# Accurate reflectance prediction in multi-angle measurement

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## Abstract

This study focuses on finding the best viewing angles so that accurate reflectance prediction could be achieved in multiangle measurement of metallic and pearlescent samples. The root mean square error (RMSE) produced by the reconstruction from the first seven Principle component vectors (PCV), the cumulative contribution being 99.92 percent, were analyzed to find the best viewing angles  $10^{\circ}$ ,  $65^{\circ}$ ,  $95^{\circ}$ ,  $120^{\circ}$ ,  $145^{\circ}$ ,  $155^{\circ}$  and  $170^{\circ}$ in clock wise direction from the surface for illumination angle of  $45^{\circ}$ . The error difference resulted by prediction using cubic interpolation and proposed Principle component analysis (PCA) based method were compared. The prediction by PCA based method outperforms the prediction by cubic interpolation. The method can be employed not only to metallic and pearlescent samples but to all non lambertian surfaces.

### Introduction

Accurate reflectance prediction is necessary for the quality assessment and quality control during production and inspection process of paint finishes. Integrating sphere and 45°/0° geometry have been used traditionally for most of paints that absorb incident light and the rest is diffusely scattered as a result perceived color is independent of measuring geometry including the illumination and viewing angles. In contrary to this, the brightness of the metallic coating depends on the viewing angles but is independent of the illumination angles and in pearl interference pigments or pearlescent coating, perceived chroma, hue and brightness depend on both illumination and viewing angles [4]. So, multi-angle measurement is essential for metallic and pearlescent samples to assess the reflectance accurately in different viewing angles. The ASTM recommends the aspecular angles (reference line is across specular direction) of  $15^\circ$ ,  $45^\circ$  and  $110^\circ$  and DIN recommends the aspecular angles of  $25^{\circ}$ ,  $45^{\circ}$ , and  $75^{\circ}$  for the metallic samples [1]. Aspecular angles of 15°, 35°, 45°, 70° and  $85^{\circ}$  viewing angles for illumination direction of  $15^{\circ}$ ,  $45^{\circ}$  and 65° have been proposed for pearlescent pigment [4]. Similarly Aspecular angles of 10°, 18°, 28°, 40° and 90° viewing angles for illumination of  $60^\circ$  have been proposed for all painted surface [3]. Our study also includes the reflectance characteristics behind the specular direction (aspecular angles of  $0^\circ$  to  $-45^\circ$  ) and far flop region.

Up to this point our study has focused on the method of accurate reflectance prediction in multi-angle measurement by choosing few number of best viewing angles. For the purpose multi-angle reflectance characteristics, with in the visible range of 380 *nm* to 780 *nm* with 5 *nm* resolution, of metallic and pearlescent samples were studied. In total 123 different viewing angles of 10° to 35°, 55° to 125° and 145° to 170° with one degree step were used to analyze the reflectance characteristics with the light source adjusted at 45° as shown in Fig. 1. The reflectance measured at the angles between 0° to 10°, 35° to 55°,

 $125^\circ$  to  $145^\circ$  and  $170^\circ$  to  $180^\circ$  were not included in the training set. Consideration of reflectance across that directions results the noise in reflectance prediction process.

The results of our studies show that the reconstruction of reflectance in all 123 different angles is possible by using principle components up to  $7^{th}$ , the cumulative contribution being 99.92 percent. On that basis the reflectance measured at seven best viewing angles should be enough to predict accurate reflectance in all 123 viewing angles. But the problem is to find the best angles. The maximum and minimum points of principle component vectors(PCV) were proposed to choose the best angles [3]. In this study we have analyzed the RMSE curve resulted by PCA based reconstruction of training set in all viewing angles. We have assumed that the angles corresponding to local minimum and local maximum points of RMSE curve may be the candidate of the best angles. The reflectance of every combination of candidate angles were employed to predict the reflectance in all angles. The combination of angles that produce the minimum error has been chosen as the best angles. In the prediction process, the basis vectors corresponding to given viewing angles has been used as the new basis vectors to find the weight function (Inner product matrix) in PCA of given reflectance. Our method is capable of predicting  $1^{st}$  to  $n^{th}$  best angles based on  $1^{st}$  to  $n^{th}$ principle component vectors. The seven best viewing angles 10°,  $65^{\circ}$ ,  $95^{\circ}$ ,  $120^{\circ}$ ,  $145^{\circ}$ ,  $155^{\circ}$  and  $170^{\circ}$  were found. The result of reconstruction by 1<sup>st</sup> to 7<sup>th</sup> principle component vectors and the result by  $1^{st}$  to  $7^{th}$  best angles are almost same, the results are shown in Table 1 and Table 2. The predicted reflectance by PCA and by cubic interpolation for the same angles were compared with measured reflectance in all angles. The results suggest that prediction by PCA method outperforms the cubic interpolation method.



