

Image Segmentation and Pigment Mapping in Spectral Imaging

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Abstract

Spectral imaging techniques have been well developed in the last ten years for art conservation science. Spectral reconstruction algorithms have achieved sufficiently high accuracy to predict specific pigments and their concentrations of each pixel on works of art. Digital rejuvenation can be promptly performed on works of art based on the pigment mapping to correct changed color or repaint discolored parts. In our pilot experiment, the painting was made of ten Gamblin artist oil paints plus white paint. A spectral image of the painting was derived from multi-channel camera signals. To overcome the difficulty of unmixing a large spectral image, the image was first segmented using k-Means classification in CIELAB color space. Within each segmented region, based on its colorimetric property, a subgroup of pigments was selected from a predefined pigment database. Pigment mapping was then implemented for each pixel in this segmented region with this subgroup of pigments based on two-constant Kubelka-Munk theory. By focusing on a subgroup of pigments rather than unmixing with the entire pigment database for each pixel, the computation efficiency was greatly improved.

Introduction

The characterization of materials constituting paintings is essential for the historical knowledge of the painting and for retouching (i.e., inpainting) the lost or damaged areas in the painting. Modern analytical techniques provide comprehensive information on the chemical composition of the materials by means of minute quantities taken from the objects.^[1] However, there is a clear desire to use non-destructive methods. There are two main visible-spectrum noninvasive approaches: spot spectroscopy and imaging spectroscopy. Though spot spectroscopy is expected to have higher accuracy than imaging spectroscopy, it is only possible to measure the color at a limited number of points on the surface of the painting over a fixed aperture. This means that the measurement sites have to be selected and marked carefully. On the other hand, imaging spectroscopy avoids the difficulty by simply measuring the whole surface. With enormous development of imaging spectroscopy in the last ten years, the spectral accuracy of this technique has been improved to a great extent so that spectral images have been used for documentation, analytical assessment and digital rejuvenation.^[2] Additionally, it is possible to identify the pigments and quantify their constituents for each pixel of the spectral image.^[3] This paper presents further investigation into the potential of spectral imaging techniques for pigment mapping.

Pigment mapping is of great importance for conservators to inpaint the lost or damaged areas of paintings. It is generally difficult to avoid metamerism if those areas are restored by visual color matching to the surrounding undamaged surface. Berns^[4] suggested that the inpainted areas should ideally have identical

optical (spectral, color and transparency) and geometric (gloss, texture and impasto) properties. In this pilot experiment, spectral matching, rather than conventional color matching, was achieved by pigment mapping.

Reference [6] investigates the potential of multispectral imaging for pigment identification in paintings. It assumes that there are only pure pigments or mixtures of these pigments with either a white or black colorant. It also assumes that these mixtures transform the reflectance spectrum of a pigment in an approximate linear fashion. However, it is known that the logarithm of the absorption **K** and scattering **S** ratio is the most invariant to changes in concentration.^[4] Thus, pigment mapping should not be done in reflectance space, but in **K/S** space.

The Kubelka-Munk (K-M) theory has been widely used in the paint industry for over 50 years.^[7,8] It is an optical model that establishes the relationship between surface reflectance and colorant formulation, layer thickness and substrate reflectance. References [4] and [5] applied single-constant K-M theory to select multiple pigments for inpainting using spot spectroscopy. Reference [9] used a computer-match prediction model based on K-M theory to select pigment recipes that give non-metameric matches, but only give prime attention to blue pigments.

In this experiment, the test target was a small oil painting made of ten chromatic pigments and titanium white. It was assumed that every pixel was made of at most four pigments. Thus, it makes more sense to map each pixel using a subgroup rather than all of the pigments. The image was first segmented using k-Means^[10] classification into five different clusters in CIELAB (a*b*) color space. Then, up to four pigments were selected to map every pixel in each cluster based on colorimetric information. This approach successfully and efficiently identified and spatially mapped pigments for each pixel in the image.

