Estimating Surface Reflectance Functions from Tristimulus Values

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ABSTRACT

Information about the spectral reflectance of a color surface is useful in many applications. Assuming that reflectance functions can be adequately approximated by a linear combination of a small number of basis functions, we address here the recovery of a surface reflectance function, given the tristimulus values under one or more illuminants.

1. Introduction

Information about the spectral reflectance of a color surface is useful in many applications. It can, for example, be helpful in simulating the change in appearance of a colored object under changing illuminants in CAD applications; or provide the input of computer programs for the matching color formulation of paints, inks, plastics, and textiles; or serve as input for many general computer graphics applications that require a wavelength-based approach to specify colors. Unfortunately, the surface reflectance is not often specified; most of the time, surface color information is given as RGB or XYZ tristimulus values. We address here the problem of estimating plausible reflectance spectra from tristimulus values for a variety of representations of reflectance functions through linear models. The main assumptions of our work are that the illuminant spectrum is known, that reflectance spectra are smooth functions of wavelength in the range of reflectance values between 0 and 100, and that no phenomena of fluorescence occur. Linear models represent reflectance functions with a good to high degree of accuracy, depending on the number of basis functions considered. There are many studies on the dimensionality of linear models based on Principal Component Analysis (PCA) for real reflectance spectra approximation. In general, for natural surfaces, a dimension of 6 to 9 bases is considered sufficient [1][2][3], while, for skin reflectance, three basis functions are enough [4]. Most of the methods available for the estimation of reflectance from tristimulus values assume it is possible to represent the spectral reflectance functions with a three-dimensional linear model, e.g. [5][6][7], do not allow the simultaneous exploitation of tristimulus values referred to different illuminants, and employ a fixed pre-defined set of basis functions to model
reflectance spectra. Unfortunately, using three PCA basis functions to estimate a reflectance spectrum from tristimulus values may still not offer a good solution. While the reflectance spectrum obtained may be perfectly metameric with respect to the unknown spectrum under the given illuminant and with the given observer, it may exhibit poor colorimetric matching with a different illuminant or observer, indicating that the underlying spectral match required has not been obtained. Since the spectral matching cannot be addressed directly, a method that allows the synthesis of a surface reflectance spectrum by taking into account colorimetric information referred to different illumination or observation conditions can increase the similarity between the estimated and the unknown reflectance spectrum.

We have applied genetic algorithms to formulate the problem of reflectance estimation for the simultaneous optimization of several constraints. We have also investigated, in the framework of the proposed method, the performance of different basis sets for reflectance function representation.

In Section II we provide a formal formulation of the problem addressed. Section III describes the basis functions considered here, while Section IV is a brief overview of the genetic algorithm proposed. The performance of the algorithm and of the basis functions is examined in Section V, where standard datasets are used for benchmarking.

2. Problem Formulation

A color stimulus is related to the CIE XYZ tristimulus values by the following equations:

\[ X = K \int_{\lambda} R(\lambda)I(\lambda)\bar{x}(\lambda)d\lambda \]
\[ Y = K \int_{\lambda} R(\lambda)I(\lambda)\bar{y}(\lambda)d\lambda \]
\[ Z = K \int_{\lambda} R(\lambda)I(\lambda)\bar{z}(\lambda)d\lambda \]  \hspace{1cm} (1)

where \( R(\lambda) \) is the reflectance spectrum, \( I(\lambda) \) is the illuminant’s spectral power distribution, \( \bar{x}(\lambda) \), \( \bar{y}(\lambda) \) and \( \bar{z}(\lambda) \) are the color matching functions that define the CIE 1931 standard colorimetric observer. If the reflectance function is represented in the range of \([0,1]\), and a luminance of 100 is attributed to the light source in the scene, then the normalization factor \( K \) is:

\[ K = \frac{100}{\int_{\lambda} I(\lambda)\bar{y}(\lambda)d\lambda} \]  \hspace{1cm} (2)

Equation (1) indicates that an infinite number of different reflectance functions may generate the same tristimulus values. The reflectance function may be expressed through a linear model as a weighted sum of a set of basis functions:

\[ R(\lambda) = \sum_{j=1}^{N} w_j b_j(\lambda) \]  \hspace{1cm} (3)
where $\tilde{N}$ is the number of bases in the linear model, $b_j(\lambda)$ is the base function of index $j$, and $w_j$ is the corresponding weight. We have considered $\lambda_{\text{min}} = 400$ nm, $\lambda_{\text{max}} = 700$ nm and $\Delta \lambda = 10$ nm here. Approximating the three integrals in equations (1) as summations over a limited range of wavelengths, and applying equation (3), the tristimulus values equations become:

\[
X = K \sum_{j=1}^{\lambda_{\text{max}}} \sum_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} w_j b_j(\lambda) I(\lambda) \tilde{x}(\lambda) \Delta \lambda \\
Y = K \sum_{j=1}^{\lambda_{\text{max}}} \sum_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} w_j b_j(\lambda) I(\lambda) \tilde{y}(\lambda) \Delta \lambda \\
Z = K \sum_{j=1}^{\lambda_{\text{max}}} \sum_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} w_j b_j(\lambda) I(\lambda) \tilde{z}(\lambda) \Delta \lambda
\]

