Predicting precision matrices for color matching problem

Takayoshi Nakamoto^{*,§}, Ryuei Nishii[†] and Shinto Eguchi[‡]

**Department of Vehicle Development
 Mazda Motor Corp., 3-1 Shinchu, Fuchu-cho
 Aki-gun, Hiroshima 730-8670, Japan*

*†Institute of Mathematics for Industry
 Kyushu University, 744 Motooka
 Nishi-ku, Fukuoka 819-0385, Japan*

*‡The Institute of Statistical Mathematics
 10-3 Midori-cho, Tachikawa, Tokyo 190-8562, Japan
[§]nakamoto.tak@mazda.co.jp*

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In this paper, as data, ellipsoids in a color coordinate called the Commission Internationale de l'Eclairage (CIE)-Lab system are given as data for 19 colors. Each ellipsoid is a region where all points are visually recognized as the same color at the center of the coordinate system. Our aim here is to predict the shape of an ellipsoid whose center is given by a new color. We proposed two prediction methods of positive definite matrices determining ellipsoids.

The first one is a nonparametric method with Gaussian kernel. The prediction is provided as a weighted sum of positive definite matrices corresponding to 19 ellipsoids in the training data. The second one is to use a matrix-valued regression model applied to a logarithm of positive definite matrices where explanatory variables are three elements of color centers. The best result was obtained by the nonparametric methods with three bandwidth parameters. The log normal regression had a weaker performance, but even so the model estimation was easily carried out.

Keywords: Color matching problem; kernel regression; log normal regression; nonparametric estimation; positive definite matrix; Riemannian metric.

1. Introduction

When car motor companies develop a new color or texture, it is very important to ensure color matching between the various products or parts in

order to provide a sophisticated appearance and design. First, we briefly review the color coordinate systems here.

One example of a color coordinate system is the Commission Internationale de l'Eclairage (CIE)

Lab system.¹ Each color in this system is represented by L (lightness) and a for the green-red and b for the blue-yellow color components.² An example is shown in Fig. 1(a), where L takes a value from 0 to 100 and a and b range from -90° to 90° .

The human visual system has a dead zone characteristic in that a set of colors with little difference is visually recognized as the same color.³ This dead zone is represented by an ellipsoid in the Lab space with the color center of interest.⁵ Therefore, predicting a dead zone ellipsoid corresponding to a new color is required in the Lab space in order to know the acceptable zone. This is known as **the color matching problem**.

The DuPont dataset⁶ gives 19 pairs of colors and ellipsoids in the Lab space. See Fig. 1(b) for color centers and corresponding ellipsoids. Note that the shapes of the ellipsoids are different from color to color. Moreover, similar colors have similar shapes in Lab space.⁷ For example, “Strong orange yellow” and “Moderate yellow” have similar shapes (long and thin for the b coordinate), and “Moderate green”, “Moderate bluish green”, and “Dark bluish green” have similar shapes (long and thin for the a coordinate).

The dataset is represented as $(\mathbf{u}_i, \mathbf{G}_i)$ for $i = 1, 2, \dots, 19$, where $\mathbf{u}_i = (a_i, b_i, L_i)^T$ denote color centers and $\mathbf{G}_i = (g_{ijk})$, $j, k = 1, 2, 3$ denote precision matrices (positive definite matrices) giving ellipsoids for colors $\mathbf{u}_i$. The dataset will be given in Sec. 2.

The problem considered here is how to predict an ellipsoid or a positive definite matrix for a new color center given as $\mathbf{u}_0 = (a_0, b_0, L_0)^T \in [-90, 90]^2 \times [0, 100]$. Then, the tolerance ellipsoid for the color with center $\mathbf{u}_0$ is given by an ellipsoid:

$$(\mathbf{v} - \mathbf{u}_0)^T \mathbf{G}(\mathbf{u}_0) (\mathbf{v} - \mathbf{u}_0) \leq 1, \quad (1)$$

where $\mathbf{v} = (a, b, L)^T$ is a vector of variables in the Lab space, and

$$\mathbf{G}(\mathbf{u}_0) = \begin{pmatrix} g_{11}(\mathbf{u}_0) & g_{12}(\mathbf{u}_0) & g_{13}(\mathbf{u}_0) \\ g_{12}(\mathbf{u}_0) & g_{22}(\mathbf{u}_0) & g_{23}(\mathbf{u}_0) \\ g_{13}(\mathbf{u}_0) & g_{23}(\mathbf{u}_0) & g_{33}(\mathbf{u}_0) \end{pmatrix}, \quad (2)$$

is a positive definite matrix corresponding to the color with center $\mathbf{u}_0$. We will estimate $\mathbf{G}(\mathbf{u}_0)$ through nonparametric and parametric methods in Secs. 2 and 3, respectively.

