Spectral Divergence for Cultural Heritage applications

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Abstract

Using reflectance spectra allows to compare the pigment mixtures in paintings. In order to improve the actual subjective spectral comparison, we propose to use spectral similarity measures. The Kullback-Leibler spectral Pseudo-Divergence (KLPD) is selected due to his expected metrological properties. The comparison between a subjective assessment and the objective assessment is developed for mixture of pigments coming from a cultural heritage painting. The obtained results show the good quality of the relationship between the subjective results and the objective ones using the KLPD.

Introduction

Acquiring spectra from artwork is now a current task for cultural heritage preservation or conservation [7, 10, 6, 17, 5, 8] . Nevertheless, comparing spectra in a metrological way is actually a challenge. Even if such results are expected in order to improve the detection of copies, to assess the degradation evolution or to propose solutions for restoration purposes. Actually the main response to this challenge are based on subjective assessment of the spectral variations [4, 2, 9] or by translating the purpose into the trichromatic domain [14, 23], loosing so all the spectral accuracy.

In parallel, recent advances in the metrology of spectral data allowed to produce a first metrologically valid measure of spectral similarity : the Kullback-Leibler spectral Pseudo-Divergence (KLPD)[22]. One of the particularity of this measure is to naturally split the spectral difference into a sum of an intensity and a shape difference. Thanks to this decomposition, the authors proposed to define bi-dimensional histograms of spectral differences (BHSD) in order to analyse the spectral diversity in hyperspectral images[11].

Inside this work, we propose to study the quality of the relationship between a subjective comparison of the spectrum similarities and an objective measure of these similarities using the KLPD. Bi-dimensional representations (objective and subjective) of the spectral differences are used to perform the comparison. In addition, we ask ourselves about the necessity to use this recent measure in confront with the most used ones (Spectral Angle Mapper and Euclidean distances). This work is developed in a real case coming from our cultural heritage.

After having shortly defined the relationship between the spectra and the optical properties of the pigments, we expose the used spectral difference and similarity measures (Euclidean, SAM and KLPD). Then, we develop the used dataset, coming from acquired and expertised data from a real painting and the parameters of the comparison. The comparison results are provide and commented before a short conclusion.

Spectra in Cultural Heritage (CH)

The protection, conservation or restoration require accurate scientific analysis, and if possible using non-destructive testing. In this way, characterizing materials, mixing products and pigments is crucial to study the provenance, the authentication and to improve the datation of artworks. In this way, the spectrometry methods based on the electromagnetic radiation and considered as non-invasive for the support, present efficient solutions.

When an electromagnetic radiation interacts with the matter, the energy is decomposed in absorbed, transmitted and reflected parts. The spectrometry methods registers the correlation between the reflectance of the energy and the wavelength. The reflectance (R) of a surface is usually expressed in percentage of the reflected light I_r from the incident one I_i:

$$S = \frac{I_r}{I_i} \tag{1}$$

The reflectance measure is fundamental in the study of the materials, because the properties of absorbance, and so the ones of reflectance, are linked to the chemistry of the matter and also to the thickness of the painted layer:

$$\frac{I_1}{I_0} = e^{-k_\lambda l} \tag{2}$$

The physical nature of the reflectance spectrum S induces to consider it as a function over the wavelength λ defined on a fixed spectral support, $S : s(\lambda), \forall \lambda \subset [\lambda_{\min}, \lambda_{\max}]$

$$s : \quad \mathbb{R} \mapsto \mathbb{R} \\ \lambda \mapsto r, \text{ with } r \subset [0.0, 1.0] \text{ for reflectance values} \tag{3}$$

The spectral acquisition is performed by digital system using spectral sampling. Nevertheless, in order to be independent from the spectral acquisition sensor and his specific spectral sampling, we will keep the continuous integrals in the following parts of this work.

