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Is Multispectral enough? An evaluation on the performance of multispectral images in pigment unmixing task

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Abstract

Multispectral imaging in contrast with hyperspectral imaging is a cheaper and more accessible method with a feasibly mobile setup. However, the restrained spectral resolution of multispectral images is a limitation that influences the applicability of this method in different fields. In this study, we tried to answer the question of whether multispectral images are suitable enough to be used in the spectral unmixing task. For this specific application, we explore spectral unmixing of an oil painting to obtain pigment maps. We observe that the performance of the multispectral imaging system in the pigment unmixing task is significantly influenced by two key factors: the number of bands in the multispectral imaging system and the spectral range covered by these bands in relation to the spectral features of the pigments present in the spectral library.

Introduction

Having specific information about the materials used in a painting is a powerful tool in various aspects of art studies ranging from authentication to restoration and conservation [1]. A painting can consist of colorants (pigments or dyes), binders, and support preparation materials, among which colorants are of great importance in the restoration process [2]. Common pigment identification techniques can be categorized based on area of analysis and invasiveness. In the case of the area of analysis, methods can be categorized into point analysis or imaging techniques. In general, any method that would require pigment or cross-section sampling is considered an invasive technique; therefore, chemical analysis and electronic microscopy methods (i.e. SEM) would fall into this category. On the other hand, imaging and optical fiber spectroscopy methods are categorized among the non-invasive methods. The high value of cultural heritage paintings makes the non-invasive techniques more favorable for pigment identification tasks. Additionally, the full-painting nature of the imaging techniques makes these analysis methods one of the most suitable techniques for this task [3].

Among the varying imaging techniques, hyperspectral imaging has been vastly used in tackling pigment identification and mapping tasks [4, 5, 6, 7]. In the hyperspectral imaging technique, the spectral reflectance of the painting can be captured in spectral ranges varying from ultraviolet (UVA: 330-380 nm) to visible (380-700 nm) on to infrared (near IR: 700-1000 nm and short wavelength IR: 900 to 2500 nm). The captured spectra later on can be processed to achieve pigment maps [4, 5, 6, 7]. Pigment mapping can be achieved through several algorithms. Among these algorithms, there are approaches such as machine learning algorithms [8] or spectral metric thresholding [4], which try to classify each pixel based on the similarity of its spectrum to the spectrum of each library member. These methods do not address the fact that the spectrum in each pixel is in fact the physical mixture of different materials spectra captured by the camera sensors. The physical models that describe this mixture phenomenon are known as spectral mixing models [9]. These mixing models are the basis of the spectral unmixing algorithm for pigment mapping. Unlike the pixel-classification methods, the output of spectral unmixing is a concentration vector that predicts the concentration of each member of the spectral library in the unmixed pixel, leading to separate concentration maps for each member.

In numerous studies, hyperspectral images of paintings have been used for pigment unmixing purposes [7, 10, 11]. Although hyperspectral imaging is a commonly used technique, the method suffers from several practical drawbacks. Hyperspectral imaging devices are expensive. Additionally, the instances with high spatial and spectral resolutions are commonly line-scanning cameras and require motorization (either a stage for the sample or a motorized camera holder) which makes their mobility complicated. In contrast, multispectral imaging is a less expensive a more mobile member of the spectral imaging devices family. However, multispectral imaging lacks spectral resolution. While hyperspectral images have a spectral resolution of less than 5 nm and uniformly cover the spectral range, the spectral resolution of the multispectral images is dependent on the number of bands, and the range of the spectral sensitivity of the bands present in the multispectral device. In this work, we investigate the possibility of using multispectral images to tackle spectral unmixing tasks. We explore the effect of band number and spectral range on the quality of spectral unmixing.

Materials and Methods

Sample Painting

The painting ($22 \times 16\ cm^2$) used in this study, which will be referred to as “The House”, was an artwork created previously by an artist (Fig. 1). The paints used in this painting were linseed oil-based paints produced by “Sang” and “Winsor & Newton”. No further preparation steps were carried out on the pre-primed canvas and the painting was well-dried when captured.

Figure 1. *The RGB-Representation of ”The House” painting.*

Hyperspectral Imaging

The imaging was carried out using a HySpex VNIR1800 line-scanner camera (Norsko Elektro Optikk). The spectral range of the capture covered 400 to 1000 nm with a sampling interval of 3.26 nm. The lens used for this capture had a working distance of 1 m and a resolution of 1800 pixels per line. As a result, each pixel covered a $168 \times 168\ \mu m^2$ of the painting. The illumination-capture configuration for this capture was set to 45:0 and the painting was illuminated by two Halogen Smart Light 3900e light sources as shown in Figure 2. The $Spectralon^{®}$ white calibration tile was used in the capture setup for reflectance calculation. Additionally, a gray tile with uniform diffuse reflectance was used to perform flat-field correction since the Spectralon tile was not wide enough.