We consider three metrics between positive definite matrices as the accuracy assessment of the estimated ellipsoids. We also consider three normalizing methods for Gaussian weights to the observed positive definite matrices. To this end, we developed a nonparametric method of Nadaraya–Watson type estimation based on Gaussian kernel with several bandwidth parameters. Furthermore, we propose a matrix-valued regression to logarithm of positive definite matrices as response variables and three elements of color centers as explanatory variables.

The best result was obtained by the nonparametric methods with three bandwidth parameters. The log normal regression showed weaker

Fig. 1. CIE Lab color coordinate system and ellipsoid shapes.

performance, but even so, its model estimation could easily be carried out. Both of the proposed methods can greatly reduce the cost of color matching compared with the conventional cut-and-try method, which would make the development of new colors more efficient.

2. Nonparametric Prediction of Positive Definite Matrices

Ellipsoid (1) of color $\mathbf{u}_i = (a_i, b_i, L_i)^T$ ($i = 1, 2, \dots, 19$) in the DuPont dataset is rewritten as

$$(\mathbf{v} - \mathbf{u}_i)^T \mathbf{V}_i^{-1} (\mathbf{v} - \mathbf{u}_i) \leq 1, \quad (3)$$

where $\mathbf{v} = (a, b, L)^T$ and

$$\mathbf{V}_i = \begin{pmatrix} v_{i11} & v_{i12} & v_{i13} \\ v_{i12} & v_{i22} & v_{i23} \\ v_{i13} & v_{i23} & v_{i33} \end{pmatrix}, \quad (4)$$

is a positive definite matrix corresponding to the variance-covariance matrix. Table 1 lists the color names, centers $\mathbf{u}_i$, and matrices $\mathbf{V}_i$ of the DuPont dataset.

2.1. Normalization of input vectors

Hereafter, color centers $\mathbf{u}_i = (a_i, b_i, L_i)^T$ are used for the expression of $\mathbf{V}_i$. Table 2 summarizes the basic statistics of Table 1. It is clear here that the sample means are significantly different. Therefore, we consider the following normalization methods for deriving Gaussian kernel weights.

2.1.1. First normalization method

Let $\mathbf{u} = (a, b, L)^T \in [-90, 90]^2 \times [0, 100]$ denote a color in Lab space. Then, we define the following normalization:

$$\psi_1(\mathbf{u}) = \left(\frac{a}{90}, \frac{b}{90}, \frac{L}{50} - 1 \right) \in [-1, 1]^3, \quad (5)$$

where we take denominators 90 or 50 so that the transformed values belong to an interval $[-1, 1]$.

2.1.2. Second normalization method

The second normalization is based on sample means and standard deviations.

$$\psi_2(\mathbf{u}) = \left(\frac{a - \bar{a}}{s_a}, \frac{b - \bar{b}}{s_b}, \frac{L - \bar{L}}{s_L} \right) \in \mathbb{R}^3, \quad (6)$$

where $\bar{a}$ and s_a^2 denote the sample means and the sample variance of a_i , $\bar{b}$, s_b^2 , $\bar{L}$, and s_L^2 are similarly defined.

2.1.3. Third normalization method

The third normalization is to transform $\mathbf{u}$ into the unit cube as

$$\psi_3(\mathbf{u}) = \left(\frac{a - a_{\min}}{a_{\max} - a_{\min}}, \frac{b - b_{\min}}{b_{\max} - b_{\min}}, \frac{L - L_{\min}}{L_{\max} - L_{\min}} \right) \in [0, 1]^3, \quad (7)$$

where $a_{\min} = \min\{a_1, \dots, a_n\}$. Similarly, $a_{\max}$, $b_{\min}$, $b_{\max}$, $L_{\min}$ and $L_{\max}$ are defined.

