Spectral Colorimetry Using LabPQR – An Interim Connection Space

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Abstract

A method of converting reflectance spectra to a convenient intermediate form introduced as LabPOR is used as an Interim Connection Space (ICS) within a spectral color management system. The LabPQR ICS makes use of a spectral encoding that explicitly incorporates colorimetry with additional dimensions that define spectral error corrections that allow an inverse transformation to approximate the original spectra. Consistent with a spectral previously defined color management transformation chain, the PQR dimensions of the ICS can be optimally formulated to suit any specific output device's spectral characteristics. Several example transformations are demonstrated using various output devices with spectral gamut visualizations. Observations are made, and from these observations, a possible method of performing spectral gamut mapping is proposed.

Introduction

Color image reproduction systems have traditionally been based upon colorimetry which relies on the fact that there are only three cones in the human visual system. Two colors can be thought of as matching when the sensations of the cones are the same. However, metamers exist. These are spectrally different colors that under one illuminant are colorimetrically equivalent, but may not appear the same under different viewing conditions or to different observers. To attenuate the impact of metamerism, the printing industry has established guidelines for comparing color reproductions that specify viewing and lighting conditions to be used while making evaluations. Color management using ICC profiles relies on colorimetry as basis for its profile connection space (PCS). Colors reproduced using such color management systems are only guaranteed to match under the viewing conditions for which the profile was prepared. There are times when it is desirable to produce reproductions that match under all illuminants.²⁻⁴ This is accomplished when reproduced spectra are the same as the original. One of the difficulties encountered in reproducing spectral images is the high dimensionality of spectral data.5 The techniques employed by ICC profiles using multi-dimensional look-up tables do not work well for the many dimensions that are

needed to represent spectral data. Additionally, the problems of gamut mapping become vague and unwieldy.

In previous work^{6,7} a spectral image processing workflow from scene to print was described. The proposal included the use of a low-dimensional Interim Connection Space (ICS) as a critical aspect of spectral color management. The ICS provides a logical way-station during the transition between a full-dimensional spectral space and device-dependent units. Thus, ICS logically sits on the output side of a spectral PCS. Conceptually, this allows the space to be device dependent if it were to be parameterized within a destination spectral profile.

Desirable characteristics of an ICS include a reasonably small number of dimensions and a computationally inexpensive calculation from spectra. This paper uses a method for deriving an ICS that adds the additional valuable increased compatibility feature of with current colorimetrically-based color management by explicitly incorporating colorimetry into its spectral representation. Converting spectral data to vectors of lower resolution with colorimetric parts have previously been discussed in the literature for use as a spectral image storage space.⁸ This paper introduces the use of such encoding, which we call spectral colorimetry, as a spectral data transformation space. Encoding an ICS with spectral colorimetry leads to novel approaches for spectral gamut visualization and spectral gamut mapping.

Spectral Colorimetry

The conversion from spectra to normalized tristimulus values can be expressed using matrix notation:

$$c = Ds \tag{1}$$

where a distillation matrix D represents the concatenation of a standard observer matrix O, the spectral power distribution of the illuminant matrix L, and a normalization based upon a perfect white under a chosen illuminant (matrix N). Thus:

$$\boldsymbol{D} = \boldsymbol{NOL} \tag{2}$$

Spectral vectors *s* and corresponding tristimulus vectors *c* can be grouped into matrices. Thus (1) can be re-written as:

$$C = DS \tag{3}$$

A reconstitution matrix **R** can conceptually be thought of as the inverse of the distillation matrix **D** in (2). By using an **S** and the corresponding **C** calculated from (3) **R** can be found by multiplying **S** by the pseudo-inverse of **C**. Thus:

$$S = RC \tag{4}$$

$$\boldsymbol{R} = \boldsymbol{S}\boldsymbol{C}^{T}(\boldsymbol{C}\boldsymbol{C}^{T})^{-1}$$
(5)

Since R is calculated using a pseudo-inverse it will not be an exact inverse of D in (2). An error difference matrix can be calculated between the spectral matrix set and its round-trip through distillation and reconstitution can be calculated.

$$\boldsymbol{E} = (\boldsymbol{I} - \boldsymbol{R}\boldsymbol{D})\boldsymbol{S} \tag{6}$$

The resulting error matrix can be characterized and quantified by performing principal component analysis on E. The resulting eigenvectors (v) correspond to basis functions in spectral error space from applying the simple spectral reconstitution matrix R to normalized tristimulus vectors. Taking the most significant eigenvectors allows one to quantify the most significant errors as spectral error coordinates.

$$p = V(I-RD)s \tag{7}$$

The dimensionality of the spectral coordinate vector p is determined by how many eigenvector rows are in matrix V. LabPQR would use three.

Putting Everything Together

To Convert (Distill) a Spectral Reflectance Vector to a Multichromatic LabPQR Vector:

- 1. Calculate distillation matrix D, reconstitution matrix R, & error basis matrix V using regression analysis and PCA. (Note this step only needs to be performed once. The D, R & Vmatricies can be cached).
- 2. Calculate a normalized XYZ vector *c* using (1).
- 3. PQR can be calculated using (7).
- 4. LabPQR can be calculated from an XYZPQR vector using CIE equations.