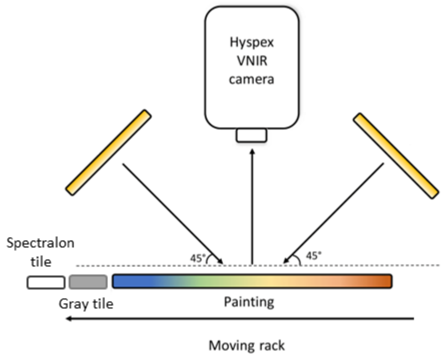

Figure 2. The scheme of the imaging setup.

Multispectral imaging simulation

Initially, a set of 16 hypothetical bands were selected. While the bands in the NIR range are completely artificial the visible bands are taken from an LED-base multispectral camera. The bands were defined in a way that they would cover the full spectral range of the VNIR hyperspectral camera [9]. Figure 3 presents the spectra of the bands used in this study.

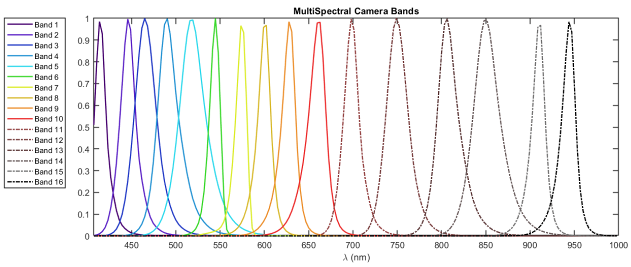

Figure 3. The Spectral sensitivity of the simulated multispectral camera.

Mixing Models

Theoretically, the mixing of the pigments' spectra can have three configurations. The first case is when the pigments are present in two completely separate regions without overlapping. In this case, the mixing happens only optically and at the camera level which is the dominant mixing configuration in the case of the pointillism painting style [12]. The second configuration happens when two layers consisting of a single type of pigment, overlay each other. Finally, there can be a mixture of various types of pigment particles (at a microscopic level) dispersed in the binder. In this case, more complex mixing phenomena are present [10].

In the case of the first configuration, since the spectra are mixed only at the camera level the mixing phenomenon would have an additive nature [11]. In contrast, the second configuration, where the light reflected from one layer would interact with

Table 1: Mixing models suggested by Grillini et al. [11]

Label	Model type	Equation
M_{Add}	Additive	$R = \sum_{i=1}^{q} R_i c_i$
M_{Sub}	Subtractive	$R = \prod_{i=1}^{q} R_i^{c_i}$
M_{Hyb}	Hybrid (Subtractive-Additive)	$R = \left(\sum_{i=1}^{q} R_i^{\tau} c_i\right)\left(\prod_{i=1}^{q} R_i^{c_i(1-\tau)}\right)$

the pigments in the other layer as it transmits through the later layer, has a subtractive nature [11]. Finally, in the third configuration (suggested by Grillini et al. [11]), both phenomena are to some extent present and can be modeled by a Subtractive-additive hybrid model. It is worth mentioning that the mixing models used in this study do not model the inter-scattering effect at the particle level. Table 1 summarizes the mentioned mixing models where q is the number of members in the spectral library, τ is a constant that defines the extent of hybridity ranging from 0 (fully additive) to 1 (Fully subtractive), R_i is the spectrum of i^{th} member of the spectral library, and c_i is its concentration in the mixture. Grillini et al. [10, 11] had shown that the subtractive model or a hybrid model with the τ value of 0 could outperform the two other models when used in an unmixing algorithm. As a result, the subtractive mixing model was used for unmixing purposes in this study.