Figure 1. Measurement geometry, thick lines show the proposed viewing angles

#### Measurement

The intensity signal (*S*) of the samples at different angles were calculated using Hamamatsu Photenic Multichannel Analyzer within the visible range of 380 to 780 nm with 5 nm step under the light source halogen lamp with D65 filter. The position of the light source was set at  $45^{\circ}$  from the surface for all viewing

directions. The reflectance of the samples was calculated using Eq. (1).

$$R_{x}(\lambda,\theta) = \frac{S_{x}(\lambda,\theta) - S_{k}(\lambda,\theta)}{S_{w}(\lambda,\theta) - S_{k}(\lambda,\theta)} R_{w}(\lambda,\theta)$$
(1)

Where  $\lambda$  and  $\theta$  are the wavelength and the angles of viewing direction respectively.  $S_x$ ,  $S_w$  and  $S_k$  are the measured signals from samples, standard white and dark respectively.  $R_x$  and  $R_w$  are the reflectance for the sample and calibrated value for a white standard. The reflectance for the sample may exceed value one in specular direction since the sample is more glossy and specular than that of used white reference. All together thirty different samples were used in training set. Out of thirty samples, nine samples were pearlescent and remaining were metallic. Each sample for the training set was measured in 123 different viewing angles  $[10^{\circ} \text{ to } 35^{\circ} 55^{\circ} \text{ to } 125^{\circ} 145^{\circ} \text{ to } 170^{\circ}]$ . Fig. 1 shows the measurement geometry setup. The reflectance measured between  $0^{\circ}$  to  $10^{\circ}$  and  $70^{\circ}$  to  $180^{\circ}$  produces the noise due to low reflectance value near to zero, sometimes goes to negative value so these angle were not considered for the measurement. Similarly reflectance between angles  $35^\circ$  to  $55^\circ$  could not be measured since camera obscures the light source and produces the shadow in the surrounding angles. In the proximity of specular direction between 125° to 145° the reflectance gets saturated for large number of samples so these angles were not considered for the measurement. The reflectance characteristics of metallic and pearlescent samples are shown in Fig. 2.



Figure 2. Reflectance characteristics of metallic and pearl sample (left to right)

# **Reconstruction by PCA**

The idea of PCA is to reduce the dimensionality of a data set, consisting of large number of interrelated variables, while retaining as much as possible variations present in the data set. This is achieved by transforming to a new set of uncorrelated variables called the principle components (PC). The PC are ordered so that first few dimension retains most of the variations present in all of the original variables [2]. Here PCA deals with reconstruction of original data set using PC (inner product matrix) and eigen vector also called principle component vector (PCV).

The first step of PCA is to have original data preferably mean subtracted data. In our case the data is reflectance. The mean subtracted reflectance of *m* different samples at wavelenght  $\lambda$  for *n* different viewing angles is represented in 2D matrix form in Eq. (2).

$$R_{\lambda} = \begin{bmatrix} R_{1}^{\lambda}(\theta_{1}) & \dots & \dots & R_{m}^{\lambda}(\theta_{1}) \\ \vdots & \vdots & \vdots & \vdots \\ R_{1}^{\lambda}(\theta_{n}) & \dots & \dots & R_{m}^{\lambda}(\theta_{n}) \end{bmatrix} - \begin{bmatrix} M^{\lambda}(\theta_{1}) \\ \vdots \\ M^{\lambda}(\theta_{n}) \end{bmatrix} I (2)$$

Where *I* is the unit matrix of size  $1 \times m$  and  $M^{\lambda}(\theta_j)$  is the mean value of reflectance for wavelength  $\lambda$  for viewing direction  $(\theta_j)$ ,

j goes from 1 to n. The mean value of reflectance across each angle is calculated in Eq. (3).

$$M^{\lambda}(\theta_{j}) = \frac{1}{m} \sum_{i=1}^{m} R_{i}^{\lambda}(\theta_{j})$$
(3)

The correlation matrix  $K_{\lambda}$  for each wavelength is calculated as  $K_{\lambda} = \frac{1}{m} R_{\lambda} R_{\lambda}^{T}$ .