Spectral Distance and Similarity

The easiest and the most used way to process the difference between two spectra is to consider them as vectors. In a direct reaction, the most used distance between spectra is a L_2 Minkowski norm [15, 3, 13].

$$d_{L2}(S_1, S_2) = \sqrt{\int_{\lambda_{min}}^{\lambda_{max}} (s_1(\lambda) - s_2(\lambda))^2 \, d\lambda} \tag{4}$$

Following this consideration of vectors, some authors searched to be independent from the white mixing, using a vector angle as measure rather than the *L*2 distance. The Spectral angle Mapper (SAM) measure is then naturally defined as the normalised dot product between two multivariate vectors[16, 21]:

$$d_{SAM}(S_1, S_2) = \arccos(1 - P) \quad (5)$$

$$P = \frac{\int_{\lambda_{min}}^{\lambda_{max}} s_1(\lambda) s_2(\lambda) d\lambda}{\int_{\lambda_{min}}^{\lambda_{max}} s_1(\lambda)^2 d\lambda \cdot \int_{\lambda_{min}}^{\lambda_{max}} s_2(\lambda)^2 d\lambda} \quad (6)$$

In [20], Nidamanuri wondered about the limits of such approaches for spectrum intraclass and interclass discrimination. In particular, the authors developed the fact that SAM measure is more adapted to discriminate dissimilar materials (vegetation from non-vegetation). And in an opposite manner, the Euclidean distance (L_2 norm) was identified as more adapted to measure variations inside spectral groups. Thanks to these considerations, Nidamanuri constructed empirically a similarity score combining the two measures (Normalised Spectral Similarity Score).

Following a parallel way, in [22], the authors proposed a spectral similarity measure combining also a shape ΔC and an intensity difference ΔW. However, this construction inherits from the Kullback-Leibler divergence measure (known as spectral divergence [19, 18]). The theoretical construction induced to adapt the Kullback-Leibler divergence using normalised spectra $\overline{S}$ (eq. 8). The obtained Kullback-Leibler spectral pseudo-divergence is then defined by:

$$div_{KL'}(S, S_{ref}) = \Delta C(S, S_{ref}) + \Delta W(S, S_{ref}) \quad (7)$$

$$\text{with} \begin{cases} \Delta C(S, S_{ref}) = k1 \cdot KL(\overline{S}, \overline{S_{ref}}) + k2 \cdot KL(\overline{S_{ref}}, \overline{S}) \\ \Delta W(S, S_{ref}) = (k_1 - k_2) \log\left(\frac{k_1}{k_2}\right) \end{cases}$$

considering the normalised spectrum $\overline{S}$ and the total energy k of S as defined by:

$$\overline{S} = \left\{ \overline{s}(\lambda) = \frac{s(\lambda)}{k}, \forall \lambda \in [\lambda_{min}, \lambda_{max}] \right\} \quad (8)$$

$$\text{with } k = \int_{\lambda_{min}}^{\lambda_{max}} s(\lambda) d\lambda.$$

Splitting the spectral difference in two combined measures attached to basic spectral characteristic, present a direct interest in the analysis of spectral set, in particular in the relationship with the human judgement of spectral similarities. Thanks to this construction, we propose to display bi-dimensional representations of the spectral differences, interrogating so the similarity measure ability to discriminate spectral groups.

In [12, 22] it was shown that the KLPD is, for the moment, the only one spectral difference measure respecting the metrological constraints, by opposition to the used approaches based on Minkoswki metrics, and associated spectral angles. Nevertheless, following the Nidamanuri construction, we search to identify if such metrological property must be necessary. So, in the following, we propose another kind of bidimensional representation based on the d_{SAM} and d_{L2} measure. As the d_{SAM} measure assesses the spectral shape variations (dot product), it can be compared to the spectral shape difference ΔS. In the same manner, the L_2 difference is more sensitive to the intensity change, as the ΔW measure. This empirical construction induced two theoretical limits. Firstly the two axis are not independent.

Figure 1: Analysed artwork: *Copy of Traiano's Justice* (unknown author) and spatial locations of the considered spectra acquired using a FORS system.

A first Experiment

The dataset

The spectral data   The used dataset comes from the analysis of a painting (*Copy of Traiano's Justice* coming from an unknown author) of a private collection. The analyses devoted to elemental and optical characterization of pigments were developed by the *DIART Laboratory - diagnostica per l'arte*, physics department, University of Milan.

