On the spectral dimensionality of object colours

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Abstract

How many components are needed to represent the spectral reflectance of a surface? What is the dimension of a spectral reflectance? How many image channels are needed for the acquisition of a multispectral colour image? Such and similar questions have been discussed extensively in the literature. We have done a survey of the literature concerning this topic, and have seen that there is a large variation in the answers. We propose a method to quantify the effective dimension of a set of spectral reflectances. The method is based on a Principal Component Analysis, and in particular on specific requirements for the accumulated energy of the principal components. We apply the analysis to five different databases of spectral reflectances, and conclude that they have very different statistical properties. The effective dimension of a set of Munsell colour spectra is found to be 18, that of a set of natural object reflectances 23, while the effective dimension of a set of reflectances of pigments used in oil painting was only 13.

1. Introduction

For example in the design of a multispectral colour imaging system,[1–4] it is of strong interest to have knowledge about the nature of the spectral reflectances that are going to be imaged. One particular design choice that is relevant to this study is the number of image channels.

The effective dimension of reflectance spectra, that is, the number of components needed to describe a spectrum in a vectorial space has been discussed extensively in the literature, and we review this literature briefly in Section 2. We see that the existing conclusions concerning the dimension of spectral reflectances, and also the number of channels needed to acquire multispectral colour images, are rather dispersed. Furthermore, quite often, the applied statistical analysis is quite elementary, and conclusions are drawn without clear objectives.

In Section 3 we therefore propose a method for a comparative analysis of sets of spectral reflectances, using statistical tools such as the Principal Component Analysis. In particular, we define the *effective dimension* of a set of spectral reflectances. In Section 4 we apply this analysis to five different sets of spectral reflectances, and in Section 5 we discuss the results and draw some conclusions.

2. Literature review

Possibly the first attempt to fit a linear model to a set of empirical surface spectral reflectances was performed by Joseph Cohen[5] of the University of Illinois in 1964. He analysed a subset of 150 out of 433 Munsell chips, and concluded that their reflectances depend on only three components, which account for 99.18% of the variance. Among later studies on Munsell colours, Eem et al.[6] propose four, Maloney[7] proposes five to seven, Burns[8,9] proposes five or six, Lenz et al.[10,11] use six, and Parkkinen et al.[12] and Wang et al.[13] claim that eight components are necessary.

For human skin, the use of three components is proposed by Imai et al.[14,15] and Sun and Fairchild[16]. For oil painting, five is proposed by Miyake et al.[17,18], while Maître et al.[19] claim that ten to twelve factors are needed. García-Beltrán et al.[20] use a linear basis of seven vectors to represent the spectral reflectance of acrylic paints. For data including reflectances of natural objects, Dannemiller[21] and Chiao et al.[22] state that three is sufficient, Vrhel et al.[23] proposes three to seven basis functions, Praefcke[24] proposes five, while Keusen[25,43] states that up to ten is needed. Laamanen et al.[26] recently stated that if a general basis should be used to represent spectral reflectances, the dimensionality might be around 20.

For the realisation of a multispectral colour image acquisition system, the choices of the number of image channels are also many: three by Miyake's group[14,15,27,28] — four by Chen and Trussell[29] and Hauta-Kasari et al.[30] — five by Haneishi et al.[17,18,31] and Kollarits and Gibbon[32] — six by Tominaga[33,34], Herzog et al.[35], and Imai and Berns[36] — seven by Saunders and coworkers[37,38], Abrardo et al.[39], Burns[8,9], and Ribés et al.[40] — five to ten by Hardeberg et al.[41,42] — ten to twelve by Maître et al.[19] — twelve to fourteen by Keusen[25,43] — sixteen by König[44,45] and Yamaguchi et al.[46,47] — and twenty-nine by Baronti et al.[48]. We have previously evaluated several set-ups using from three to seventeen channels and a Liquid Crystal tunable filter[1–3], without drawing firm conclusions concerning the optimal number of channels.

