

Analysis-synthesis transforms versus orthogonal transforms for coding reflectance spectra

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Abstract

In this paper we present a comparison of different schemes for transform coding of reflectance spectra. Aiming for representing the spectra with a small number of coefficients, we first concentrate on schemes using orthonormal sets of basis vectors. In this case the basis vector sets used for analysis and synthesis of the spectra are identical. Regarding the mean squared spectral error, the optimal basis function set for a given set of test spectra can be calculated analytically.

We then allow the vector bases for analysis and synthesis to be different and give an example for creating appropriate sets. We show that the best vector set strongly depends on the error measure that is to be minimized. It is not efficient to replace the error in a visually uniform color space by the mean squared spectral error. Minimizing these two error measures yields different sets of vectors as they can not be minimized simultaneously. Furthermore we show the superiority of the approach using separate analysis and synthesis vector sets over orthonormal basis vector sets.

In order to verify the results of the analytically derived vector sets, we compare them with those of vector sets derived by optimization algorithms.

1. Introduction

The notation is chosen in accordance with the work of Trussell [1]. We sample a spectrum equally spaced over the visible range and form a column vector $\mathbf{f}$ with n elements. The color matching functions, which are linear combinations of the sensitivity characteristics of the three different cone types of the human eye, form an $n \times 3$ matrix $\mathbf{A} = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$. By multiplication we get the color impression as a 3-vector $\mathbf{c} = \mathbf{A}^{\mathrm{T}}\mathbf{f} = (X, Y, Z)^{\mathrm{T}}$.

The physical spectrum $\mathbf{f} = \mathbf{D}\mathbf{r}$ depends on the reflectance spectrum $\mathbf{r}$ of the object and the spectrum $\mathbf{D}$ of the illumination, where $\mathbf{D}$ is an $n \times n$ diagonal matrix with the spectrum on the diagonal. For the color vector we have $\mathbf{c} = \mathbf{A}^{\mathrm{T}}\mathbf{D}\mathbf{r} = \mathbf{A}_d^{\mathrm{T}}\mathbf{r}$, using the abbreviation $\mathbf{A}_d = \mathbf{D}\mathbf{A}$.

Now the reflectance spectra $\mathbf{r}$ are approximated by the weighted sum of synthesis functions $\mathbf{r} \approx \sum_{i=0}^{m-1} w_i \mathbf{s}_i = \mathbf{F}_s\mathbf{w}$. The synthesis vectors $\mathbf{s}_i$ are represented in the columns of the $n \times m$ matrix $\mathbf{F}_s$. The weighting coefficients form the m-vector $\mathbf{w}$.

These weighting coefficients are calculated as scalar products of the reflectance spectrum $\mathbf{r}$ and the analysis vectors $\mathbf{t}_i^{\mathrm{T}}$ which are represented in the rows of the analysis $m \times n$ matrix $\mathbf{F}_a$. We have

$$\mathbf{w} = \mathbf{F}_a\mathbf{r}, \quad \mathbf{r} \approx \hat{\mathbf{r}} = \mathbf{F}_s\mathbf{w} = \mathbf{F}_s\mathbf{F}_a\mathbf{r} \qquad (1)$$

Analysis and synthesis vector sets $\mathbf{F}_a$ and $\mathbf{F}_s$ are to be constructed such, that an error measure is minimized. $\mathbf{F}_a$ and $\mathbf{F}_s$ have to meet the following two conditions:

1. The repeated application of analysis and synthesis must not change the vector $\mathbf{r}$. Therefore $\mathbf{P} = \mathbf{F}_s\mathbf{F}_a$ has to be a projection: $(\mathbf{F}_s\mathbf{F}_a)^2 = \mathbf{F}_s\mathbf{F}_a$.

2. It immediately follows the orthonormality condition in form of $\mathbf{F}_a\mathbf{F}_s = \mathbf{I}$, the $m \times m$ identity matrix.