Theory

The general model of K-M theory can be simplified for an opaque surface.^[8] The simplified version describes the relationship between the optical (spectral reflectance) and material properties (the ratio between absorption and scattering coefficients), as follows:

$$\left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda} = \frac{(1 - \mathbf{R}_{\lambda})^2}{2\mathbf{R}_{\lambda}} \quad (1)$$

where \mathbf{R}_{λ} is spectral reflectance of a surface and $(\mathbf{K}/\mathbf{S})_{\lambda}$ is the spectral ratio between absorption **K** and scattering **S**. Further, for two-constant K-M theory, the ratio of absorption and scattering of a mixture sample can be expressed using the pigment concentration *c*, the number of pigments in a mixture *n*, the absorption **k** and scattering **s** of pigments at unit amount. The scattering coefficient for white paint $\mathbf{s}_{\lambda,w}$ was assumed to be unity independent of wavelength,^[8] and its absorption coefficient $\mathbf{k}_{\lambda,w}$

was equal to the ratio $(\mathbf{K}/\mathbf{S})_{\lambda,w}$, calculated using Eq. (1) from the reflectance measurement.

$$\left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda} = \frac{\left(1 - \sum_{i=1}^n c_i\right) \mathbf{k}_{\lambda,w} + \sum_{i=1}^n c_i \mathbf{k}_{\lambda,i}}{\left(1 - \sum_{i=1}^n c_i\right) \mathbf{s}_{\lambda,w} + \sum_{i=1}^n c_i \mathbf{s}_{\lambda,i}} \quad (2)$$

The unit absorption and scattering coefficients for each pigment can be calculated based on a pure pigment (masstone) and its mixture with white paint, as described by the following two equations, readily derived from Eq. (2).

$$\left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda, \text{mixture}} = \frac{(1-c) \mathbf{k}_{\lambda,w} + c \mathbf{k}_{\lambda}}{(1-c) \mathbf{s}_{\lambda,w} + c \mathbf{s}_{\lambda}} \quad (3)$$

$$\left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda, \text{masstone}} = \frac{\mathbf{k}_{\lambda}}{\mathbf{s}_{\lambda}} \quad (4)$$

The unit absorption \mathbf{k} and scattering \mathbf{s} of this pigment can then be deduced.

$$\mathbf{k}_{\lambda} = \mathbf{s}_{\lambda} \cdot \left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda, \text{masstone}} \quad (5)$$

$$\mathbf{s}_{\lambda} = \frac{1-c}{c} \frac{\left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda, \text{mixture}} \cdot \mathbf{s}_{\lambda,w} - \mathbf{k}_{\lambda,w}}{\left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda, \text{masstone}} - \left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda, \text{mixture}}} \quad (6)$$

After the unit absorption and scattering coefficients for each pigment are calculated using Eqs. (5) and (6), the database has been completely developed. Characterization of any unknown mixture sample requires knowledge of both constituents of pigments and their concentrations, the solutions to which demand multiple linear regression. This is more obvious by rewriting Eq. (2) as Eq. (7).^[11] Assuming that some pigments in the regression model were more important than others, stepwise regression could be used to select the most important pigments that contribute to the unknown mixture. This regression has to be applied to each and every pixel using all pigments of interest.

$$\sum_{i=1}^n c_i \left[\left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda} (\mathbf{s}_{\lambda,i} - \mathbf{s}_{\lambda,w}) - (\mathbf{k}_{\lambda,i} - \mathbf{k}_{\lambda,w}) \right] + \left[\mathbf{s}_{\lambda,w} \left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda} - \mathbf{k}_{\lambda,w} \right] = 0 \quad (7)$$

In this paper, image segmentation was applied first to divide the entire image into several color clusters based on colorimetric information, with each cluster only consisting of up to four pigments. Compared with stepwise regression, this approach avoids the difficulty of iteratively selecting the pigments.

To obtain pigment information of each pixel, optimization was used to minimize root-mean-square (RMS) error between measured and predicted spectral reflectance. It is very important to apply optimization in reflectance space, rather than in K/S space. It is because small differences in K/S space can result in large reflectance differences, and in turn large color differences, caused by the nonlinear relationship between these two spectral descriptions.