The applied technique is the FORS (Fiber Optic Reflectance Spectroscopy). The data were collected using an Ocean Optics spectrophotometer (HR4000), with spectral sensitivity ranging between 360 and 1100 nm (spectral resolution of $0,27$ nm, see table 1). The selected lightning is a Xenon source (HPX-2000). The lightning/acquisition angle between the surface to acquire, the reflection and backscattering probes is fixed to 45° thanks to a dedicated support. A *Y QR400-7-VIS-NIR* fibre model, that avoids specular reflection, was used for the acquisition. The calibration protocol used a white ($R \approx 99\%$) and a black ($R \approx 2\%$) references. The table 1 resume the used acquisition parameters. In this work only the visible part of the spectra (380-780 nm) was taken into account.

Table 1: FORS parameters

Integration Time	100 (ms)
Spectral Average	5 (nm)
Time	100 x 5 = 500 (ms)
Boxcar	7

Table 2: Identified composition of the colours thanks to the human analysis of the acquired spectra

| Spectra's Name	Color	Pigment
12.Dead	Rosy	Vermilion and lead white
16.Flag	Red	Vermilion
21.CapeL	Red	Vermilion
28.TCape	Red	Red varnish
37.Blower	Rosy	Vermilion and lead white
38.TFace	Rosy	Vermilion, red varnish and lead white
39.TKnee	Rosy	Red varnish and lead white

Subjective pigment analysis Several pigments were analysed, inducing spectral acquisition at different locations in the painting (fig. 1). In this work, we are focusing on a particular red, and more specifically to colours close to the *vermilion*. The corresponding spectral responses were compared to pigment references (dedicated database from the IFAC [1]) by two experts. Table 2 presents the proposed pigment nature and mixing when necessary.

In order to improve the pigment characterization/discrimination, an Energy-dispersive X-ray fluorescence spectroscopy (*ED-XRF*) was performed in order to obtain a chemical characterization of the painting surface, so the pigments. A portable XRF spectrometer (LITHOS 3000, Assing) employing the monochromatic radiation of molybdenum ((Mo,$K = 17,4KeV$) was used. The *ED-XRF* detected a great presence of *lead* (*Pb*) in all the analysed locations. This presence is characteristic from the white lead and from the common preparation layer in paintings. The red points under *ED-XRF* analysis were *12.Dead, 16.Flag* and *38.TFace* and the instrument detected the presence of *mercury* (*Hg*), characteristic of the *vermilion* and *iron* (*Fe*), typical element for the *ochre*, but also trace element of many pigments and preparations.
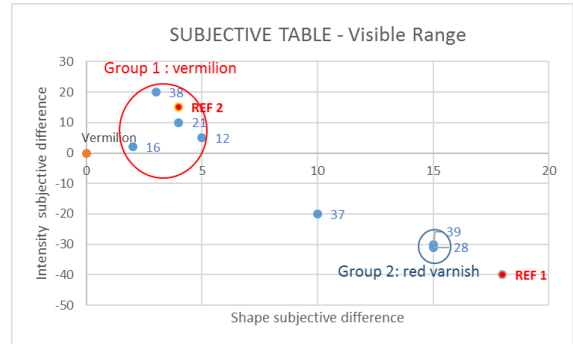
Subjective Bidimensional representation of the spectral similarities Our objective is to compare the experts way to discriminate pigments by spectra with the proposed approach using the Kullback-Leibler spectral pseudo-divergence (KLPD). So, we ask to the expert to organize in a bidimensional representation the spectral differences using the notion of intensity and shape differences. In such construction, the quantitative values have no sense, but the order on each axis are preserved in front of the expert judgement.

The value of intensity correspond to the increase of reflectance associated with the white lead, than, the shape difference value is based on the shape difference between the analysed spectrum and the vermilion reference from the Milano's Laboratory database. The obtained bidimensional representation can be observed in figure 2b.