We see that the existing conclusions vary over a broad range, both concerning the dimension of spectral reflectances, and the number of image channels needed in order to capture appropriate information about the spectral re-

flectance in a scene. For a more in-depth literature review concerning the dimension of spectral reflectances, refer to Appendix F of reference 1.

3. Analysis of spectral reflectance data sets

3.1. Principal Component Analysis

According to Jolliffe [49], the central goal of a principal component analysis (PCA) is to reduce the dimensionality of a data set which consists of a large number of interrelated variables, while retaining as much as possible of the variation present in the data set. The reason for applying PCA to a set of spectral reflectances is mainly twofold:

- To acquire information about the dimensionality of the data. Are all the reflectances of the set linearly independent, or in which way are they dependent? How many factors are required to represent a spectral reflectance? This may give an indication on the number of channels to be used in a multispectral colour imaging system.
- To allow compression of spectral information. A spectral reflectance can be approximated using a reduced number of principal components. This is particularly important for multispectral colour imaging since the image file sizes tend to be prohibitively large.

To implement the PCA analysis, we use the Singular Value Decomposition (SVD) algorithm. Numerous variants of the SVD algorithm exist. We apply here the version implemented in Matlab. We recall that for any arbitrary (N-line $\times$ P-column) matrix $\mathbf{X}$ of rank R, there exist an $(N \times N)$ unitary matrix $\mathbf{U}$ and a $(P \times P)$ unitary matrix $\mathbf{V}$ for which

$$\mathbf{X} = \mathbf{U}\mathbf{W}\mathbf{V}^{\mathbf{t}}, \tag{1}$$

where $\mathbf{W}$ is an $(N \times P)$ matrix with general diagonal entries w_i, $i = 1 \ldots R$, denoted *singular values* of $\mathbf{X}$, and the columns of the unitary matrix $\mathbf{U}$ are composed of the eigenvectors $\mathbf{u_i}$, $i = 1 \ldots N$, of the symmetric matrix $\mathbf{X}\mathbf{X}^{\mathbf{t}}$. (Note that the *singular values* correspond to the square roots of the *eigenvalues*.)

For our PCA analysis, we denote our data set of P reflectances $\mathbf{r_i}$ as the $(N \times P)$ matrix $\mathbf{R} = [\mathbf{r_1}\mathbf{r_2} \ldots \mathbf{r_P}]$, and we define the matrix $\mathbf{X}$ as

$$\mathbf{X} = \begin{bmatrix} \mathbf{r_1} - \bar{\mathbf{r}} & \mathbf{r_2} - \bar{\mathbf{r}} & \cdots & \mathbf{r_P} - \bar{\mathbf{r}} \end{bmatrix}, \tag{2}$$

where $\bar{\mathbf{r}}$ is the mean values of the reflectance spectra,

$$\bar{\mathbf{r}} = \frac{1}{P} \sum_{j=1}^{P} \mathbf{r_j}. \tag{3}$$

Applying the SVD, the resulting matrix $\mathbf{U}$ (*cf.* Eq. 1) is a $(N \times N)$ column-orthogonal matrix describing an orthogonal basis of the space spanned by $\mathbf{X}$ or equivalently by $\mathbf{R}$. We denote this space by $R(\mathbf{R})$, the *range* of $\mathbf{R}$, and note that $R(\mathbf{R}) = \mathbf{R}(\mathbf{X}) = \mathbf{R}(\mathbf{U})$. We will denote the columns of $\mathbf{U}$, called *nodes* in PCA terminology, as the *characteristic reflectances* of the data set. $\mathbf{W}$ is a diagonal matrix containing on its diagonal the singular values w_i, in order of decreasing magnitude.

In accordance with previous studies, we have observed that there is a strong concentration of variance/energy in the first few singular values (see Figure 3). This suggests that the spectral reflectances may be approximated using a small number of components, as described in the following section.