We must now find the weights in equation (4), given the tristimulus values and assuming that no fluorescence occurs. Once the weights have been estimated, the reflectance spectrum can be computed using equation (3). We considered different types of basis sets, all of which require the estimation of a variable number of parameters.

### 3. The Basis Set Considered

The different sets of basis functions experimented included those obtained by Principal Component Analysis performed on the datasets studied and Gaussian basis functions.

**Principal Component Analysis** allows the computation of basis functions for linear model representation. A PCA basis set corresponds to directions having maximum variance in the data space; the idea is to account for the direction in which the measured data has the most variance. The use of PCA implies the assumption that the distribution of the data has a Gaussian form.

The number of components needed to accurately represent a set of reflectance spectra depends on the characteristics of the data set. The reflectance spectra of most objects found in nature are smooth functions of wavelength; the same is true of spectra produced using photography, printing, or paints. These spectra can, therefore, be accurately represented by a limited number of basis functions[8]. Various studies have estimated that three to seven principal components will provide a satisfactory reconstruction of the reflectance spectra in most cases, while increasing the number does not guarantee a better performance[9]. We have set the number of basis functions at six, in accordance with Maloney[2], who has demonstrated that a linear model with as few as six basis functions provides essentially perfect fits for almost all natural surface spectral reflectance functions. Consequently the reflectance function here is represented by the following equation:

\[
R(\lambda) = \sum_{j=1}^{6} A_j b_j(\lambda)
\]
where $b_j(\lambda)$ is the basis function of index $j$, and $A_j$ is the corresponding weight.

**Gaussian Basis Functions.** Angelopoulou et al. [10] have used an approximation of reflectance spectra with Gaussian functions to model skin reflectances. A Gaussian basis set has also been used by Dupont [11]. We considered a basis set composed of 15 Gaussian functions obtained with the following equation:

$$g_j(\lambda) = \exp\left[-\frac{4 \ln(2)(\lambda - \lambda_j)^2}{40}\right]$$  \hspace{1cm} j = 1..15 \hspace{1cm} (6)$$

where $\lambda_j$ ranges from 400 to 700 with a step of 20. The reflectance function is represented by the equation

$$R(\lambda) = \sum_{j=1}^{15} D_j g_j(\lambda)$$  \hspace{1cm} (7)$$

where $D_j$ are the fifteen weights of the linear model to be estimated.

We refer to this basis as the “Fixed Gaussian” case (FG). We have also investigated a “Variable Gaussian” (VG) approach, in which the reflectance function is modeled using a constant term and three Gaussian functions:

$$R(\lambda) = E_0 + E_1 \exp\left[-\frac{(\lambda - \lambda_{\text{min}} - E_2)^2}{E_3^2}\right] +$$

$$+ E_4 \exp\left[-\frac{(\lambda - \lambda_{\text{min}} - E_5)^2}{E_6^2}\right] + E_7 \exp\left[-\frac{(\lambda - \lambda_{\text{min}} - E_8)^2}{E_9^2}\right]$$  \hspace{1cm} (8)$$

where the unknowns are the weights $E_0$, $E_1$, $E_4$, and $E_7$, the mean terms $E_2$, $E_5$, and $E_8$, and the terms $E_3$, $E_6$, and $E_9$ correlated with the standard deviation.

### 4. Genetic algorithms

Genetic algorithms (GA) are a general method for solving optimization problems, inspired by the mechanisms of evolution in biological systems (see e.g. [12], [13] for an introduction to GA and their applications). In the basic genetic algorithm, every candidate solution is represented by a sequence of binary, integer, real, or even more complex values, called an individual. A number of individuals are randomly generated as an initial population. The GA then iterates a procedure that produces a new population from the
current one, until a given "STOP" criterion is satisfied. At each iteration, the value of a suitable "fitness" function is computed for every individual in the current population; the goal of the GA is to generate an individual with the best value of fitness. Given the problem described in Section II, and assuming that only a triplet of tristimulus values is available, fitness is the squared sum of the perceptual differences between the CIELab values computed on the input color and those computed on the estimated reflectance spectrum, plus a term of range violation, with no perceptual meaning, to account for the bounds the solution must respect in order to match physical reflectance properties:

\[
\text{fitness} = \left[ (L^* - L_{\text{input,ill}}^*)^2 + (a^* - a_{\text{input,ill}}^*)^2 + (b^* - b_{\text{input,ill}}^*)^2 \right]_{\text{ill}} + \delta_1(R(\lambda)) + \delta_2(R(\lambda)) \quad (9)
\]

where \( \delta_1(R(\lambda)) = D_1 \left[ \max_A(R(\lambda)) - 100 \right] \) iff \( \max_A(R(\lambda)) \geq 100 \), else \( \delta_1(R(\lambda)) = 0 \) and \( \delta_2(R(\lambda)) = -D_2 \min_A(R(\lambda)) \) iff \( \min_A(R(\lambda)) < 0 \), else \( \delta_2(R(\lambda)) = 0 \).

Parameters \( D_1 \) and \( D_2 \) must be positive, and define the weight in the optimization function of the range violation error with respect to the colorimetric perceptual error. In our experiment we set \( D_1 = D_2 = 1 \). No term of smoothness has been considered in the fitness function; the smoothness of the reflectance spectrum is not an issue, due to the characteristics of the linear model basis employed. Many different spectra can generate the same XYZ triplet. If we assume that the tristimulus values referred to different illuminants are also known, a more effective fitness function can be designed:

\[
f = \sum_{k=1}^{K} \left[ (L^* - L_{\text{input,ill}_k}^*)^2 + (a^* - a_{\text{input,ill}_k}^*)^2 + (b^* - b_{\text{input,ill}_k}^*)^2 \right]_{\text{ill}_k} + \delta_1(R(\lambda)) + \delta_2(R(\lambda)) \quad (10)
\]

where \( K \) is the number of illuminants considered, and the other symbols are those used in equation (9).

5. Experiments and Results

Different data sets of reflectance functions have been used for benchmarking: the Macbeth ColorChecker Chart, the whole Munsell Atlas [14], a set of 120 Dupont paint chips [15] and of a set of 1000 silk color samples [16]. The following experiments were performed. For each dataset, given \( R(\lambda) \) we computed the tristimulus values for three illuminants: D65, A, and F2. Then, for each type of basis set, we estimated the weights of equation (4) by means of a genetic algorithm using the fitness function described in (10). We conducted three experiments for each basis set and for each dataset: one considering only the D65 illuminant, a second considering the D65 and the A illuminants, and a third considering all three illuminants (D65, A and F2). The results for the different basis sets are described in Section III.

We computed four basis sets by applying Principal Component Analysis to the datasets used for benchmarking. We then estimated the reflectance spectra for each dataset, using the corresponding basis set. Table I reports the statistics of results obtained using the PCA basis set of each dataset considered.
<table>
<thead>
<tr>
<th>Variable</th>
<th>ΔE D65</th>
<th>ΔE A</th>
<th>ΔE F2</th>
<th>MAE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>avg</td>
<td>M</td>
<td>sdv</td>
<td></td>
</tr>
<tr>
<td>Macbeth, D65</td>
<td>0.00</td>
<td>0.09</td>
<td>0.02</td>
<td>2.72</td>
</tr>
<tr>
<td>D65,A</td>
<td>0.19</td>
<td>0.60</td>
<td>0.14</td>
<td>0.20</td>
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<tr>
<td>D65,A,F2</td>
<td>0.18</td>
<td>0.66</td>
<td>0.14</td>
<td>0.26</td>
</tr>
<tr>
<td>Munsell, D65</td>
<td>0.00</td>
<td>0.08</td>
<td>0.01</td>
<td>1.67</td>
</tr>
<tr>
<td>D65,A</td>
<td>0.13</td>
<td>0.87</td>
<td>0.11</td>
<td>0.14</td>
</tr>
<tr>
<td>D65,A,F2</td>
<td>0.18</td>
<td>2.21</td>
<td>0.17</td>
<td>0.29</td>
</tr>
<tr>
<td>Dupont, D65</td>
<td>0.06</td>
<td>0.72</td>
<td>0.13</td>
<td>3.65</td>
</tr>
<tr>
<td>D65,A</td>
<td>0.35</td>
<td>1.55</td>
<td>0.36</td>
<td>0.40</td>
</tr>
<tr>
<td>D65,A,F2</td>
<td>0.47</td>
<td>2.68</td>
<td>0.58</td>
<td>0.77</td>
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<tr>
<td>Silk, D65</td>
<td>0.01</td>
<td>0.38</td>
<td>0.04</td>
<td>1.92</td>
</tr>
<tr>
<td>D65,A</td>
<td>0.23</td>
<td>1.13</td>
<td>0.18</td>
<td>0.24</td>
</tr>
<tr>
<td>D65,A,F2</td>
<td>0.28</td>
<td>1.29</td>
<td>0.21</td>
<td>0.46</td>
</tr>
</tbody>
</table>

### Table I: Statistics of results obtained using the PCA basis set of each of the dataset considered (MAE = mean absolute error, avg = mean value, M = maximum value, sdv = standard deviation).