We seek for analysis and synthesis vector sets that lead to a minimal error for a test set of reflectance spectra. We consider two error measures:

1. The mean spectral error is defined by

$$E\left(\frac{1}{n}(\mathbf{r} - \hat{\mathbf{r}})^{\mathrm{T}} \cdot (\mathbf{r} - \hat{\mathbf{r}})\right). \qquad (2)$$

2. The mean color error is evaluated in a visually uniform color space taking a set of different illuminants $\mathbf{D}$ into account. We use the modified Euclidean distance of the two colors to be compared in the CIELab color space as proposed in the ΔE_{94}^* formula [2].

In the following two sections we propose analytical derivations of orthogonal basis vector sets as well as analysis-synthesis vector sets. Afterwards we employ optimization algorithms to be able to verify the results.

2. Orthogonal Systems

In this case we claim the analysis and synthesis vector sets to be identical, $\mathbf{F}_s = \mathbf{F}_a^{\mathrm{T}} = \mathbf{F}$. From the two above conditions it follows that $\mathbf{F}$ needs to be an orthonormal basis.

For minimizing the mean squared spectral error we know the analytical solution in form of the Karhunen-Loève transform (KLT). The transform vectors are the eigen vectors according to the k largest eigen values of the autocorrelation matrix of the test spectra set under consideration. To be comparable to transform schemes that do not subtract the mean spectrum prior to the transform, we take the eigen vectors of the *autocorrelation matrix* instead of those of the *autocovariance matrix*.

3. Analysis-Synthesis Systems

With a large number of given test spectra and a given set of test illuminants we can analytically derive transform systems that minimize the mean squared error regarding the color values. This approach, which is based on a singular value decomposition of the matrix of color values, was introduced as the *one-mode analysis* [3].

Therefore we have to choose a color space for the minimization. The $L^*a^*b^*$ space is obviously more uniform to the visual perception of color differences than the *XYZ* space, but it is derived by a nonlinear transform. We can only seek the best linear approximation of this transform for a given set of spectra.

After collecting the p test reflectance spectra $\mathbf{r}$ in an $n \times p$ matrix $\mathbf{R}$, we get the $3 \times p$ matrix of color values $\mathbf{C} = \mathbf{A}^{\mathrm{T}}\mathbf{R}$. Given the nonlinear transform $\mathcal{L}(\mathbf{c}) = \mathbf{e}$ we obtain the color vector $\mathbf{e} = (L^*, a^*, b^*)^{\mathrm{T}}$. Applying this transform to the whole matrix of spectra yields $\mathcal{L}(\mathbf{C}) = \mathbf{E}$, again a $3 \times p$ matrix. We approximate $\mathbf{E} \approx \hat{\mathbf{E}} = \mathbf{T}\mathbf{C}$ using the 3×3 matrix $\mathbf{T}$. The minimal error in $\hat{\mathbf{E}}$ is achieved by $\mathbf{T} = \mathbf{E}\mathbf{C}^{\mathrm{T}}(\mathbf{C}\mathbf{C}^{\mathrm{T}})^{-1}$. Then the transform from a reflectance spectrum into the resulting color space is given by $\mathbf{e} = \mathbf{T}\mathbf{A}^{\mathrm{T}}\mathbf{r}$.

Combining the $n \times 3$ matrix $\mathbf{A}\mathbf{T}^{\mathrm{T}}$ of the color matching functions of the resulting color space with the predefined set of l test illuminants $\mathbf{D}_{d=0\ldots l-1}$ we build the $n \times 3l$ matrix of the weighted color matching functions $\mathbf{A}_* = (\mathbf{D}_0\mathbf{A}\mathbf{T}^{\mathrm{T}}, \mathbf{D}_1\mathbf{A}\mathbf{T}^{\mathrm{T}}, \ldots, \mathbf{D}_{l-1}\mathbf{A}\mathbf{T}^{\mathrm{T}})$.