Experimental

The input device of the spectral image acquisition system is a Sinarback 54H digital camera that has a Kodak KAF-22000CE CCD with a resolution of 5440 × 4880 pixels. The camera employed a color-filter-array (CFA) and a filter slider with two customer-designed filters that improved both color and spectral accuracies over the production camera.^[12] In each position of the filter wheel, a three-channel image was collected, producing six-

channel camera images. A calibration target (GretagMacbeth ColorChecker DC) was measured using a bidirectional spectrophotometer and imaged. A reconstruction model was derived to convert the multi-channel camera data to spectral reflectance data for each pixel.^[12] The model consists of both colorimetric and spectral transformations, which can achieve high spectral and colorimetric accuracies simultaneously for a certain viewing and illuminating condition. Following camera calibration, spectral reflectance as a function of spatial position can be estimated for any imaged target.

For this experiment, the test target was a small oil painting, featured with flowers in a blue vase, which was made of Gamblin artist oil paints. The following pigments were used: Cadmium Yellow Medium, Indian Yellow, Cadmium Red Medium, Venetian Red, Quinacridone Red, Phthalocyanine Green, Chromium Oxide Green, Cobalt Blue, Phthalocyanine Blue, Ivory Black and Titanium White. Reference [4] suggested that the logarithm of the absorption and scattering ratio was the most invariant to changes in concentration. The $\log(\mathbf{K}/\mathbf{S})$ spectra of these pigments are plotted in Figure. 1.

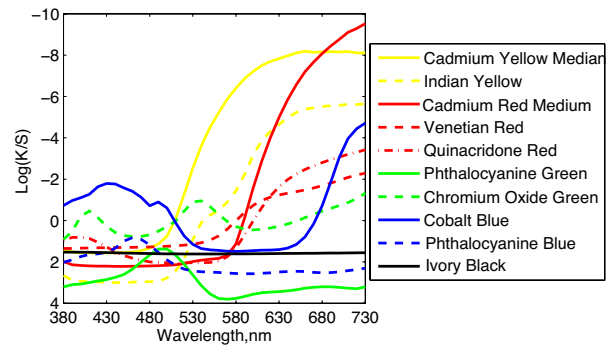


Figure 1 The $\log(\mathbf{K}/\mathbf{S})$ spectra of ten Gamblin artist oil paints

Since the resulting spectral image from the two RGB camera images was too large (about 1.5 GB), the RGB images were cropped and down-sampled by 90%.

Results and Discussions

Database Development

For each pigment, one masstone and two mixture samples were prepared according to the concentrations listed in Table I.

Table I Measured and predicted weight concentrations for each pigment mixed with white paint

Golden Artist Oil Pigments	Concentrations (Mass, %)			
	#1	#2	#3	#3 Pred.
Cadmium Yellow Medium	100	51.0	20.0	22.5
Indian Yellow	100	52.4	18.5	22.9
Cadmium Red Medium	100	51.1	79.6	68.6
Venetian Red	100	52.3	78.9	89.0
Quinacridone Red	100	50.0	21.4	21.4
Phthalo Green	100	52.1	20.5	27.4
Chromium Oxide Green	100	60.5	20.4	22.1
Cobalt Blue	100	60.3	20.6	21.0
Phthalo Blue	100	59.7	20.3	27.1
Ivory Black	100	59.2	19.6	24.7

The masstone (#1) and one mixture sample (#2) per pigment were used to calculate unit absorption and scattering coefficients. The other mixture sample (#3) was used to evaluate the accuracy of the prediction model. Table I also lists the predicted concentrations for these verification mixture samples. The errors between measured and predicted concentrations are quite reasonable. The concentration errors may result from measurement inaccuracy, incomplete mixing, surface non-smoothness and limitations of the Kubelka-Munk theory.