Here *T* denotes the transpose of the matrix. Since  $R_{\lambda}$  is mean subtracted data so correlation matrix is exactly covariance matrix of original data. For the correlation matrix  $K_{\lambda}$ , the eigen equation  $K_{\lambda}v_{\lambda} = \sigma_{\lambda}v_{\lambda}$  gets satisfied.  $v_{\lambda}$  and  $\sigma_{\lambda}$  are eigen vectors and eigen values respectively for each wavelength of size  $n \times n$ . The eigen value  $\sigma_{\lambda}$  is a diagonal matrix. The eigen vectors corresponding to *p* largest eigen values are orthogonal basis function  $B_{\lambda}$ . The size of basis matrix  $B_{\lambda}$  is  $n \times p$ . The number of eigen vectors as basis functions were chosen according to the information content termed as fidelity ratio. The fidelity ratio *f* for the first *p* eigen values to the sum of total eigen values as shown in Eq. (4).

$$f = \frac{\sum_{i=1}^{p} \sigma_i}{\sum_{i=1}^{n} \sigma_i} 100 \tag{4}$$

(5)

During the data reduction process inner product matrix IP is calculated in eqn.(5).

 $IP = B_{\lambda}^T R_{\lambda}$ 

$$B_{\lambda} = \begin{bmatrix} v_1^{\lambda}(\theta_1) & \dots & \dots & v_p^{\lambda}(\theta_1) \\ \vdots & \dots & \cdots & \vdots \\ \vdots & \ddots & \dots & \vdots \\ v_1^{\lambda}(\theta_n) & \dots & \dots & v_p^{\lambda}(\theta_n) \end{bmatrix}$$

The reconstruction of reflectance is calculated from eq. (6).

$$R_{\lambda} \approx \tilde{R_{\lambda}} = B \, IP \tag{6}$$

The reconstruction result is the mean subtracted result so the final result is calculated by adding the mean of each wavelength across each angle. The error of reconstruction using 1<sup>st</sup> to 7<sup>th</sup> principle component vectors up to fidelity  $\geq$  99.9 has been shown in Table 1. The 1976 *CIE* L\*a\*b\*(CIELAB) [2] color difference (Lab  $\Delta$ E) and Root mean square error (RMSE) of reflectance are the average results calculated between measured reflectance and predicted reflectance of 30 different samples and 123 different angles (in total 3690 reflectance).

# Primary angle selection and Prediction by PCA

The primary angles have been selected by analyzing the root mean square error as a result of reconstruction by first to seven principle component vectors. The different primary angles might be generated for different wavelength since we have separate principle component vectors for each wavelength. To avoid this ambiguity, we have to calculate principle component vectors collectively for all wavelength and for all samples in the process of primary angle selection. After having primary angles, we can predict reflectance collectively for all wavelengths or each by each wavelength. Our experiment shows small improvement by the wavelength by wavelength prediction and reconstruction than collective prediction and reconstruction. Wavelength by wavelength prediction generate Lab  $\Delta E = 0.464$  and RMSE = 0.005

against Lab  $\Delta E = 0.603$  and *RMSE* = 0.006 by collective prediction using seven best angles.

To ascertain the characteristics of overall wavelength lightness sensed by the naked eye has been used in reference [3]. But in the case of pearl sample, not only the perceived lightness, but also perceived chroma and hue depends on viewing and illumination angle [4]. Therefore only the lightness can not ascertain the characteristics of overall wavelength. However we need eigen vectors and values considering all wavelength at a time but only across the direction of viewing angles. For the purpose the mean subtracted reflectance of *m* different samples including all wavelengths for *n* different angles has been arranged in two dimensional matrix form in Eq. (7).

$$R = \begin{bmatrix} R_1(\theta_1) & \dots & R_m(\theta_1) \\ \vdots & \vdots & \vdots & \vdots \\ R_1(\theta_n) & \dots & R_m(\theta_n) \end{bmatrix} - \begin{bmatrix} M(\theta_1) \\ \vdots \\ M(\theta_n) \end{bmatrix} I \quad (7)$$

Where  $R_i(\theta_j)$  is the reflectance value in all wavelengths of  $i^{th}$  sample at  $j^{th}$  viewing angle and is represented as  $R_i(\theta_j) = [R_i^{380}(\theta_j) - -R_i^{780}(\theta_j)]$ . Here size of matrix R is  $n \times N$ , where  $N = m \times k$ , m is number of samples and k is number of wavelengths. Eq. (8) shows the mean value calculation including all wavelength at angle  $\theta_j$ .

$$M(\boldsymbol{\theta}_j) = \frac{1}{m \times k} \sum_{i=1}^{m} \sum_{\lambda=380}^{780} R_i^{\lambda}(\boldsymbol{\theta}_j)$$
(8)

The principle component vectors and its contribution were calculated. It was found that seven principle component corresponding to seven largest eigen values contributes > 99.9 percent

Table 1. *Reconstruction result:* Principle component vectors (PCV), total contributions (TC), mean values ( $\mu$ ) and maximum values (m) of CIELAB color differences (Lab  $\Delta E$ ), and Root mean square errors (RMSE).