The $3l \times p$ matrix $\mathbf{G} = \mathbf{A}_*^{\mathrm{T}}\mathbf{R}$ gives us all the color values that we wish to reproduce with minimal error using the approximated spectra.

$$\mathbf{G} \approx \hat{\mathbf{G}} = \mathbf{A}_*^{\mathrm{T}}\hat{\mathbf{R}} = \mathbf{A}_*^{\mathrm{T}}\mathbf{F}_s\mathbf{F}_a\mathbf{R} \qquad (3)$$

Applying the singular value decomposition we get the expression $\mathbf{G} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathrm{T}}$. Let the set of test spectra be sufficiently large: $p > 3l$. Then the decomposition yields the orthogonal $3l \times 3l$ matrix $\mathbf{U}$, the diagonal $3l \times 3l$ matrix $\mathbf{S}$, and the orthogonal $p \times 3l$ matrix $\mathbf{V}$. The elements s_i on the diagonal of $\mathbf{S}$ (which are the eigen values of $\mathbf{G}$) are sorted in decreasing order $s_i > s_{i+1}$. Replacing the smallest eigen values $s_k, s_{k+1}, \ldots s_{3l-1}$ with zero value leads to an approximation for $\mathbf{G}$ in a least mean square sense:

$$\mathbf{G} \approx \hat{\mathbf{G}} = \mathbf{U}\mathbf{S}_k\mathbf{V}^{\mathrm{T}} = \mathbf{A}_*^{\mathrm{T}}\mathbf{F}_s\mathbf{F}_a\mathbf{R} \qquad (4)$$

Solving $\mathbf{U}\mathbf{S}_k = \mathbf{A}_*^{\mathrm{T}}\mathbf{F}_s$ for $\mathbf{F}_s$ and $\mathbf{V}^{\mathrm{T}} = \mathbf{F}_a\mathbf{R}$ for $\mathbf{F}_a$ yields the analysis and synthesis functions that we need. It can be easily shown that replacing all but the first k eigen values of $\mathbf{S}$ with zeros is equivalent to taking only the first k rows of $\mathbf{F}_a$ and the first k columns of $\mathbf{F}_s$. In other words, we code the spectra with the first k coefficients of the transform.

The rows of the $3l \times p$ matrix $\mathbf{V}^{\mathrm{T}}$ span a subspace of the space formed by the rows of the $n \times p$ matrix $\mathbf{R}$. Therefore there exists a solution of $\mathbf{V}^{\mathrm{T}} = \mathbf{F}_a\mathbf{R}$, which is unique and given by

$$\mathbf{F}_a = \mathbf{V}^{\mathrm{T}}\mathbf{R}^{\mathrm{T}}(\mathbf{R}\mathbf{R}^{\mathrm{T}})^{-1}. \qquad (5)$$

Herewith we have already defined the analysis vectors for the transform coding kernel.

On the other hand, equation $\mathbf{U}\mathbf{S}_k = \mathbf{A}_*^{\mathrm{T}}\mathbf{F}_s$ consists of $3l \times 3l$ single equations to solve the $3l \times n$ variables of $\mathbf{F}_s$. Since usually $3l < n$, it is underdeterminate. Therefore we can employ further constraints to the solution. Here we try to minimize both the aforementioned error criteria. At first we concentrated on the construction of vectors to minimize the color error. Now we can determine the synthesis vectors such, that also the spectral error is reduced. For natural spectra, which are relatively smooth, we obtain the best approximation if we use "smooth" synthesis vectors. In order to achieve these vectors we employ a Wiener inverse expression under the assumption of an AR(1) model for the spectra together with a correlation coefficient $0 < \rho < 1$. For such a statistical model we can calculate the covariance matrix $\mathbf{K}$. This matrix is square ($n \times n$) and of Toeplitz structure with $\rho^{|k|}$ on the k-th secondary diagonal. Amongst all possible solutions the Wiener inverse yields the one that has minimal deviation from the assumed model.

$$\mathbf{F}_s = \mathbf{K}\mathbf{A}_*(\mathbf{A}_*^{\mathrm{T}}\mathbf{K}\mathbf{A}_*)^{-1}\mathbf{U}\mathbf{S} \qquad (6)$$

4. Systems Derived by Optimization

For minimizing the mean visual color error over a set of different illuminants there is no analytical solution. There-

fore what we have calculated so far is suboptimal in a visual color error sense because we only minimized the mean squared spectral error and the mean squared color error in a color space which is close to a visually uniform color space. For comparison we calculated the mean ΔE^*_{94} error by means of optimization algorithms. We applied a combination of stochastic optimization to find a good starting point followed by a gradient scheme.