Pigment Unmixing Algorithm

The pigment unmixing was carried out by solving a concentration optimization problem per pixel using the mixing models presented in table 1. The optimization was carried out using the non-linear optimization function "fmincon()" with a sequential quadratic programming algorithm in MATLAB (The MathWorks Inc., Natick, MA, USA.). As for the cost function, the optimization was penalized based on the mean square of the difference between the mixture spectra and the predicted mixture spectrum (Eq. 1); where the predicted mixture spectrum was the output of the mixing model. The optimization was carried out while considering two main constraints: non-negativity and sum-to-one. The optimization was initialized with an equal concentration of the library members while maintaining the sum-to-one constraint.

$$MSE = \sum_{i=1}^{n} \left(\left(R_{prediction,i} - R_{unmixed,i}\right)^2 / n \right) \tag{1}$$

Spectral Library

Table 2 shows the pigments present in the painting. The spectra of the spectral library were taken from the Fiber Optics Reflectance Spectra (FORS) of Pictural Materials database provided by the Institute of Applied Physics (Italy) [14]. The spectra were obtained using fiber optics spectroscopy of pure pigments dispersed in linseed oil and painted over wood panels of 15 mm thickness. The spectra were interpolated using cubic interpolation to match the sampling intervals of the spectral image. Figure 5 shows the spectra of the members of the spectral library. Here is the table 2.

Based on the points made by the artist, the dark blue patches only contained ultramarine blue, while in the case of light blue patches were mixed with white paint. The windows contained

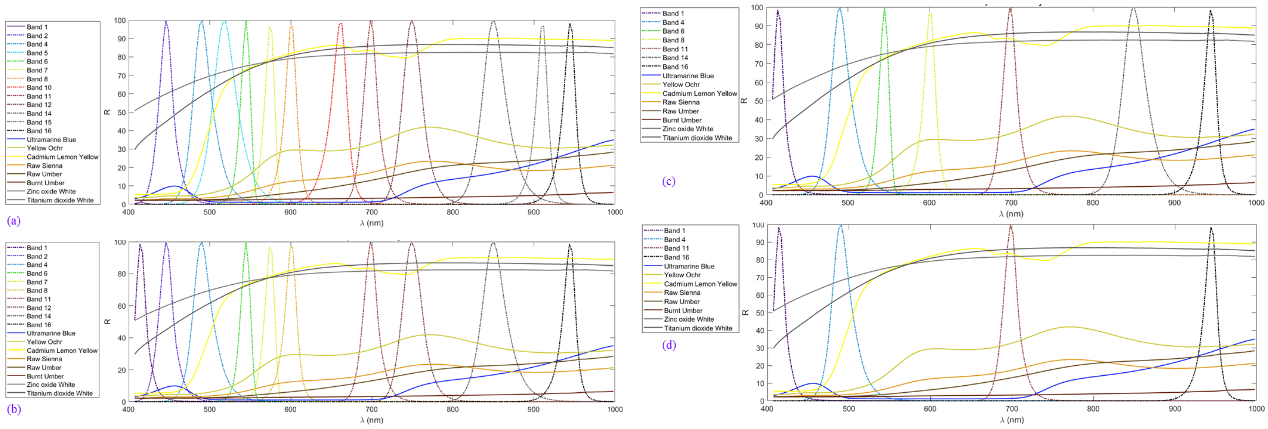

Figure 4. Simulated camera sensitivities and the spectra of spectral library members: a)13-band camera, b)10-band camera, c) 7-band camera, d) 4-band camera

Table 2: List of members of the spectral library.

Paint	Pigment	Binder	Title of library member
Blue	Ultramarine	Linseed oil	Ultramarine Blue
Yellow	Ochre	Linseed oil	Ochre Yellow
Lemon Yellow	Cadmium	Linseed oil	Cadmium Lemon Yellow
Brown 1	Raw Sienna	Linseed oil	Raw Sienna
Brown 2	Raw Umber	Linseed oil	Raw Umber
Brown 3	Burnt Umber	Linseed oil	Burnt Umber
White	Zinc Oxide	Linseed oil	Zinc White
White	Titanium dioxide	Linseed oil	Titanium White

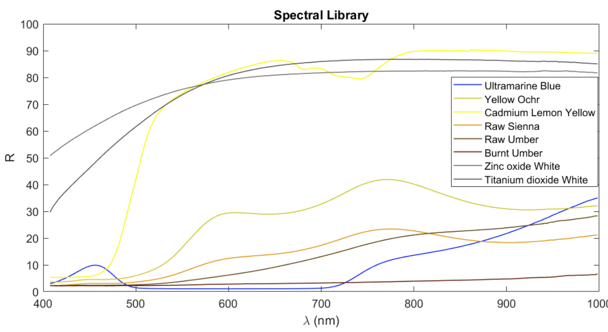

Figure 5. Spectra of the spectral library members.

cadmium lemon yellow, while the walls were mostly painted using ocher yellow. The roof and the door were mostly painted using burnt umber and the light brown lines were painted using raw sienna and raw umber. According to the supplier the white paint contained titanium dioxide and zinc oxide.