Firstly, we observe that naturally more than one half of the red pigments (red circle) are close from the representation origin (*vermilion*). Secondly, the closest colours are the pure *vermilion* (12.*Dead* and 16.*Flag*). Then the 3 others are organised in front of the quantity of the added and mixed pigments. Thirdly, a second group of colour appears at the bottom right of the representation (inside the blue circle), including the 28.*TCape* and 39.*TKnee* locations. These two colours was identified as formed by red varnish. The observed spectra in figure 2a shown why the spectral shape and intensity was judged as very different (28.*TCape* and 39.*TKnee* are the two lowest spectra). Finally, the
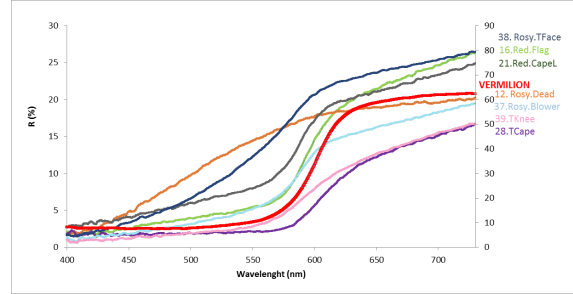
(a) Acquired spectra (*vermilion* used the dynamic range on the right)

(b) Bidimensional Representation of subjective shape and intensity differences

Figure 2: Acquired spectra from the selected location pointed out in figure 1 and the subjective representation of the spectral differences between the acquired spectra.

colour corresponding to 37.*Blower* is located between the vermilion and the varnish group. This behaviour of the spectrum could be due to the presence of a third pigment or to a mixture of the first two.

Results

The references Before to draw the bidimensional representation of spectral differences (BHSD), we need to select the reference to use. As defined previously, the reference must be outside the spectral dataset and stay close from it in order to increase the discrimination ability. In a first consideration, we could imagine to choose the vermilion spectrum as reference. Unfortunately, this spectrum don't respect the second constraint (his intensity level is too important and the considered spectrum is then too far from the spectral data to analyse, see figure 5).

In order to respect the defined constraints, we selected to analyse the spectra using two references framing the spectral set. The reference $Ref1$ is selected to be under the spectra with a shape (the step part) slightly sliced to the right of the 28.*TCape* spectrum. The second reference $Ref2$ is by opposition located upper the spectra 38.*TFace*. Thanks to this direct construction, the constraints are solved and the spectra can be compared using the bidimensional representation of spectral differences.

As previously expressed, we propose two kinds of representation. First ones (fig. 3) are based on a combination of an Euclidean and a spectral angle mapper measures (SAM). The second ones (fig. 4) are based on the two parts of the Kullback-Leibler spectral pseudo-divergence. In the two cases, we mark using blue and red ellipsods, the spectral groups identified using the FORS
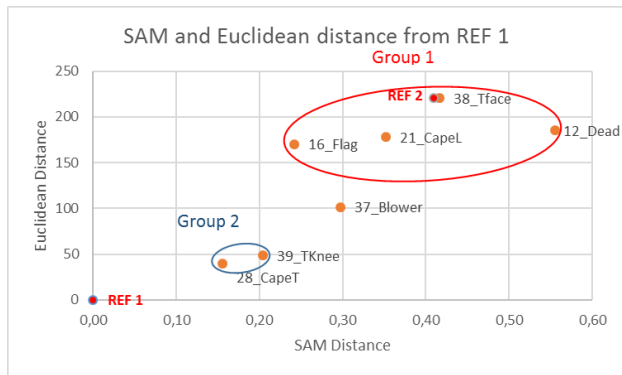
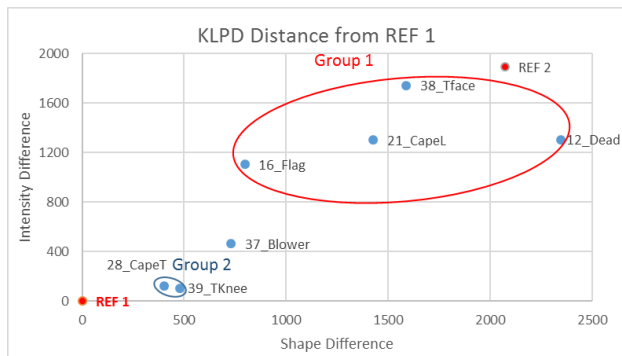(a) spectral difference to reference 1
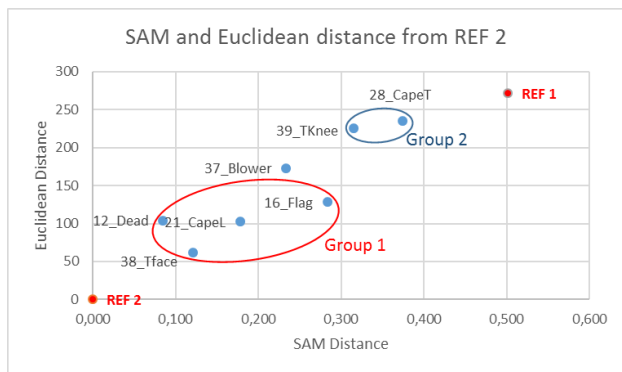
(b) spectral difference to reference 2