3.2. Effective dimension

The dimension D of the space $R(\mathbf{R})$ is rigorously determined by $D = \mathrm{rank}(\mathbf{R})$, which is given by the number of non-null singular values. If the columns of $\mathbf{R}$, the reflectance spectra, are linearly independent, then $D = N$. (This supposing that $N < P$. If $N > P$, then $D = P$.) However, if some singular values are very close to zero, which is often the case, the *effective* dimension of the space, denoted D_e, may be much smaller. That is, it is possible to construct an adequate representation of the spectral data in a more compact form, using merely D_e principal components, D_e being generally significantly smaller than D. Given a reflectance spectrum represented by the N-vector $\mathbf{x} = \mathbf{r} - \overline{\mathbf{r}}$, the vector of principal components $\mathbf{z} = [\mathbf{z_1}\mathbf{z_2} \ldots \mathbf{z_{\tilde{P}}}]^{\mathbf{t}}$ is given by

$$\mathbf{z} = \tilde{\mathbf{U}}^{\mathbf{t}}\mathbf{x}, \tag{4}$$

$\tilde{\mathbf{U}}$ being defined as the first $\tilde{P} < P$ characteristic reflectances, $\mathbf{z}$ thus being a $\tilde{P}$-vector. The reconstruction of an approximation $\tilde{\mathbf{r}}$ of the original reflectance is obtained by

$$\tilde{\mathbf{x}} = \tilde{\mathbf{U}}\mathbf{z} = \tilde{\mathbf{U}}\tilde{\mathbf{U}}^{\mathbf{t}}\mathbf{x}, \tag{5}$$

and consequently

$$\tilde{\mathbf{r}} = \tilde{\mathbf{U}}\mathbf{z} + \overline{\mathbf{r}} = \tilde{\mathbf{U}}\tilde{\mathbf{U}}^{\mathbf{t}}(\mathbf{r} - \overline{\mathbf{r}}) + \overline{\mathbf{r}}. \tag{6}$$

The spectral reconstruction error is thus identified as

$$d_E = \|\mathbf{r} - \tilde{\mathbf{r}}\| = \|\mathbf{r} - \tilde{\mathbf{U}}\tilde{\mathbf{U}}^{\mathbf{t}}(\mathbf{r} - \overline{\mathbf{r}}) - \overline{\mathbf{r}}\| \tag{7}$$

To determine an estimation of the effective dimension of the space $R(\mathbf{R})$, that is, a good choice of D_e, we need to determine how many principal components that must be taken into account to represent the data. To this end, in addition to the measurement of spectral reconstruction errors, the notion of *accumulated* energy $E_a(\tilde{P})$ turns out to be useful. Accumulated energy is defined as the ratio of the energy or variance represented by the first $\tilde{P}$ singular vectors, to the total energy, as follows:

$$E_a(\tilde{P}) = \frac{\sum_{i=1}^{i=\tilde{P}} w_i}{\sum_{i=1}^{i=P} w_i}. \tag{8}$$

We may also define the *residual* energy $E_r(\tilde{P}) = 1 - E_a(\tilde{P})$, that is, the energy represented by the principal components that are *not* taken into account. As an example, we present in Figure 1 the mean and maximal spectral reconstruction error $\|\mathbf{r} - \tilde{\mathbf{r}}\|$, over a set of spectral reflectances, compared to the residual energy, using $\tilde{P}$ principal components. We see that the mean spectral reconstruction error is highly correlated to the residual energy, while the maximal error shows a more random variation, although still correlated.