In addition to prediction of concentration, the performance of spectral estimation for these mixtures was quantified using three metrics. These metrics included RMS spectral error between measured and estimated reflectances, CIEDE2000 color difference for CIE illuminant D65 and the 2-degree observer, and a metameric index from D65 to CIE illuminant A. Both the spectral and colorimetric performances were quite well.

Table II Performance metrics for estimation accuracy of the mixture samples (#3)

Statistics	Spectral % RMS Error	Color Difference (ΔE_{00} D65)	Index of Metamerism (ΔE_{00} D65 \rightarrow A)
Average	1.1	1.0	0.1
Std. Dev.	0.8	0.6	0.1
Maximum	3.0	2.1	0.3
90% Percentile	2.4	1.9	0.3

Image Segmentation

The spectral image of the test target was obtained from two raw camera RGB images using the reconstruction method described in Reference [12]. It was then transformed to a CIELAB image for CIE illuminant D65 and the 2-degree observer. Unsupervised k-Means clustering method was used to segment the CIELAB image into five clusters in a^*b^* space. The clustering process was implemented by the *kmeans* function in MATLAB.

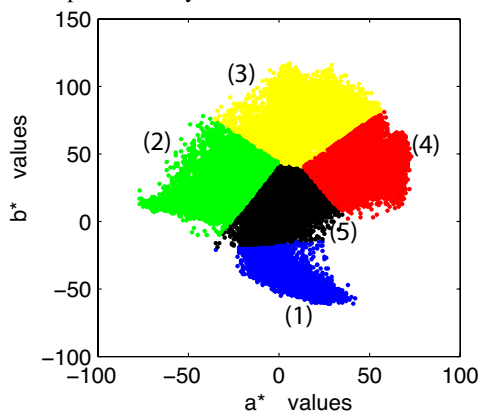


Figure 2 Scatter plot of five segmented clusters in a^*b^* space

Figure 2 shows the scatter plot of the five segmented clusters in a^*b^* space. Figure 3 illustrates each segmented image separately. The k-Means clustering method successfully segmented the image based on colorimetric information. The number of clusters was determined to be five through trial-and-error. Four clusters were insufficient to separate certain colors. On the other hand, six or more clusters provided more detail than was necessary

for the test target. Cluster 5 consists of all low chroma colors and locates in the center of a^*b^* space (Figure 2).

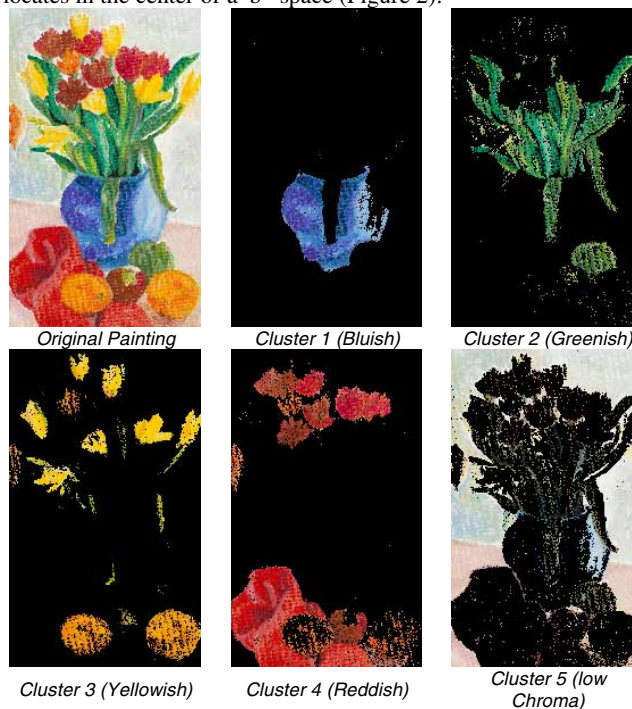


Figure 3 Original image of the oil painting and five segmented images

Pigment Mapping

In this small oil painting, only a small portion consisted of pure pigments, the majority being mixtures. Several assumptions were made: (1) the painting was totally opaque; (2) most mixtures were made of only one chromatic pigment with white paint, and some mixtures were made of no more than four chromatic pigments with white. Because Cluster 5 was somewhat transparent and appeared to consist of more than four pigments, it was eliminated from the following analysis.

