{ab} > 2$ and ≤ 2.7); D) between 50:50% replacement point and the largest color difference with no mismatches observed ($\Delta E_{ab} > 2.7$ and ≤ 3.7); and E) mismatch ($\Delta E_{ab} > 3.7$).

The VC was already well established in the market when dentists surveyed indicated a need for the development of a new and systematic shade guide.[32] Nonetheless, VC was chosen for comparison because it has been a gold standard in dentistry for decades. A wide range of dental products on the market were keyed to VC: shade guides, various types of dental ceramics and resin composites, compomers, glass ionomer cements, hybrid ionomer cements, and temporary dental materials. The same is true for the output information from a majority of dental handheld shade matching devices.[1] In addition, the

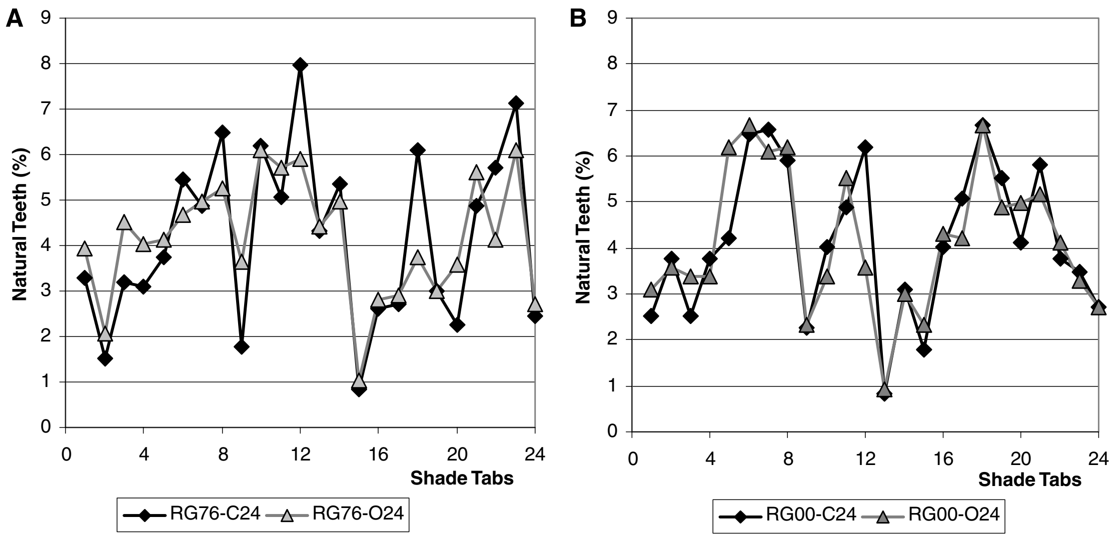

Figure 1. Percentage of natural teeth represented by each tab of *(A)* $RG_{ab} - C_{24}$ (SD 1.9) and $RG_{ab} - O_{24}$ (SD 1.3); and *(B)* $RG_{00} - C_{24}$ (SD 1.6) and $RG_{00} - O_{24}$ (SD 1.5).

measuring device used in this study (made by the same manufacturer as VC) provided ΔE_{ab} values between natural teeth and VC tabs, which was not the case with three-dimensional (3D), where the closest tab was displayed without numerical quantification of color difference. There is evidence that 3D covers a wider color range than VC;[4] however, it was reported that 55% of natural teeth had a of $\Delta E_{ab} \geq 3.7$ as compared with the closest 3D tab; in 20%, color difference was from 2.0 to 3.7. Even though a $\Delta E_{ab} \leq 2$ was recorded in 25% of cases, minimal color difference ranged from 0.6 to 12 ΔE_{ab} units.[33] In an experiment on 500 maxillary central incisors, 57% of teeth had a $\Delta E_{ab} > 2$ as compared with the closest 3D tab.[12]