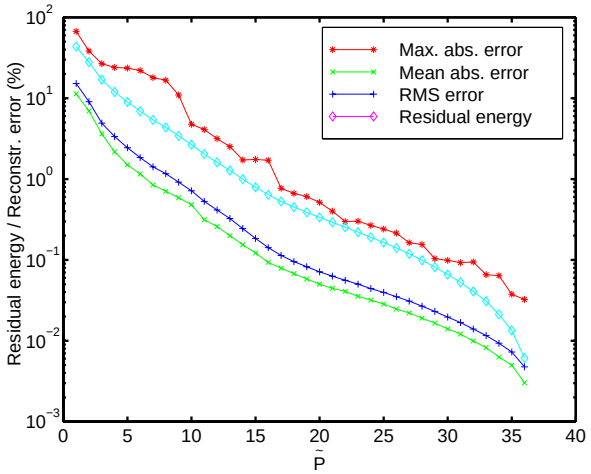

Figure 1: *Example of mean and maximal spectral reconstruction error using the $\tilde{P}$ first principal components, compared to the residual energy, using the* PIGMENTS *data.*

This result suggests that we may use the accumulated energy as a criterion to define an appropriate choice of dimensionality D_e. We define thus

$$D_e \stackrel{\text{def}}{=} \min\{\tilde{P} | E_a(\tilde{P}) \geq E_{\text{req}}\}. \quad (9)$$

The definition of the effective dimension depends thus on the choice of required accumulated energy E_{req}. A typical value seen in the literature [9,17] is $E_{\text{req}} = 99\%$, and we propose therefore to use this as a default value when calculating the effective dimension.

4. Experimental Results

We have applied the proposed analysis to five sets of spectral reflectances (Figure 2). PIGMENTS; a set of reflectances from a target made using 64 different oil pigments used in the restoration of old paintings. The target was provided to the ENST by the National Gallery in London (courtesy of David Saunders). [19,37] MUNSELL; a set of reflectances of 1269 matte finish Munsell colour chips measured and made available by Jussi Parkkinen and his colleagues at the University of Joensuu, Finland [12,50]. NATURAL; the reflectances of 218 coloured samples collected

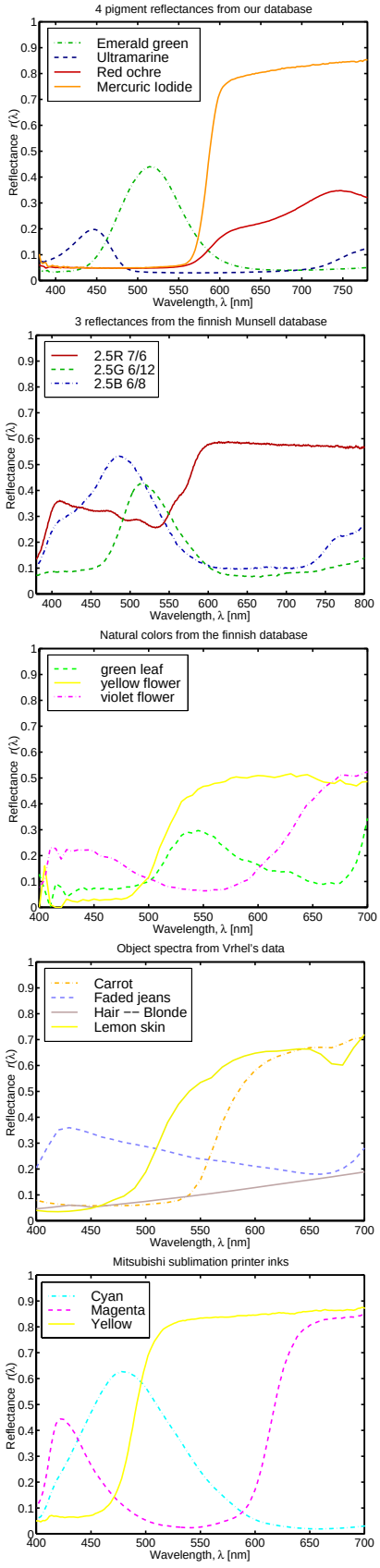

Figure 2: *Examples of reflectance spectra from the different databases:* PIGMENTS, MUNSELL, NATURAL, OBJECT, *and* SUBLIM.

from the nature, obtained from the same source. OBJECT; 170 reflectances of various natural and man-made objects provided by Michael Vhrel.[23] SUBLIM; 125 reflectances from a Mitsubishi S340-10 CMY sublimation printer.[1] To be able to compare these different reflectance sets, we have resampled all data to a common wavelength resolution of 10nm, and a wavelength interval from 400nm - 700nm. For more details about the sets, such as the measurement equipment used, see reference 1.