Because the analytically derived vectors offer the possibility to be used in a hierarchical way we also optimized the vector sets, such that they can be used hierarchically. Let (mean $\Delta E^*_{94,i}$) be the mean visual color error averaged over a set of illuminants and over a set of test spectra using only i coefficients of the transform. Then for a set of I vectors we would like to minimize all $\Delta E^*_{94,i}$ for $i = 1 \ldots I$ simultaneously. This can be accomplished by taking their product

$$\text{total error} = \prod_{i=1}^{I} \text{mean } \Delta E^*_{94,i} \tag{7}$$

as the measure to be minimized. It was observed that the single error values $\Delta E^*_{94,i}$ were not much worse than the error values that remain after minimizing the $\Delta E^*_{94,i}$ individually. That means by minimizing the above error measure we gain the benefit of hierarchical usage with almost no loss of reconstruction quality. The small degradation of quality can be due to the difficulty in finding the global optimum in this high dimensional problem.

We started the optimization with the analytically derived vectors. First we performed a stochastic optimization using the Threshold Accepting algorithm [4] and took the result as the initial point for a gradient scheme which is referred to as the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm in [5].

To comply the two conditions given in Section 1 we need additional steps in the optimization.

At first we add a step to each iteration of the optimization that performs an orthonormalization of the basis vectors, respectively an orthonormalization of the analysis vectors to the synthesis vectors.

In the case of the analysis-synthesis system it is possible to substitute the synthesis vectors $\mathbf{F}_s$ by smoother vectors $\mathbf{F}_{s,\mathrm{smooth}}$, provided that they yield the same projection onto the space spanned by matrix $\mathbf{A}_*$. Like we did in Section 3 we incorporate the desired smoothness by modeling the spectra with an AR(1) model with a predefined correlation coefficient ρ and a corresponding covariance matrix $\mathbf{K}$. The smooth versions of the synthesis vectors are given by

$$\mathbf{F}_{s,\mathrm{smooth}} = \mathbf{K}\mathbf{A}_*(\mathbf{A}_*^{\mathrm{T}}\mathbf{K}\mathbf{A}_*)^{-1}\mathbf{A}_*^{\mathrm{T}}\mathbf{F}_s. \tag{8}$$

Both synthesis vector sets lead to the same color error, while with the smoother vectors $\mathbf{F}_{s,\mathrm{smooth}}$ at the same time the mean squared spectral error is decreased.

To include the smoothing into the optimization we perform this projection of the synthesis vectors in each iteration of the optimization followed by the aforementioned orthonormalization of the analysis set to the synthesis set. It was observed that the optimization algorithm works very well with this supplement, that means the results in terms of the color error are not affected whereas the spectral error is decreased significantly.

5. Results

The following figures were obtained using a set of 1269 reflectance spectra of Munsell chips, sampled between 400 and 700 nm in 5 nm intervals [6]. Our set of illuminants consisted of the standard illuminants A, C, D65, Xe, and F11. We compare the following transforms:

1. Orthogonal transform, minimizing the mean squared spectral error, KLT.

2. Orthogonal transform, minimizing Eq. (7), derived using the above given optimization.

3. Analysis-synthesis vector set, according to Section 3, spectra AR(1) modeled with $\rho = 0.99$.

4. Analysis-synthesis vector set, minimizing Eq. (7), derived using the above given optimization, synthesis vectors AR(1) modeled with $\rho = 0.99$.

Figures 1 and 2 show the first 5 basis vectors for both the orthogonal transforms. Figures 3 and 4 show the first 5 analysis and synthesis vectors which were analytically derived as given in Section 3. Figures 5 and 6 show the first 5 analysis and synthesis vectors which were derived using the optimization.

The error evaluation is divided into the mean squared spectral error (Table 1) and the mean $\Delta E^*_{94,i}$ color error (Table 2) for a number of $i = 1 \ldots 7$ coefficients. Because of the stochastic optimization different optimization runs render results which are not identical. Although the results are only slightly differing it should be noted that they are only exemplary as well for the error values as for the shape of the vectors.