Ground truth

To obtain a ground truth for the performance of the hyperspectral image in pigment unmixing, the discussed unmixing algorithm was carried out on the spectrum of each pixel using the subtractive mixing model. Figure 6.a illustrates the result of the unmixed hyperspectral image.

Results and Discussion

Multispectral simulation

To evaluate the performance of different multispectral images in the pigment unmixing task, initially, several hypothetical multispectral cameras were created by selection of various combinations of the bands described in figure 3. To simulate the response (I) of each multispectral camera from the hyperspectral cube equation 2 was used where s_i is the spectral sensitivity of the band at the i^{th} wavelength and n is the total number of the bands. In order to resample the spectral library, equation 2 was used to calculate each band's response to the members of the spectral library and the responses were used in the unmixing process.

$$I_{band} = \sum_{i=1}^{n} (R_i - s_i) / \sum_{i=1}^{n} s_i \quad (2)$$

Study on the effect of band number

To investigate the effect of the number of the bands on the unmixing performance, the unmixing was carried out in several steps, and in each step, a new camera was simulated by removing one band from the range of 400-600 nm, one band from the range of 600-800 nm and one band from the range of 800-1000 nm. These spectral ranges were decided based on the location of the spectral features of the members of the spectral library and were chosen to make sure that even after the removal of several bands no important spectral range would remain uncovered. In the first trial, a 13-band camera was simulated by removal of the 3rd, 9th, and 13th bands. Figure 4a shows the remaining bands along the spectra of the spectral library. The same approach was followed to simulate a 10-band camera by removing the 5th, 10th, and 15th bands (Fig. 4b). In the next steps, a 7-band and a 4-band camera were simulated by removal of the 2nd, 7th, 12th band (Fig. 4c) and the 6th,8th, and 14th (Fig. 4d) respectively. The simulated camera sensitivities were then used to calculate the camera response through equation 3 and the unmixing optimization was carried out based on the subtractive mixing model.

Figure 6 shows the pigment maps obtained from the simulated response of the two extremes of multispectral band numbers in comparison to the pigment maps obtained from the hyperspectral cube. As it can be seen, while the pigment maps obtained

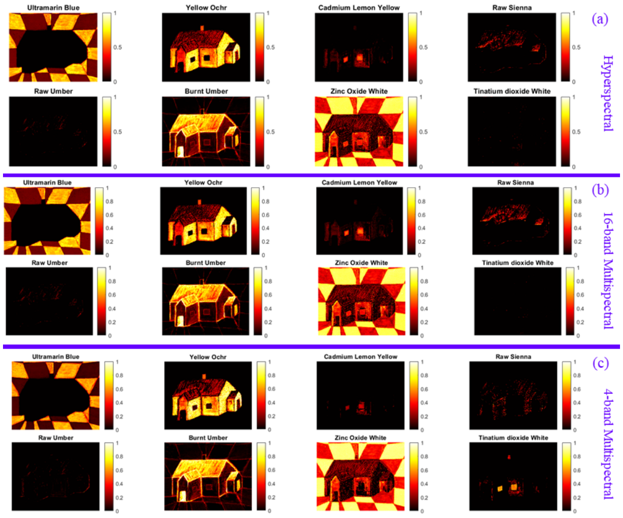

Figure 6. Comparison of the pigment maps obtained from: a) Hyperspectral camera, b) 16-band Multispectral camera, c) 4-band Multispectral camera

from both cameras show a similar structure as in the ground truth (hyperspectral cube's pigment maps), it is visible that the 4-band multispectral camera responses have considerable confusion in the case of raw sienna, titanium white, cadmium lemon yellow and zinc white.

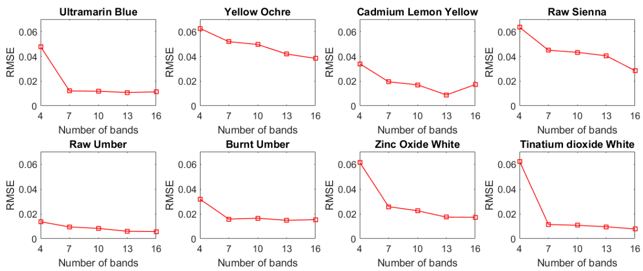

Figure 7. Evaluation of the unmixed pigment maps in the presence of different numbers of spectral bands in terms of RMSE for the members of the spectral library

Figure 7 quantitively summarizes the performance of each simulated camera in comparison to the ground truth in terms of RMSE (Eq. 3). According to these diagrams, a general decrease in the number of channels leads to a higher level of inaccurate concentration prediction. The most drastic changes were observed in the case of ultramarine blue, titanium white, zinc white, and raw sienna.