We apply the PCA analysis to the different databases. The relative magnitude of the singular values, that is, the eigenvalues of the covariance matrix $\mathbf{X}\mathbf{X}^{\mathbf{t}}$ are shown in Figure 3. In Figure 4 and Table 1, the accumulated energy represented by the $\tilde{P}$ first characteristic vectors is shown.

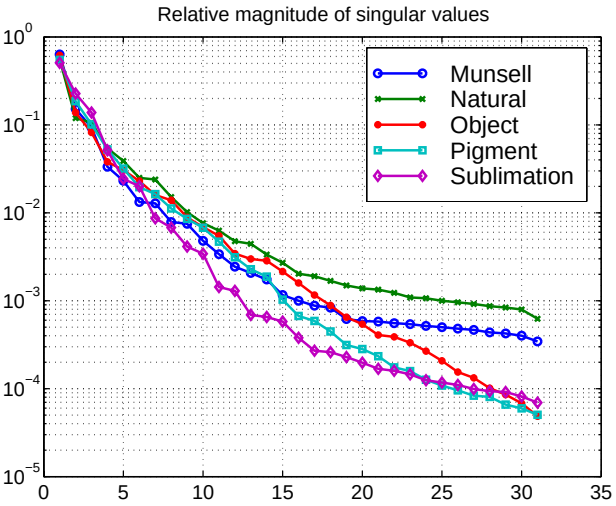

Figure 3: *Comparison of singular values of the 5 different databases in logarithmic scale. The steeper the curves decrease, the more the energy is concentrated in the first singular vectors.*

Analysing the data reported in Table 1, we may conclude that a different number of basis vectors should be chosen, depending on the database used to calculate the covariance matrix, see Table 2. As expected, the NATURAL data shows the highest dimensionality, and the SUBLIM data the lowest, but they do exhibit a rather similar behaviour. If we require that $E_{\text{req}} = 99\%$ of the signal variance should be accounted for, we can encode the spectra using 10 components for the SUBLIM reflectances, while as many as 23 components would be needed for the NATURAL data. The MUNSELL data set has an effective dimension of 18, the OBJECT data 15, and the PIGMENT set 13. Especially if we consider the two largest sets, MUNSELL and NATURAL, we see that the results comply fairly well with Laamanen's recent paper, [26] in which it was suggested that the dimensionality of a general spectral basis was around 20.

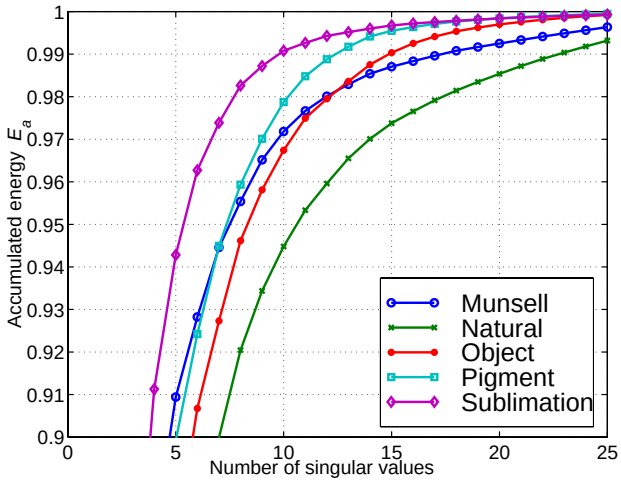

Figure 4: *Comparison of the accumulated energy $E_a(\tilde{P})$ of the different databases. For example if $E_{req} = 99\%$ of the signal energy should be preserved, 23 singular vectors should be used for the* NATURAL *data, while 10 is enough for the* SUBLIM *data.*

5. Discussion and Conclusion

We have proposed a new method to quantify the effective dimension of a set of spectral reflectances. The method uses the Principal Component Analysis algorithm, and a criterion on the required accumulated energy in the retained principal components. In alignment with previous studies, we propose to use 99% accumulated energy in the definition of the effective dimension, even if this choice is rather heuristic.