Concerning both the orthogonal transforms (transforms 1. and 2.) it can be stated that the mean squared spectral error (minimized by the KLT) and the mean $\Delta E^*_{94,i}$ error (minimized with the optimized basis vectors) are contrary to each other. Minimizing the color error is by no means equivalent to minimizing the spectral error.

	transform			
i	1.	2.	3.	4.
1	9.0701	26.2012	9.9268	10.3316
2	2.8990	21.6506	4.4168	5.0851
3	0.5618	19.7249	0.8736	1.0106
4	0.2648	19.3786	0.6987	0.8237
5	0.1229	19.1538	0.3788	0.4409
6	0.0779	19.1458	0.1860	0.2391
7	0.0425	19.1400	0.1575	0.2070

Table 1: *Mean squared spectral error [*$\times 1000$*]*

	transform			
i	1.	2.	3.	4.
1	16.5787	16.4859	16.1975	16.1081
2	10.8818	10.3858	9.6435	9.4431
3	1.6416	0.8544	0.5304	0.4261
4	1.2552	0.4119	0.2709	0.2335
5	0.5801	0.1691	0.1266	0.1024
6	0.5302	0.0903	0.0570	0.0500
7	0.1967	0.0429	0.0181	0.0169

Table 2: *Mean* $\Delta E^*_{94,i}$ *error*

Using the proposed scheme for obtaining separate vector sets for analysis and synthesis (transform 3.), the color error can be further reduced. This is accompanied by only a moderate increase of the spectral error compared to the KLT. As far as the mean $\Delta E^*_{94,i}$ color error is concerned, we observe that with only three coefficients we get the same accuracy as with six coefficients using the KLT.

Generally the analysis-synthesis transforms perform better than the orthogonal transforms. Even the analytically derived analysis-synthesis vectors (transform 3.) yield smaller color errors throughout than the best achievable orthogonal basis vectors (transform 2.).

We have developed a scheme to analytically derive analysis-synthesis transform vectors for coding reflectance spectra, which outperform the best possible orthogonal transform in terms of mean color error, and which nearly reach the error values of the best achievable analysis-synthesis vectors that can be derived by optimization.

6. References

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6. Reflectance spectra of 1269 matt Munsell color chips. Available via anonymous FTP at Lappeenranta University of Technology, Finland. ftp.lut.fi/pub/color/spectra/mspec/