PCV	TC	$Lab\Delta E$		RMSE		
101	10	μ	m	μ	т	
1 <i>st</i>	73.98	11.66	24.86	0.110	0.180	
1 <sup>st</sup> -2 <sup>nd</sup>	90.99	5.620	14.044	0.054	0.130	
1 <sup>st</sup> -3 <sup>rd</sup>	97.60	3.871	11.682	0.031	0.080	
$1^{st}-4^{th}$	98.90	2.284	11.516	0.021	0.079	
$1^{st}-5^{th}$	99.56	1.190	2.368	0.013	0.037	
1 <sup><i>st</i></sup> -6 <sup><i>th</i></sup>	99.84	0.738	1.777	0.007	0.017	
$1^{st} - 7^{th}$	99.92	0.667	1.814	0.006	0.012	

Table 2. *Prediction result:* Mean values ( $\mu$ ) and maximum values (m) of CIELAB color differences (Lab  $\Delta$ E) and the Root mean square errors (RMSE) according to best angles.

Rest angles	La	b∆E	RMSE	
Dest angles	μ	т	μ	т
1 <sup><i>st</i></sup>	9.35	18.97	0.101	0.171
$1^{st} - 2^{nd}$	6.005	13.810	0.063	0.242
$1^{st}-3^{rd}$	2.726	14.043	0.029	0.132
$1^{st}$ - $4^{th}$	1.968	13.406	0.019	0.092
$1^{st}$ - $5^{th}$	1.074	3.633	0.013	0.082
$1^{st}$ - $6^{th}$	0.733	2.53	0.008	0.051
$1^{st} - 7^{th}$	0.603	2.501	0.006	0.021

fidelity ratio. The principle component analysis was computed to the training set consisted both metallic and pearl sample.

The primary angles could be selected by picking the angles whose reflectance produce the minimum prediction errors applied to the reflectance of training set. In that process, the combination of angles which produce minimum prediction error are the required primary angles. Nevertheless this process is computationally slow since process should be repeated for all possible combinations. The number of computations required for selecting *n* best angles from *N* set of angles is given by Eq. (9).

$$\binom{N}{n} = \frac{N!}{(N-n)!n!} \tag{9}$$

The sign ! indicates factorial. As the number of total angles and choice of best angles increases, this method goes rather slow since in every iteration, there should be prediction for each combination. To make computation faster total angles have been sampled at candidate angles. The candidate angles are corresponding angles of local maxima and local minima of reconstruction error by Principle component analysis. Fig. 3. shows the reconstruction error (RMSE) and its local minima and maxima points.



Figure 3. Mean RMSE as reconstruction error by first seven Principle component vectors (left to right and top to down). The round dot shows local maximum and square dot shows local minimum

By using the reflectance of set of candidate angles, the best angles were chosen. The candidate angles are fewer in count than total angles so improves the computation. The candidate angles and best angles have been shown below. The first and second bracket contain angles corresponding to local minima and local maxima of error curve respectively.

- C<sub>1</sub> [35 170][10 125]
- *B*<sub>1</sub> [35]
- *C*<sub>2</sub> [25 85 165][10 35 145 170]
- B<sub>2</sub> [85 165]
- C<sub>3</sub> [30 80 120 155][10 35 110 125 170]
- *B*<sub>3</sub> [80 110 155]
- $C_4$  [30 70 90 120 155][10 35 85 110 145 170]
- *B*<sub>4</sub> [70 110 120 155]
- C<sub>5</sub> [20 80 120 155 165][10 25 105 145 160 170]
- *B*<sub>5</sub> [10 80 105 120 155]
- C<sub>6</sub> [15 35 65 95 125 160][10 25 55 85 120 150 170]
- *B*<sub>6</sub> [10 65 95 125 150 170]
- *C*<sub>7</sub> [15 35 65 95 145 155 170][10 25 55 85 120 150 165]
- *B*<sub>7</sub> [10 65 95 120 145 155 170]

Here C and B indicate candidate angles and best angles respectively. The subscript 1 to 7 indicates to the  $1^{st}$  to  $7^{th}$  best and candidate angles.