Table III Selected pigment combinations for each cluster

Pigments	Cluster Number			
	1	2	3	4
Cadmium Yellow Medium		x	x	
Indian Yellow			x	x
Cadmium Red Medium				x
Venetian Red				x
Quinacridone Red				x
Phthalocyanine Green		x		
Chromium Oxide Green		x	x	
Cobalt Blue	x			
Phthalocyanine Blue	x			
Ivory Black				

For each cluster, several candidate pigments were selected based on colorimetric information. As listed in Table III, Cluster 1 contained two blue pigments. For Cluster 2, one yellow pigment was included along with two green pigments, as visual inspection of the painting indicated the existence of yellow among the

dominant green colors. The same conclusion applied to Clusters 3 and 4. The ivory black was not selected for any cluster except for Cluster 5 because its spectrum was flat and spectrally nonselective.

Nine points on the painting were carefully selected and measured with a bidirectional spectrophotometer. In addition, the reflectance spectra of these points were estimated from the camera model only and from pigment mapping based on spectral imaging. Figure 4 compares the estimated spectra from the camera model and pigment mapping with *in-situ* spectrophotometer measurements for four chromatic pigments. It can be clearly seen that the estimated reflectance spectra from pigment mapping are more accurate and much closer to *in-situ* measurements. The same result has been obtained using the simulated camera data in reference [3]. It can be concluded that the accuracy of spectral imaging is high enough to predict specific pigments and their concentrations of each pixel of the painting, and that by incorporating pigment information, the accuracy of spectral image can be further improved.

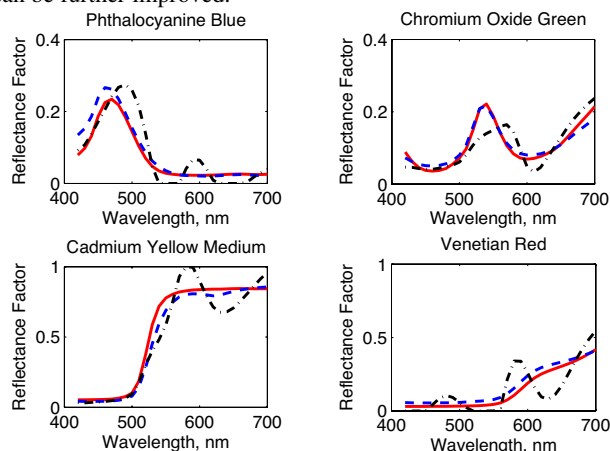


Figure 4 Measured (solid lines) and estimated spectra from camera model (dot-dashed lines) and pigment mapping (dashed lines) of four chromatic pigments

Conclusions

The CIELAB image of the test target was first segmented using K-Means classification in a^*b^* color space. Within each cluster, a subgroup of candidate pigments was selected from a ten-pigment database. After that, pigment mapping was implemented on a pixel basis using two-constant Kubelka-Munk theory to obtain a concentration map for each pigment. This technique resulted in quite good performance. By focusing on a subgroup of pigments rather than unmixing with the entire pigment database for each pixel, the computation efficiency was improved greatly. It also proves that spectral imaging techniques have the potential to identify pigments and determine their concentrations image-wise.

The fundamental basis of the technique presented in this research is the spectral accuracy of the camera model. The choice of calibration target greatly affects estimation accuracy and it is critical that the target should span both the spectral and colorimetric description of the painting.^[5] Since the current calibration target (ColorChecker DC) does not satisfy the above requirements, better spectral accuracy should be expected with a more appropriate target.^[13] It is also possible to develop an

automatic selection routine for candidate pigments instead of the manual process used for this research. Finally, it is more common that the pigments in a painting are unknown. This problem can be solved in two steps: (1) select candidate pigments from a larger database; and (2) mapping each pixel using the described technique.

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