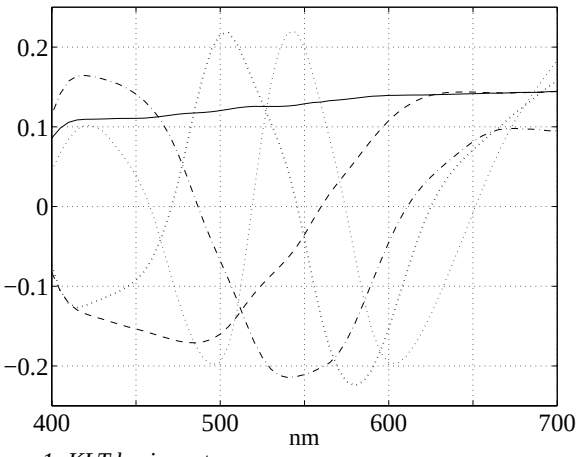

Figure 1: *KLT basis vectors.*

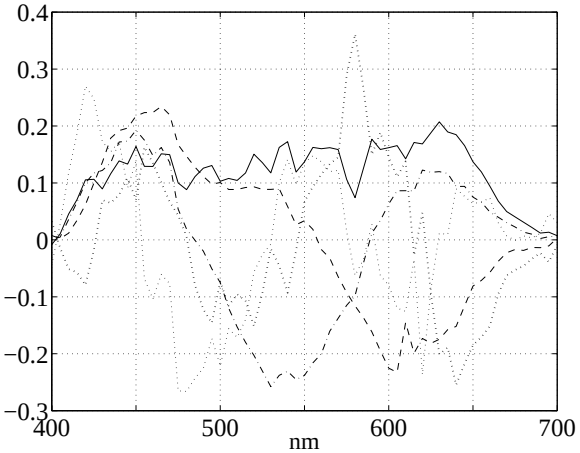

Figure 2: *Basis vectors minimizing Eq. (7).*

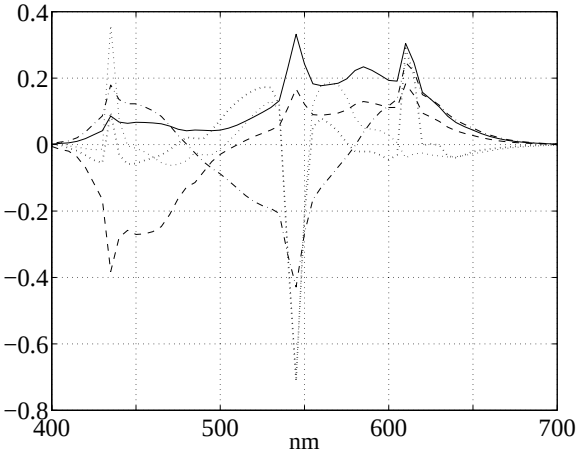

Figure 3: *Analysis vectors according to Section 3.*

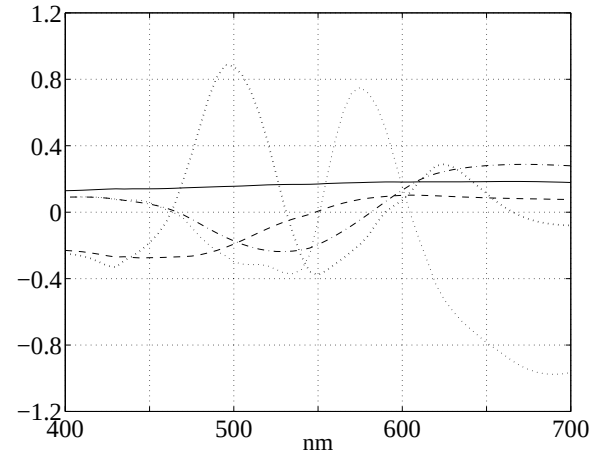

Figure 4: *Synthesis vectors according to Section 3.*

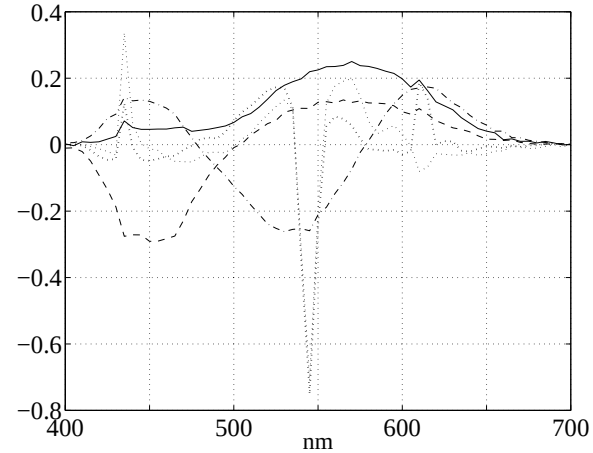

Figure 5: *Optimized analysis vectors minimizing Eq. (7).*

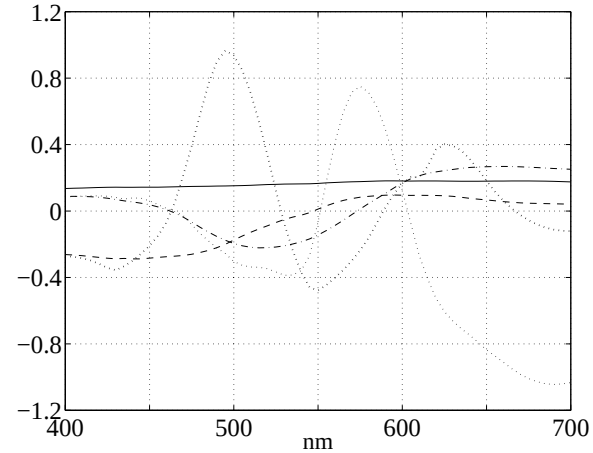

Figure 6: *Optimized synthesis vectors minimizing Eq. (7).*