The selection of best angles are based on reconstruction and prediction of spectra in all wavelength by PCA. For the prediction process of test set we have principle component vectors calculated from training set and we have reflectance from test set measured in some few angles and our goal is to predict reflectance in all viewing angles from 10° to 170°. Reflectance are best estimated by the linear combination of first *p* principle components as shown in Eq. (6). But the inner product matrix *IP* is not known for the reflectance of given angles. The inner product matrix *IP* is solved as shown in Eq. (10)using angles of mean subtracted reflectance of test set and basis function corresponding to given angles of test set. Here the angles of test set are  $\alpha = (\alpha_1, ..., \alpha_p)$  and test angles  $\alpha$  should be the element of set of total angles  $\theta$ .

$$IP = \begin{bmatrix} v_1^{\lambda}(\alpha_1) & . & v_p^{\lambda}(\alpha_1) \\ \vdots & . & \vdots \\ \vdots & . & . \\ v_1^{\lambda}(\alpha_p) & . & v_p^{\lambda}(\alpha_p) \end{bmatrix}^T \begin{bmatrix} R_1^{\lambda}(\alpha_1) - M^{\lambda}(\alpha_1) \\ \vdots \\ R_p^{\lambda}(\alpha_p) - M_p^{\lambda}(\alpha_p) \end{bmatrix} (1)$$

The reflectance value of each wavelength in all viewing angles  $R_{\lambda} = [R_{\lambda}(\theta_1), \dots, R_{\lambda}(\theta_n)]^T$  can be predicted easily by inserting IP from Eq. (10) in Eq. (6). Then the mean value from training sets corresponding to each angles should be added. The error of prediction from reflectance from first to seventh best angles has been shown in Table 2. The results predicted by PCA using reflectance of best angles are almost the same as the result of reconstruction by PCA. The prediction results by PCA was compared with the results by cubic interpolation. The results by PCA outperforms the results by cubic interpolation. Fig. 4 shows the RMSE error by PCA based prediction and the comparison of error by PCA based prediction to the cubic interpolation. All the reflectance of training sets were used for error calculation using seven best angles. Figs. 5 and 6 show the results by PCA based prediction and cubic interpolation using seven best applied to metallic and pearlescent samples respectively. The continuous transitions of reflectance in specular direction between angles of 130° to 140° could estimated by doing the interpolation of principle component vectors of the training set or by doing the linear regression. The same method can be applied to get continuous transitions of reflectance between  $35^{\circ}$  to  $55^{\circ}$ . The extrapolation using time series analysis can be applied to the principle component vector to retain the reflectance between  $0^{\circ}$  to  $10^{\circ}$  and  $170^{\circ}$ to 180°.



Figure 4. RMSE error by PCA based prediction and its comparison to the cubic interpolation method (left to right)

# **Error Measures**

In this study, we used root-mean-square error (RMSE) and  $CIEL^*A^*B^*$  color difference (Lab $\Delta E$ ) to measure disparity between measured and predicted reflectance factors. The RMSE was calculated as shown in Eq.(11).

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (R_m(i) - R_p(i))^2}{n}}$$
(11)

In Eq. (11)  $R_m$  and  $R_p$  are the measured and predicted reflectance factors at the same angle and *n* is the number of wavelengths. The color difference was calculated using Eq. (12). Day light source *D*65 and CIE 1931 standard observer were employed to calculate luminance  $L^*$ , and chrominance  $a^*$  and  $b^*$  of the reflectance factor.

$$Lab\Delta E = \sqrt{(L_m^* - L_p^*)^2 + (a_m^* - a_p^*)^2 + (b_m^* - b_p^*)^2}$$
(12)

In Eq. (12) the subscript *m* and *p* are the notations for the measured and predicted ones. Since the reflectance of some samples in specular direction are greater than one,  $Lab\Delta E$  fails to measure the accurate color difference.

### 0) Conclusions

We have presented PCA based reflectance prediction method in multi-angle measurement. The best viewing angles for metallic and pearlescent samples were selected depending on the minimum reconstruction error of training set. Our future work will consider the multi-angle reflectance characteristics of glossy plastic surface and ceramic tiles too. our work will also investigate the best primary illumination angle or angles so that minimum color difference could be achieved in the reflectance prediction process between 0° to 180° viewing angles.

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*Figure 5.* Reflectance characteristics of metallic sample, results predicted by PCA and cubic interpolation using seven best angles.



*Figure 6.* Reflectance characteristics of pearlescent sample, results predicted by PCA and cubic interpolation using seven best angles.