By our analysis we have shown that spectral reflectances from different databases have different statistical properties. When fixing the amount of signal variance that should be accounted for, approximately twice as many components are needed to encode a spectrum from the NATURAL database than for the SUBLIM data.

One of the goals of this study was to analyze the importance of the data set being adapted to the application. Our conclusion is that the different reflectance data set have very different statistical properties, and that, therefore, for a given application, an appropriate set should be used. Our results have important practical consequences when designing a multispectral image acquisition system. However, one should be careful in applying the results directly to the design of imaging systems, since many other factors come into play in that context, such as imaging noise and intent.

Directions for further studies on this subject could be to apply the analysis to other spectral databases [51,52] and to further study the relationship between the linear bases designed from the different data sets. Is it important to use oil painting reflectances when designing a multispectral image acquisition system for paintings, or could a standard set of Munsell reflectances equally well be used?

Table 1: *Accumulated energy $E_a(\tilde{P})$ of the different databases. The entries corresponding to design choices of $E_{req} = 0.90$ and $E_{req} = 0.99$ are underlined, and reported in Table 2.*

$\tilde{P}$	MUNSELL	NATURAL	OBJECT	PIGMENT	SUBLIM
1	0.4783	0.4235	0.4833	0.4344	0.4005
2	0.6955	0.5836	0.6710	0.6714	0.6724
3	0.8288	0.7265	0.7841	0.7944	0.8491
4	0.8763	0.7953	0.8345	0.8583	0.9108
5	0.9094	0.8363	0.8750	0.8992	0.9426
6	0.9282	0.8695	0.9067	0.9242	0.9626
7	0.9446	0.8999	0.9273	0.9449	0.9737
8	0.9554	0.9204	0.9462	0.9593	0.9825
9	0.9652	0.9344	0.9581	0.9701	0.9871
10	0.9718	0.9448	0.9674	0.9788	0.9907
11	0.9767	0.9533	0.9749	0.9848	0.9926
12	0.9801	0.9596	0.9795	0.9888	0.9943
13	0.9829	0.9655	0.9836	0.9917	0.9951
14	0.9854	0.9701	0.9875	0.9942	0.9960
15	0.9871	0.9738	0.9903	0.9955	0.9967
16	0.9883	0.9766	0.9925	0.9963	0.9972
17	0.9896	0.9791	0.9941	0.9971	0.9975
18	0.9908	0.9814	0.9954	0.9977	0.9978
19	0.9917	0.9835	0.9962	0.9981	0.9981
20	0.9925	0.9854	0.9970	0.9984	0.9984
21	0.9933	0.9872	0.9976	0.9987	0.9986
22	0.9941	0.9889	0.9981	0.9989	0.9988
23	0.9949	0.9904	0.9985	0.9991	0.9990
24	0.9956	0.9918	0.9989	0.9993	0.9991
25	0.9963	0.9932	0.9992	0.9994	0.9993
26	0.9970	0.9945	0.9994	0.9996	0.9994
27	0.9977	0.9957	0.9996	0.9997	0.9996
28	0.9983	0.9969	0.9997	0.9998	0.9997
29	0.9989	0.9981	0.9998	0.9999	0.9998
30	0.9995	0.9991	0.9999	0.9999	0.9999
31	1.0000	1.0000	1.0000	1.0000	1.0000

Table 2: *Effective dimension D_e for the different databases for required accumulated energy of 0.90 and 0.99.*

E_{req}	MUNSELL	NATURAL	OBJECT	PIGMENT	SUBLIM
0.90	5	8	6	6	4
0.99	18	23	15	13	10

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Biography

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