Table 1. Color names, centers and ellipsoids from the DuPont dataset.

i	Center Names	a	b	L	v_{11}	v_{22}	v_{12}	v_{13}	v_{23}	v_{33}
1	Moderate blue	-1.403	-27.81	35.338	1.784	5.015	-1.166	-0.053	0.268	0.850
2	Moderate greenish blue	-16.374	-11.263	50.259	2.564	2.340	0.118	-0.065	-0.030	0.618
3	Medium gray	-0.782	1.049	59.334	0.779	1.955	-0.131	0.033	0.134	0.777
4	Moderate bluish green	-27.549	2.374	55.618	5.892	1.752	-0.362	-0.300	0.154	0.950
5	Light brown	12.606	20.571	62.928	1.735	2.302	0.369	0.024	0.145	0.878
6	Grayish purple	12.153	-13.079	46.389	2.109	3.725	-0.962	0.030	-0.084	0.810
7	Dark reddish orange	35.646	21.403	42.315	3.661	2.801	0.587	-0.093	0.114	1.039
8	Moderate yellow	1.937	35.638	78.023	1.645	4.131	0.249	-0.020	0.214	1.285
9	Grayish yellow green	-10.011	13.281	64.938	1.433	2.357	-0.277	-0.144	0.135	0.762
10	Black	-0.453	0.421	14.14	0.627	2.096	-0.064	0.007	-0.057	1.520
11	Light bluish green	-30.732	-5.03	68.678	6.132	4.070	-1.127	-0.418	0.108	1.091
12	Moderate reddish brown	21.121	17.804	28.893	1.243	2.630	0.411	-0.093	-0.199	1.027
13	Dark bluish green	-33.638	-5.012	31.683	21.938	1.522	1.586	-1.519	0.019	1.267
14	Brilliant greenish blue	-13.44	-25.897	59.904	3.119	5.599	-1.249	-0.042	-0.538	1.299
15	Very dark red	25.237	3.409	17.357	4.261	2.691	-0.182	-0.262	0.264	1.248
16	Moderate purplish pink	31.509	-0.183	58.109	5.831	3.988	-0.422	0.080	-0.123	1.742
17	Dark blue	6.826	-31.146	30.186	1.769	3.030	-1.096	-0.006	-0.011	1.074
18	Light gray	0.307	0.214	83.481	1.099	5.275	-0.507	0.146	-0.100	1.899
19	Strong orange yellow	18.226	79.894	76.057	3.468	19.339	-0.025	0.187	0.657	2.398

Table 2. Basic statistics of color centers.

	Sample means	Standard deviations	Minimum	Maximum
a_i	1.641	20.236	-33.638	35.646
b_i	4.034	25.276	-31.146	79.894
L_i	50.717	20.289	14.140	83.481

2.2. Metrics between positive definite matrices

Let $\mathbf{L} = (l_{jk})$ and $\mathbf{M} = (m_{jk})$ be positive definite matrices of order 3. We use the following three metrics for evaluating the positive definite matrices in order to obtain the best Gaussian kernel estimations.

2.2.1. Frobenius norm

The Frobenius norm gives the Euclidean norm between two matrices.

$$\Delta_F(\mathbf{L}, \mathbf{M}) = \|\mathbf{L} - \mathbf{M}\|_F = \sqrt{\sum_{j=1}^3 \sum_{k=1}^3 (l_{jk} - m_{jk})^2}. \quad (8)$$

2.2.2. Riemannian metric

The Riemannian metric is obtained from the geometrical distance between two matrices.⁸

$$\Delta_R(\mathbf{L}, \mathbf{M}) = \sqrt{\sum_{j=1}^3 \{\log \lambda_j(\mathbf{L}^{-1}\mathbf{M})\}^2}, \quad (9)$$

where $\lambda_j(\mathbf{L}^{-1}\mathbf{M}) > 0$ denotes the j th largest eigenvalue of $\mathbf{L}^{-1}\mathbf{M}$.

2.2.3. Kullback–Leibler (KL) divergence

We apply the Kullback–Leibler (KL) divergence between $N(\mathbf{0}, \mathbf{L})$ and $N(\mathbf{0}, \mathbf{M})$ by regarding two matrices as the variance–covariance matrices of two independent Gaussian distributions having zero mean, as

$$\Delta_{KL}(\mathbf{L}, \mathbf{M}) = \frac{1}{2} \{\log |\mathbf{L}^{-1}\mathbf{M}| + \text{trace}(\mathbf{L}^{-1}\mathbf{M}) - 3\}. \quad (10)$$

The first two metrics satisfy the three axioms of the distance whereas KL does not.