In Table I, the results are reported as average error, maximum error and standard deviation of the distance in CIELAB space between the coordinates of the measured and the estimated spectra under the illuminants D65, A, and F2. The spectral mismatch is reported as the mean absolute error between reflectance spectra. For each dataset, the first row reports the results for the estimation, assuming the tristimulus values for the D65 illuminant are available. In this case, the colorimetric error ΔE D65 is low, while colorimetric errors for the A and F2 illuminants are larger, and indicate that the estimated spectra are metameric with respect to the original ones. The use of two or three illuminants, as reported in the second and third row of each dataset, reduces the difference between colorimetric errors. As a consequence, the spectral error is also reduced. Table II reports the statistics of results obtained using the fitness in equations (10), and the FG basis set. Tables III shows the statistics of the results obtained employing the VG basis set.

<table>
<thead>
<tr>
<th>Variable</th>
<th>ΔE D65</th>
<th>ΔE A</th>
<th>ΔE F2</th>
<th>MAE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>avg</td>
<td>M</td>
<td>sdv</td>
<td></td>
</tr>
<tr>
<td>Macbeth, D65</td>
<td>0.13</td>
<td>0.45</td>
<td>0.11</td>
<td>3.87</td>
</tr>
<tr>
<td>D65,A</td>
<td>0.45</td>
<td>0.13</td>
<td>0.23</td>
<td>0.43</td>
</tr>
<tr>
<td>D65,A,F2</td>
<td>0.45</td>
<td>1.11</td>
<td>0.24</td>
<td>0.53</td>
</tr>
<tr>
<td>Munsell, D65</td>
<td>0.12</td>
<td>0.81</td>
<td>0.10</td>
<td>4.44</td>
</tr>
<tr>
<td>D65,A</td>
<td>0.38</td>
<td>1.62</td>
<td>0.21</td>
<td>0.36</td>
</tr>
<tr>
<td>D65,A,F2</td>
<td>0.41</td>
<td>1.67</td>
<td>0.26</td>
<td>0.46</td>
</tr>
<tr>
<td>Dupont, D65</td>
<td>0.19</td>
<td>2.56</td>
<td>0.33</td>
<td>3.16</td>
</tr>
<tr>
<td>D65,A</td>
<td>0.49</td>
<td>2.68</td>
<td>0.40</td>
<td>0.47</td>
</tr>
<tr>
<td>D65,A,F2</td>
<td>0.53</td>
<td>2.57</td>
<td>0.43</td>
<td>0.64</td>
</tr>
<tr>
<td>Silk, D65</td>
<td>0.36</td>
<td>1.43</td>
<td>0.36</td>
<td>3.71</td>
</tr>
<tr>
<td>D65,A</td>
<td>0.43</td>
<td>2.40</td>
<td>0.27</td>
<td>0.42</td>
</tr>
<tr>
<td>D65,A,F2</td>
<td>0.51</td>
<td>3.57</td>
<td>0.37</td>
<td>0.55</td>
</tr>
</tbody>
</table>

### Table II: Statistics of results obtained using the Fixed Gaussian basis set (MAE = mean absolute error, avg = mean value, M = maximum value, sdv = standard deviation).

<table>
<thead>
<tr>
<th>Variable</th>
<th>ΔE D65</th>
<th>ΔE A</th>
<th>ΔE F2</th>
<th>MAE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>avg</td>
<td>M</td>
<td>sdv</td>
<td></td>
</tr>
</tbody>
</table>

### Table III: Statistics of results obtained employing the VG basis set.
The Variable basis set performs better here than the Fixed set of Gaussian functions, as can be observed by comparing Tables II and III.

6. Conclusions

We have addressed the problem of synthesizing a spectral reflectance function given the standard CIE 1931 tristimulus values and representing the unknown reflectance functions with linear models. In particular, we have investigated different types of basis functions for the linear model, and different datasets for benchmarking. No single set of basis functions can perfectly model all reflectance functions. Our results confirm that PCA basis sets provide the most effective approach to the problem. These results also indicate that when a suitable set of reflectance data for the calculus of PCA basis functions is lacking, a Gaussian basis set may be satisfactorily employed instead.

REFERENCES