Finally, even with a 4-band multispectral camera the pigment concentration map error per member remained below 7.5%. Additionally, it was observed that a minimum 7-band multispectral camera response can potentially provide pigment maps with an average error of 2.4%.

$$RMSE = \sqrt{\sum_{i=1}^{q} \left(C_{hyper,i} - R_{multi,i}\right)^2 / q} \quad (3)$$

Unmixing of the Hyperspectral Cube

To investigate the spectral range covered by the selected bands on the obtained pigment maps, two scenarios were compared. In the first, case 10 spectral bands were chosen in a way that 6 covered the visible range and 4 covered the NIR range (Fig. 4b). On the other hand, in the second scenario, the bands were selected in a way that only the visible range was covered (Fig. 8). As it can be seen in Figure 8, the absence of bands in the NIR range would mean that the imaging system would miss important spectral features which would probably lead to confusion.

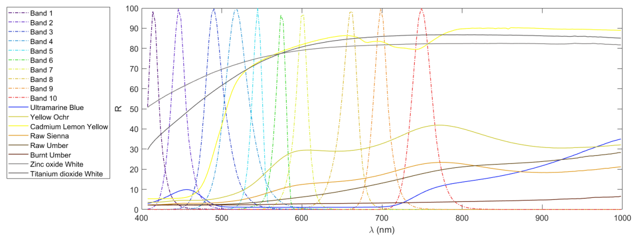

Figure 8. Simulated sensitivities of the Visible-only camera and the spectra of spectral library members.

The pigment maps obtained from the visible-only band configuration are presented in Figure 9. As shown in Figure 9, in the absence of bands in the NIR range the unmixing algorithm fails to detect raw sienna as it confuses the raw umber with raw sienna. Additionally, the algorithm confuses ultramarine blue and ocher yellow. Referring to the spectra of ultramarine blue and ocher yellow along with the spectral bands of the visible-only camera in figure 8,it can be observed that an important part of ultramarine blue's spectral features falls within the NIR range which possibly plays a role in the observed confusion.

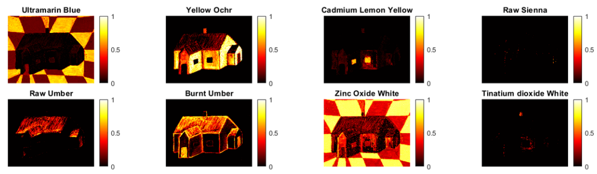

Figure 9. Pigment map of 10-band visible-only multispectral camera simulated response.

Figure 10 shows the RMSE values per library member for the two configurations. As it can be observed, the exclusion of the NIR region has led to an average of 3.9 times higher RMSE. Additionally, the absence of NIR bans has led to changes in the mostly confusing library members. While in the case of the VNIR range the most confused pigments are ochre yellow and raw sienna, in the case of visible-only configuration the most problematic pigments are raw and burnt umber.

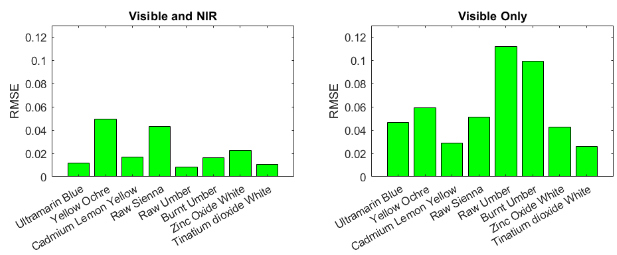

Figure 10. RMSE per library member for pigment maps obtained using the visible-only and VNIR configuration.

Conclusion

To investigate the applicability of multispectral imaging techniques for spectral unmixing tasks, several multispectral cameras with various numbers of spectral bands and spectral ranges were modeled. The camera responses in each case were simulated using the hyperspectral image of an oil painting. To obtain a ground truth for the hyperspectral image unmixing performance, a pigment unmixing algorithm based on a subtractive mixing model was used. The comparison of the pigment maps obtained from the simulated spectral cameras of varying band numbers to the ground truth pigment maps showed that an increase in the number of channels leads to better pigment map prediction. The number of suitable bands however is dependent on the desired precision. It was observed that a multispectral imaging device of 7 bands that cover the VNIR range would only incorporate a 2.4% error in the pigment maps. It was also observed that in case the spectral range of the multispectral imaging device fails to cover the spectral range in which the spectral features of pigments are present, the concentration prediction error can drastically increase. Given these observations, it is suggested to investigate the introduction of a multispectral imaging system with the most suitable number of bands and spectral range, based on the spectral features of the most commonly used pigments

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