2.3. Nonparametric estimation of a center matrix by Gaussian kernel

Gaussian kernel estimation is applied to the positive definite matrices.⁹ We set $\mathcal{V}$ as the space containing all positive definite matrices of order p . Assume that training dataset $\{\mathbf{V}_i \in \mathcal{V} \mid i = 1, \dots, n\}$ is available. Then, our aim here is to derive an ellipsoid i.e., a **matrix** $\mathbf{V} \in \mathcal{V}$ of the training data **in some sense**. The matrix is defined by minimizing the following loss function:

$$L(\mathbf{V}) = \sum_{i=1}^n w_i \Delta_{KL}(\mathbf{V}, \mathbf{V}_i) \quad \text{for weights } w_i > 0 \text{ with } \sum_i w_i = 1, \quad (11)$$

where $\Delta_{KL}(\cdot, \cdot)$ is the KL divergence defined in (10).

Proposition.

Let

$$\hat{\mathbf{V}} = \sum_{i=1}^n w_i \mathbf{V}_i \in \mathcal{V}, \quad (12)$$

be a weighted sum of the training data. Then, it holds that

$$\hat{\mathbf{V}} = \arg \min_{\mathbf{V} \in \mathcal{V}} L(\mathbf{V}). \quad (13)$$

Proof. We obtain that

$$2L(\hat{\mathbf{V}}) = \sum_i w_i [\text{trace}(\mathbf{V}_i \hat{\mathbf{V}}^{-1}) - p + \log |\mathbf{V}_i \hat{\mathbf{V}}^{-1}|].$$

By the linearity of the trace function, we have

$$\begin{aligned} 2L(\mathbf{V}) - 2L(\hat{\mathbf{V}}) &= \text{trace}(\mathbf{V}^{-1}\hat{\mathbf{V}}) - \log |\mathbf{V}| - p + \log |\hat{\mathbf{V}}| \\ &= \text{trace}(\mathbf{V}^{-1}\hat{\mathbf{V}}) - p + \log |\mathbf{V}^{-1}\hat{\mathbf{V}}| \geq 0. \end{aligned}$$

The last inequality follows from the non-negativity for KL divergence (10). Note that the equality holds if and only if $\mathbf{V} = \hat{\mathbf{V}}$. $\square$

The proposition implies that the weighted sum (12) minimizes the loss function (11). Next, determination methods of the weights w_i are proposed from different viewpoints.

2.3.1. Gaussian kernel estimation 1

In the first method for predicting the positive definite matrix for a certain color center $\mathbf{u}$, we

normalize input vector $\mathbf{u}$ and obtain $\psi_q(\mathbf{u})$ defined by (5)–(7) for $q = 1, 2, 3$. Next, we apply a single bandwidth tuning parameter $\gamma > 0$ to the nonlinear weighting function:

$$\hat{\mathbf{V}}(\psi_q(\mathbf{u})) = \sum_{i=1}^n w_i(\psi_q(\mathbf{u}), \gamma) \mathbf{V}_i, \quad (14)$$

$$w_i(\psi_q(\mathbf{u}), \gamma) = \frac{\exp\{-\gamma \|\psi_q(\mathbf{u}) - \psi_q(\mathbf{u}_i)\|^2\}}{\sum_{l=1}^n \exp\{-\gamma \|\psi_q(\mathbf{u}) - \psi_q(\mathbf{u}_l)\|^2\}}. \quad (15)$$

If $\gamma = 0$, (2.12) gives the mean matrix of $\mathbf{V}_i$. The positive definiteness of the matrix given by (14) is easily shown because it is given by the sum of positive weights on positive definite matrices.

The validity of estimation using the weighted sum in the form of (15) is ensured by the proposition. The bandwidth parameter $\gamma > 0$ is tuned by minimizing a metric between the estimated and observed positive definite matrices using leave-one-out cross-validation. We consider three types of metrics: the Frobenius norm, the Riemannian metric, and the KL divergence.

Let $\hat{\mathbf{V}}_i$ be the estimated positive definite matrix in the form of (14) with (15) using the training data while omitting $\mathbf{V}_i$. We tune parameter γ using the three metrics.

Frobenius norm

$$\hat{\gamma}_F = \arg \min_{\gamma > 0} \sum_{i=1}^n \Delta_F^2(\mathbf{V}_i, \hat{\mathbf{V}}_i), \quad (16)$$

where $\Delta_F(\cdot, \cdot)$ denotes the Frobenius norm (8).

The tuning methods using the Riemannian metric and KL divergence are used similarly. Then, $\hat{\gamma}_R$ and $\hat{\gamma}_{KL}$ are similarly defined.