Different arrangement principles of shade guides have been promoted.[21-25] Although this topic is beyond the scope of this article, it should be mentioned that tab arrangement based on increasing color difference compared with the lightest tab and the one based on decreasing lightness were found to be the most appropriate.[1] Both of these arrangement methods included tab division into certain numbers of groups: the first one by dividing a total ΔE_{ab} range into segments, and the second one by dividing a total lightness (L^*) range into segments. For the sake of simplicity, and since the largest variation was recorded as an L^* coordinate, $RG_{ab} - O_{24}$ and $RG_{ab} - O_{24}$ samples are arranged in Table 3 based on decreasing lightness, without further division into groups. Tab arrangement may influence shade-matching quality,[34] but cannot reduce coverage error. $RG_{76} - O_{01}$ shade guide (containing only one sample tab) had coverage error of $\Delta E_{ab} = 7.9$ (3.8). The coverage error of VC (containing 16 tabs) was matched with five samples in $RG_{ab} - O_{05}$. Coverage errors for VC and Vitapan 3D Master (3D) shade guides reported in the literature were 3.0 (2.3) and 2.3 (1.5), respectively.[5,6] Another study reported coverage errors of 3.1 (1.7) for VC and 2.6 (1.2) for 3D.[11] Since only the latter study employed an identical method for color measurements of teeth and shade tabs, these results were used to estimate coverage error for 3D ($\Delta E_{cov} \approx 3.5$) that is proportional to the coverage error for VC obtained in this study. This number was matched with 7 samples in $RG_{ab} - O_{07}$. Regardless of the differences in study design (1064 vs. 150 evaluated teeth, hand-held spectrophotometer in vivo vs. spectroradiometer in vitro), the coverage error of shade guide with 24 samples ($RG_{ab} - O_{24}$) designed in this study using optimization corresponded to a shade guide containing 26 tabs designed in another study using clustering.[11]

A regression equation among coverage errors in all 30 $RG_{ab} - O$ versus $RG_{00} - O$ shade guides was used for conversion of recorded CIELAB coverage error of 4.1 (VC) and approximated coverage error of 3.5 (3D) into CIE2000. Corresponding CIE2000 coverage errors were 2.7 and 2.4, respectively.

Vita Easyshade is a hand-held spectrophotometer that consists of a handpiece and a base unit.[1] This device uses a pseudocircular 0/0 measuring geometry, has a spectral resolution of 400 to 700 nm, and spectral range of 25 nm.[35] Potential concerns in tooth color measurements, especially when portable devices are used, might be associated with edge-loss error and free-hand positioning of the measuring tip. Edge-loss error occurs due to the small size of measuring window/tip and tooth translucency. As a result, a substantial amount of light reflected from the tooth emerges on the surface outside the window of measurement, rendering the measurements too dark.[16,17,35] To correct the coverage error, Vita Easyshade design requires using different measurement modes based on the measured material (tooth, crown, or shade tab). The Easyshade probe, approximately 5 mm in diameter, contains 19 1-mm diameter fiber optics. The outer ring of 12 fiber bundles is used to illuminate 5 mm (at 0 to 30°). There are two spectrometers used during the measurement process, both placed within the inner ring of the probe. These two spectrometers, combined, take into account the scattering, translucency, and thickness of the material. In addition to edge-loss, instrument design took into consideration concerns associated with free-hand positioning—three fibers in the inner ring of the probe prevent measurements if steadiness and perpendicular position of the probe are not achieved.[35]

Nonlinear optimization (minimization) requires an initial guess. In order to decrease computation time, the starting guesses used for X_j were the mean values calculated by clustering. It should be noted that the nonlinear optimization is independent of clustering, and the starting point can be chosen arbitrarily. If the system has a global minimum, multiple solutions (with the same minimum) can arise from interchange of indices of the X_j set, but it will not affect the final result (X_j values and the minimum value).

Further research on color range and distribution of human teeth should include information on vertical and horizontal color transitions of human teeth. In addition, differences among patients associated with age, gender, ethnicity, habits, oral hygiene, and bleaching history, should be more thoroughly evaluated. Appropriate methods in manufacturing new shade guides and actual esthetic materials, as well as tab arrangement of newly designed shade guides in accordance with color vision physiology and needs of clinical dentistry, will be a substantial challenge.

Dental shade guides are schematic representations of tooth color with a limited number of shade tabs. Therefore, some coverage error (the smaller, the better) is expected. Reducing the coverage error below the limit of clinical acceptability ($\Delta E_{ab} \leq 2$) with a reasonable number of tabs (26 after clustering and 24 after optimization) should be acceptable. This study demonstrated that, compared with existing shade guides, future shade guides can provide either (a) similar coverage of tooth color with fewer tabs, thus simplifying shade matching procedure, or (b) better coverage of tooth color with a similar number of tabs, in both cases increasing the chances of a satisfactory match and, consequently, better esthetics.

Conclusion

Both clustering and optimization enabled better representation of tooth color as compared with an existing dental shade guide. Optimization outperformed clustering and is therefore recommended as a method of choice for representation of tooth color and designing dental shade guides.

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