Figure 3: Bidimensional representation of the spectral difference using a combination of a Spectral Angle Mapper(SAM) as shape difference and an Euclidean measure as intensity difference.

combined with ED - XRF and the human assessment.

Spectral distribution relative to reference $Ref1$ Firstly we consider fig. 3a and 4a. The two spectral representations seems very similar. The two main groups are well separated, and the spectrum 37.*Blower* is, as expected, located between these two groups. Secondly, the spectra 28.*TCape* and 39.*TKnee* are very close from the representation origin (location of the $Ref1$ spectrum). Some differences exist between the two representations. Typically, in the relative location of the spectrum 37.*Blower* to the 16.*Flag* on the horizontal axis (shape or angle difference). Some inversions can be observed on the vertical axis (intensity difference) : $Ref2$ versus 38.*Tface* or 28.*TCape* versus 39.*TKnee*.

Spectral distribution relative to $Ref2$ Considering the second subset of representations (3b and 4b), firstly, we note that the 39.*TKnee* and 28.*TCape* spectra are located in top-right corner of the representation, farthest of the $Ref2$ spectrum. Secondly, we observe that the relative order of the spectra are not preserved from the first representations. Such fact is normal due to the problem dimensionality and to the positive nature of the difference measures. It is interesting to remark also that the intra-class dynamic in the two bidimensional representations are different due to the expressions used to assess the shape and intensity differences. In addition, we remark also the important dynamic of the KLPD representation for the shape difference by opposition to the

(a) spectral difference to reference 1
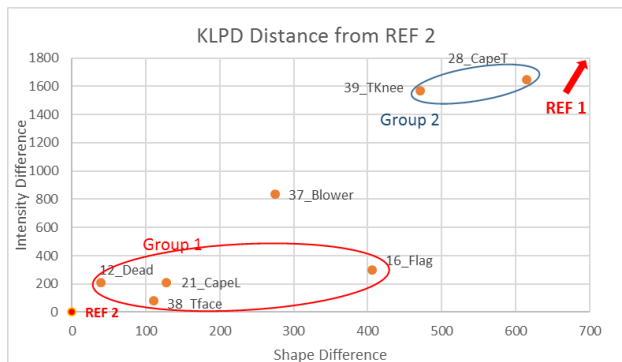
(b) spectral difference to reference 2

Figure 4: Bidimensional representation of the spectral difference using a Kullback-Leibler spectral pseudo-divergence.

SAM measures restricted to $[0, 1]$.

Discussion

Looking at the figures 4a and 3b is possible to discriminate the spectra due to their shape and intensity differences. This is an advantage when analysing pigment's spectra because the shape is strictly correlated with the absorption bands of the materials and the intensity is linked with the lightness and the presence of white in the mixture.

The results obtained through the spectral difference confirms the subjective judgement dividing the pigments in two main groups, but the KLPD gives us more interesting informations about the different spectra inside the groups. In this way, we have the certitude of two main pigments used to make the red colour, but we can also have a clear discrimination of the pigments that presents more white inside them. In fact *Group 1* forms a coherent group made with the same pigment, *vermilion*, but the differences in shape and intensity indicates us the presence of white that increase the intensity and tend to change the spectra's shape. Another interesting point is spectra 37.*Blower*, because thanks to KLPD we have the confirm that it is a mixture of two different pigment, but we can also know that it is more similar to the *Group 1*.