2.3.2. Gaussian kernel estimation 2

The diagonal elements in positive definite matrix $\mathbf{V}$ are more important than the off-diagonal elements because these parameters determine the ellipsoidal size corresponding to the color coordinates. We thus deconstruct the positive definite matrix $\mathbf{V}(\psi_q(\mathbf{u}))$ to the standard deviations and correlations as

$$\mathbf{V}(\psi_q(\mathbf{u})) = \mathbf{S}(\psi_q(\mathbf{u})) \mathbf{C}(\psi_q(\mathbf{u})) \mathbf{S}(\psi_q(\mathbf{u})), \quad (17)$$

where

$$\mathbf{S}(\psi_q(\mathbf{u})) = \begin{pmatrix} \sqrt{v_{11}(\psi_q(\mathbf{u}))} & 0 & 0 \\ 0 & \sqrt{v_{22}(\psi_q(\mathbf{u}))} & 0 \\ 0 & 0 & \sqrt{v_{33}(\psi_q(\mathbf{u}))} \end{pmatrix}, \quad (18)$$

$$\mathbf{C}(\psi_q(\mathbf{u})) = \begin{pmatrix} 1 & \rho_{12}(\psi_q(\mathbf{u})) & \rho_{13}(\psi_q(\mathbf{u})) \\ \rho_{12}(\psi_q(\mathbf{u})) & 1 & \rho_{23}(\psi_q(\mathbf{u})) \\ \rho_{13}(\psi_q(\mathbf{u})) & \rho_{23}(\psi_q(\mathbf{u})) & 1 \end{pmatrix}. \quad (19)$$

The standard deviations and correlations are estimated using different bandwidths $\gamma > 0$ and $\delta > 0$ as

$$\sqrt{v_{jj}(\psi_q(\mathbf{u}))} = \sum_{i=1}^n w_i(\psi_q(\mathbf{u}), \gamma) \sqrt{v_{ijj}}, \quad j = 1, 2, 3, \quad (20)$$

$$\rho_{jk}(\psi_q(\mathbf{u})) = \sum_{i=1}^n w_i(\psi_q(\mathbf{u}), \delta) \rho_{ijk}, \quad (j, k) = (1, 2), (1, 3), (2, 3), \quad (21)$$

and $w_i(\psi_q(\mathbf{u}), \cdot)$ is defined by (2.13). The ρ_{ijk} is the (j, k) correlation of matrix $\mathbf{V}_i$. Two bandwidths are estimated by minimizing the metric as

Frobenius norm

$$(\hat{\gamma}_F, \hat{\delta}_F) = \arg \min_{\gamma > 0, \delta > 0} \sum_{i=1}^n \Delta_F^2(\mathbf{V}_i, \hat{\mathbf{V}}_i), \quad (22)$$

where $\hat{\mathbf{V}}_i$ is derived using (17) with two parameters.

Similarly, bandwidths tuned by the Riemannian metric and KL divergence are defined. The estimated matrix is shown to be positive definite because its correlation matrix is given by the sum of positive weights of the correlation matrices (ρ_{ijk}) .

Note that the tuned parameters depend on the normalization methods $\psi_q(\cdot)$. Note also that $\hat{\mathbf{V}}_i$ is positive definite because its correlation matrix is given by a linear combination of training correlation matrices with positive weights.

2.3.3. Gaussian kernel estimation 3

The first and second estimation methods in 2.3.1 and 2.3.2 use the common parameter γ for the variances v_{11} , v_{22} and v_{33} for normalization types

$q = 1, 2, 3$. Actually, the maximum and the minimum of v_{i11} is given by 1.600 and 0.054, respectively (see Table 1). This means that v_{11} corresponding to color coordinate a and the other two variances should be modeled separately. Under this consideration, we will propose the following third model:

$$\sqrt{v_{11}(\psi_q(\mathbf{u}))} = \sum_{i=1}^n w_i(\psi_q(\mathbf{u}), \gamma) \sqrt{v_{i11}}, \quad (23)$$

$$\sqrt{v_{jj}(\psi_q(\mathbf{u}))} = \sum_{i=1}^n w_i(\psi_q(\mathbf{u}), \delta) \sqrt{v_{ijj}}, \quad j = 2, 3, \quad (24)$$

$$\rho_{jk}(\psi_q(\mathbf{u})) = \sum_{i=1}^n w_i(\psi_q(\mathbf{u}), \eta) \rho_{ijk}, \quad (j, k) = (1, 2), (1, 3), (2, 3). \quad (25)$$

Then, the three bandwidths are tuned as follows.

Frobenius norm

$$(\hat{\gamma}_F, \hat{\delta}_F, \hat{\eta}_F) = \arg \min_{\gamma > 0, \delta > 0, \eta > 0} \sum_{i=1}^n \Delta_F^2(\mathbf{V}_i, \hat{\mathbf{V}}_i), \quad (26)$$

where $\hat{\mathbf{V}}_i$ is estimated using (17) with three bandwidths.

Similarly, three bandwidths based on the Riemannian metric and KL divergence are respectively defined. Note that $\hat{\mathbf{V}}_i$ is positive definite for the same reason stated in the two-bandwidth case.

3. Regression Analysis in Matrix Log-Normal Distribution

Next, we construct a regression model between the positive definite matrices and color centers.¹¹ Recall that $\{(\mathbf{u}_i, \mathbf{V}_i) \in \mathbb{R}^3 \times \mathcal{V} \mid i = 1, \dots, n\}$ is the DuPont dataset with a set of positive definite matrices $\mathcal{V}$. In general, $\mathbf{V} \in \mathcal{V}$ has the following decomposition based on an orthogonal matrix $\mathbf{Q}$ as follows:

$$\mathbf{V} = \mathbf{Q} \mathbf{D} \mathbf{Q}^T, \quad (27)$$

$$\mathbf{D} = \begin{pmatrix} \lambda_1 & & \mathbf{0} \\ & \lambda_2 & \\ \mathbf{0} & & \lambda_3 \end{pmatrix}, \quad \lambda_i > 0. \quad (28)$$

Then, we define a logarithm of $\mathbf{V}$ by

$$\log \mathbf{V} = \mathbf{Q} \begin{pmatrix} \log \lambda_1 & & \mathbf{0} \\ & \log \lambda_2 & \\ \mathbf{0} & & \log \lambda_3 \end{pmatrix} \mathbf{Q}^T. \quad (29)$$

Now, we use the log normal regression model¹² described by

$$\log \mathbf{V}_i := \mathbf{M}_0 + a_i \mathbf{M}_1 + b_i \mathbf{M}_2 + L_i \mathbf{M}_3 + \mathbf{E}_i, \quad i = 1, 2, \dots, n, \quad (30)$$

where $\mathbf{M}_j (j = 0, 1, 2, 3)$ are unknown symmetric matrices of order 3 and $n = 19$. They are regression coefficient matrices for explanatory variables 1, a_i , b_i , and L_i . We assume that error matrices $\mathbf{E}_i$ ($i = 1, 2, \dots, n$) are distributed independently.

Let $\tilde{\mathbf{H}} = (\mathbf{H}_1, \dots, \mathbf{H}_n)^T : 3n \times 3$ with $\mathbf{H}_i = \log \mathbf{V}_i$, and $\tilde{\mathbf{M}} = (\mathbf{M}_0, \dots, \mathbf{M}_3)^T : 12 \times 3$. The design matrix $\mathbf{X}$ is set as follows:

$$\mathbf{X} = \begin{pmatrix} 1 & a_1 & b_1 & L_1 \\ 1 & a_2 & b_2 & L_2 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & a_n & b_n & L_n \end{pmatrix} : n \times 4. \quad (31)$$

Then, the log normal regression model (30) is rewritten as

$$\mathbf{H}_i = \mathbf{M}_0 + a_i \mathbf{M}_1 + b_i \mathbf{M}_2 + L_i \mathbf{M}_3 + \mathbf{E}_i, \quad (32)$$

for $i = 1, 2, \dots, n$, and we have the following simultaneous equation:

$$\begin{aligned} \tilde{\mathbf{H}} &\equiv \begin{pmatrix} \mathbf{H}_1 \\ \mathbf{H}_2 \\ \vdots \\ \mathbf{H}_n \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{I} & a_1 \mathbf{I} & b_1 \mathbf{I} & L_1 \mathbf{I} \\ \mathbf{I} & a_2 \mathbf{I} & b_2 \mathbf{I} & L_2 \mathbf{I} \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{I} & a_n \mathbf{I} & b_n \mathbf{I} & L_n \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{M}_0 \\ \mathbf{M}_1 \\ \mathbf{M}_2 \\ \mathbf{M}_3 \end{pmatrix} + \begin{pmatrix} \mathbf{E}_1 \\ \mathbf{E}_2 \\ \vdots \\ \mathbf{E}_n \end{pmatrix} \end{aligned} \quad (33)$$