From the results that we obtained, it should be possible in a quick approximation to consider the two kinds of representations as equivalent. Nevertheless the observed differences must be taken with care. If we focus on the easiest measure to analyse, the intensity difference, the expected measure will consider
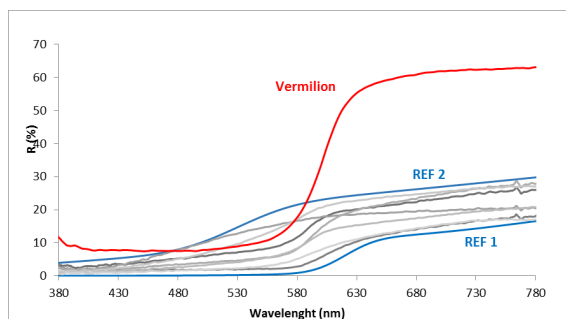
Figure 5: Reference spectra framing the spectral set and the *vermilion* spectrum .

the relative difference of intensity. This measure is naturally link to the integral of the considered spectra. Having a look on the 21.*TCape*, 39.*TKnee* and *Ref*1 spectra (figure 2a) we see that the expected order would locate 39.*TKnee* as being the closest in intensity to the *Ref*1 spectrum. Only the representation based on the KLPD measure obtains this result, that is easily confirmed by the integral values. In a more theoretical point of view, we need to not forget that the Euclidean distance embed a part of the spectral angle mapper, inducing so his own limits for the construction of the intensity axis.

So, the main advantage of KLPD measure is then to have a natural decomposition of the spectral difference into intensity and shape differences inherited from the Kullback-Liebler divergence rewriting, instead of an empirical construction. However, this construction of the KLPD allows to compute the total spectral distance in the representation as a $L1$ norm and consequently to take into account the relative position of two spectra combining the two dimensions. In an opposite manner, the empirical construction of the SAM/Euclidean constructions don't allow such total difference computation due to the dependency of the two axis. This difference is fundamental for spectral analysis, which describes the physical properties of a material.

The main limit of the presented results is link to the analysis of only one pigment from only one painting. As our purpose was to develop and analyse the relationship between theoretical spectral difference measures and our traditional way to compare pigment spectra, the database size is not a problem. We are in front of two new representations, an empirical one improving the Nidamanuri construction [20], and a construction theoretically defined for metrological purposes. One of the questions to solve was about the necessity to choose the KLPD construction, that seemed more complex. The obtained representations show that the results interpretation are direct, and more correlated to our way to consider the spectral similarity. Increasing the number of analysed pigments will not change this result.

The following question, on this way to produce tools for expert in cultural heritage, is linked to the automatic pigment detection in painting (unmixing problem), or to the statistical analysis of the spectral distributions. In such case, the bidimensional representation is transformed into a bidimensional histogram of spectral differences (BHSD)[22]. Such bidimensional histograms are adapted for clustering/classification approaches. Nevertheless, also in this case a total distance of a spectrum to a reference in the bidimensional representation is required, requiring so the KLPD distance rather than the SAM/Euclidean ones.

Conclusion

Inside this work we explored the interest of recent advances in spectral differences assessment in order to help the experts in cultural heritage for pigment analysis. Even if it exists several spectral distances and classification tools for hyperspectral data, none reach the metrological level before the Kullback-Leibler pseudo-divergence and associated histogram of differences.

One of the interests of the pseudo-divergence is to split the spectral difference into a shape and an intensity differences allowing so the bi-dimensional representation. We proven the performance of the bi-dimensional histogram of differences based on the proposed pseudo-divergence in front of an alternative using the two mainly used spectral distances (Spectral Angle Mapper and Euclidean distance). This result reinforces the limits of non-metrological approaches for spectral image/data processing.

The result confrontation to the experts judgement imposed to create bi-dimensional representation of his perception of the spectral differences. Creating so a subjective representation for which the ordering of the spectral differences were preserved under his own judgement. The construction was enabled (but not commented) by the a-priori knowledges about the pigment analysis by XRF measures. The obtained comparisons proven the direct relationship between the subjective way to proceed by the expert and the objective and metrological processing obtained by the pseudo-divergence using the histograms of differences.

Thanks to this first results, more complete works are in course in order to address the question of the spectral diversity analysis, or automatic pigment detection from these n-dimensional representations of spectral differences. Such results are expected in the scientific tools for cultural heritage analysis, in order to improve the analysis using statistical points of view.

Acknowledgement

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