$$= \tilde{\mathbf{X}} \tilde{\mathbf{M}} + \tilde{\mathbf{E}}. \quad (34)$$

The regression coefficient matrix $\tilde{\mathbf{M}}$ is estimated by the least square method by minimizing the following error function:

$$\begin{aligned} \text{trace}(\mathbf{S}^T \mathbf{S}) &= \text{trace}(\tilde{\mathbf{M}}^T \tilde{\mathbf{X}}^T \tilde{\mathbf{X}} \tilde{\mathbf{M}}) \\ &\quad - 2 \text{trace}(\tilde{\mathbf{M}}^T \tilde{\mathbf{X}}^T \tilde{\mathbf{H}}) + \text{trace}(\tilde{\mathbf{H}}^T \tilde{\mathbf{H}}), \end{aligned} \quad (35)$$

where

$$\mathbf{S} = \tilde{\mathbf{H}} - \tilde{\mathbf{X}} \tilde{\mathbf{M}}. \quad (36)$$

The derivative of the error function is defined as follows.

$$\frac{\partial \text{trace}(\mathbf{S}^T \mathbf{S})}{\partial \tilde{\mathbf{M}}} = 2\tilde{\mathbf{X}}^T \tilde{\mathbf{X}} \tilde{\mathbf{M}} - 2\tilde{\mathbf{X}}^T \tilde{\mathbf{H}} = \mathbf{O}. \quad (37)$$

Then, the regression coefficient matrix is estimated as

$$\hat{\tilde{\mathbf{M}}} = \{(\mathbf{X}^T \mathbf{X})^{-1} \otimes \mathbf{I}\} \tilde{\mathbf{X}}^T \tilde{\mathbf{H}}, \quad (38)$$

$$= (\mathbf{X}^T \mathbf{X})^{-1} \sum_{i=1}^n \begin{pmatrix} \mathbf{H}_i \\ a_i \mathbf{H}_i \\ b_i \mathbf{H}_i \\ L_i \mathbf{H}_i \end{pmatrix}. \quad (39)$$

Thus, $\log \mathbf{V}$ at a color point $(a, b, L)^T$ is estimated by

$$\log \hat{\mathbf{V}} = \hat{\mathbf{M}}_0 + a\hat{\mathbf{M}}_1 + b\hat{\mathbf{M}}_2 + L\hat{\mathbf{M}}_3. \quad (40)$$

Then, the positive definiteness of $\hat{\mathbf{V}} \equiv \exp(\log \hat{\mathbf{V}})$ is obviously satisfied because eigenvalues of $\hat{\mathbf{V}}$ are positive.

4. Numerical Experiments

4.1. Numerical experiments on DuPont dataset

The proposed nonparametric formulas up to three bandwidths based on three normalization methods were applied to the DuPont training dataset. We have 9 ($= 3^2$) possible prediction formulas for positive definite matrices. The bandwidths were tuned by the leave-one-out cross validation according to the three metrics between observed and predicted matrices.

Table 3 compares 27 ($= 3^3$) models and lists tuned bandwidths. The first row separates the models according to the number of widths one, two and three corresponding to formulas (16), (22) and (26). The second row implies the q th normalization methods with $q = 1, 2, 3$ for each block. The 2nd entry of the 4th row, 727.9, gives the minimum Frobenius norm appearing in (16) with the optimal bandwidth based on the first normalization method

Table 3. Kernel estimation results.

Number of bandwidths	One (14)			Two (20–21)			Three (23–25)		
Normalization methods: q	1 (5)	2 (6)	3 (7)	1 (5)	2 (6)	3 (7)	1 (5)	2 (6)	3 (7)
Metrics									
Frobenius norm	727.9	611.7	624.6	734.8	607.4	605.5	719.9	586.8	598.0
Riemannian metric	26.52	20.99	19.95	26.42	20.64	19.78	24.79	20.12	19.54
KL divergence	8.686	6.472	6.297	8.666	6.620	6.378	8.057	6.335	6.286
Bandwidths									
γ_F	21.89	132.1	132.1	20.31	183.4	832.1	0.031	200.1	1532
γ_R	25.59	1.771	29.80	13.47	1.563	28.63	0.031	2.250	36.78
γ_{KL}	1.217	1.506	26.18	0.031	1.656	33.47	0.031	200.0	44.59
δ_F	—	—	—	26.91	1.750	20.75	16.78	1.250	256.08
δ_R	—	—	—	18.06	1.313	17.44	11.84	0.844	15.81
δ_{KL}	—	—	—	93.25	1.250	15.72	13.19	0.938	18.50
η_F	—	—	—	—	—	—	16.47	1.813	21.00
η_R	—	—	—	—	—	—	20.19	1.281	17.13
η_{KL}	—	—	—	—	—	—	83.50	1.156	15.53

Table 4. Evaluation of the estimated results by the three metrics.

Evaluation metrics	Estimation methods			
	Nonparametric			Parametric
	Frobenius	Riemannian	Kullback–Leibler	Log normal
Frobenius	586.78	641.95	638.65	845.95
Riemannian	21.50	19.54	19.60	36.97
Kullback–Leibler	6.40	6.31	6.29	16.29

Fig. 2. True and estimated ellipsoids by the proposed methods.

$q = 1$. The 9th entry in the 4th row, 586.8 in bold face, gives the minimum Frobenius norm (26) in the same row. Similarly, numerals in bold face at the 5th and 6th rows mean that they are the minimum in the respective rows. We can see that the Riemannian metric and KL divergence chose the model with three bandwidths based on the third normalization method. The estimated bandwidths are tabulated from the 8th to 16th rows.

We can see from Table 3 that the models with three bandwidths had the best performance. Furthermore, the second and third normalization methods works well, and the difference between the second and the third normalizations is small. Table 4 compares four optimized models by the DuPont dataset. The second row shows the sum of Frobenius norms between 19 true and estimated matrices by each proposed method. The third and fourth rows are similarly derived by Riemannian and KL metrics. We use the three optimal kernel methods with three bandwidths found in Table 3. The kernel methods based on Frobenius norm gives the minimum Frobenius norm, and so on. The accuracy of the log normal regression, however, is poor for the kernel methods.

4.2. Estimated ellipsoids by the proposed methods

Figure 2 depicts the true (a) and estimated ellipsoids by the kernel methods (b)–(d) and regression model (e). As shown, all the models failed to estimate the flat-shaped ellipsoid of “Dark bluish green”. This may stem from the fact that this color is located at the edge of the 19 training colors. We can also see that the estimated ellipsoids in (e) by log normal regression are smaller than those by kernel methods in (b)–(d). The log normal regression, however, has an advantage because the linear estimation has a closed form of the solution. Also, the model can easily implement new explanatory variables such as second-order models.

5. Conclusion

It is known that each color has an ellipsoid region whose points are visually recognized as the same color. Currently, the DuPont dataset provides pairs of colors and ellipsoids in the CIE-Lab system. Of course, the shape of an ellipsoid is determined by a positive definite matrix. Therefore, in this paper, we

have proposed the methods for estimating ellipsoids with a new color center in the Lab system.

First, we considered Gaussian kernel estimation of positive definite matrices with three bandwidths at most and three types of normalization methods of explanatory variables. We found that the third as well as the second normalization methods work well for estimation. The bandwidths were tuned by minimizing the three metrics, namely, Frobenius, Riemannian, and KL. These three metrics showed similar performance for estimation. It is noted that this weighted-sum approach has a theoretical justification based on KL divergence.

Second, we used the matrix-valued log normal regression. This approach has a closed solution for regression coefficient matrices, and gives the ellipsoid of a new color easily. Unfortunately, it showed a poor performance with respect to kernel estimation. This may be improved by using additional explanatory variables derived by color features.

The paint shops at automotive factories currently need more than one month to adjust the painting conditions for synthesis of the same color. With our method, the color matching admitting tolerant ellipsoids could be easily tuned within one week because the painting condition of robot painters can be configured by applying tolerance ellipsoids. This would make it possible to mass-produce new colors with stable quality at factories around the world.

Furthermore, if human color sensitivity can be modeled, the synthesis of new colors could be developed by simulation. We plan to establish a fundamental technology enabling the efficient management of attractive new colors by developing more accurate prediction algorithms based on mathematical approaches such as support vector regression and other approximation techniques as well as on a database of colors and ellipsoids.

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Abbreviations

CIE: Commission Internationale de l'Eclairage, KL: Kullback Leibler.

Declarations

Availability of data and material.

The datasets supporting the conclusions of this article are represented in Sec. 4.

Competing Interests

The authors declare that they have no competing interests.

Author's Contributions

All authors read and approved the final manuscript.

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