To Convert (Reconstitute) a Spectral Reflectance Vector from a Multichromatic LabPQR Vector:

- 1. Convert Lab to normalized XYZ using inverse CIE equations thus creating a c vector
- 2. Calculate reconstituted spectra s' as follows:

$$s' = \mathbf{R}c + \mathbf{V}^T p \tag{8}$$

Going from PCS to ICS

LabPQR makes an excellent candidate as an ICS for the following reasons:

- 1. It is tuned to (based on) the reflectance spectra of the printer. It was previously pointed out there are "many arguments for designing an ICS so that it is particularly efficient at describing a printer's spectral gamut."^{6,7}
- 2. It is a low dimensional representation of reflectance spectra.
- 3. It is relatively computationally inexpensive to transform from spectra to LabPQR.
- 4. Because of its explicit colorimetric qualities, gamut mapping should be well served.
- 5. Although the colorimetric portion of LabPQR is illuminant dependant, the full entity represents reflectance spectra and is thus illuminant independent.
- 6. Because of where ICS falls in the spectral transformation workflow^{6,7} it is only necessary for LabPQR to describe the spectral gamut of the destination device.

Implementation

An implementation of spectral colorimetry was performed in a C++ program (SpecSep) that makes use of an open source C++ matrix library, NewMat10,⁹ that works well with large matrix sizes. For these discussions we do not differentiate between LabPQR and XYZPQR as they are considered equivalent. To evaluate the spectral round trip accuracy of taking original spectra through XYZPQR and back, a root mean squared (RMS) spectral difference calculation was made. Additionally the original spectra and reconstituted spectra were both converted to CIELAB under a Planckian 2856K illuminant and a Δ E2000 calculation was performed.

Improvements

While implementing the SpecSep program two optimizations were also found to give better results:

- 1. A feedback mechanism was put in place to add greater weight to spectra that perform poorly in a round trip. Initially, the largest RMS error was calculated to set an initial threshold at 95% of the maximum RMS. Spectra with RMS errors greater than the threshold were repeatedly given greater weight to get the maximum RMS error reduced to the threshold. If the number of times the spectral weights were incremented was fewer than 20, then the threshold was reduced by 5%, and the process repeated again. This is an attempt to account for outliers without excessive overtraining.
- 2. **XYZ+**: Using non-linear combinations of coordinates improved accuracy by adding more degrees of freedom to the analysis. In addition to X, Y, & Z coordinates, XY, XZ, YZ, & XYZ were added to form a vector *c*' that was used and substituted for as appropriate in (1) through (8).

Testing the Implementation

Several data sets were used to evaluate the implementation of spectral colorimetry in SpecSep. All the data sets tested had fairly smooth spectra, and were sampled at spectral wavelengths from 400nm to 700nm in 10nm intervals.

Two of the spectral reflectance data sets were obtained from the spectral database¹⁰ of the University of Joensuu: a "Munsell colors glossy (all)" set containing 1600 spectral colors, and an "Agfa IT.8/7.2" set containing 289 spectral colors. Additional spectral reflectance sets were obtained from measurements of prints of custom ICC profile charts that were produced from PosterShop by Onyx Graphics. Spectral readings were made using an Xrite Spectrofiler. Charts were printed both on a Mimaki JV3 solvent-based CMYKcm printer on vinyl, and a Roland HiFi Jet 540 pigment-based CMYKOGcm printer on canvas. In both cases light concentrations of cyan and magenta are treated as extensions of the dark inks. The Mimaki JV3 data set contains a complete 11x11x11 sampling of the CMY channels in uniform 10% increments and this CMY subset was used as an independent test set.

Table 1 shows the round trip results from converting spectra using data-set-specific XYZPQR transforms, and then performing the back-conversion to reflectance spectra. The number of patches in the set, Min/Ave/Max RMS values, and Min/Ave/Max Δ E2000 color differences are shown. The bottom row shows the percentage of patches that have an RMS error greater than 90% of the Maximum RMS error.

Table 1. Round Trip Results for Each Data Set Using itsOwn Optimized Transform

	Mimaki CMY	Mimaki CMYK	Roland CMYKOG	Agfa dataset	Munsell dataset
# Patches	1331	2067	2239	289	1600
Min RMS	0.001	0.0006	0.0014	0.0011	0.0007
Ave RMS	0.0041	0.0043	0.0083	0.0044	0.0089
Max RMS	0.0151	0.015	0.0199	0.0072	0.0285
Min ΔE2000	0.0005	0.0015	0.0014	0.0008	0.0015
Average ΔE2000	0.0556	0.0607	0.081	0.0764	0.045
Max ΔE2000	0.6879	0.7052	0.5961	0.2805	0.5169
High Patches	0.45%	0.44%	1.34%	5.88%	0.81%

It is possible to round trip reflectance spectra to and from each of the specific XYZPQR spaces, even those that were designed from other data sets. Table 2 shows one such case.

For visualization purposes the columns in the reconstruction matrices R & V can be expressed as spectral graphs. Figures 1 & 2 show results from two data sets.

 Table 2. Round Trip Results using Munsell Optimized

 Transform

	CMY	CMYK	CMYKOG	Agfa
Min RMS	0.0064	0.0004	0.001	0.0024
Ave RMS	0.0217	0.0187	0.0143	0.0249
Max RMS	0.0496	0.0498	0.0442	0.0848
Min ΔΕ2000	0.0039	0.0015	0.0034	0.0044
Average ΔE2000	0.0967	0.0903	0.0967	0.0729
Max ΔΕ2000	0.3356	0.3356	0.3982	0.2054
High Patches	0.60%	0.73%	0.22%	3.46%



Figure 1. R matrix columns for estimating XYZ+. Munsell data set left, Roland CMYKOG right



Figure 2. V matrix columns for estimating PQR. Munsell data set left, Roland CMYKOG right

The following two figures show LabPQR coordinates as scatter plots of two simultaneous projections of Lab and PQR coordinates.

Evaluating the Implementation

The round trip errors on PQR's customized to a particular dataset or printer were rather low. Even using a PQR space optimized for a different printer showed surprisingly robust results. The Munsell optimized transform performed best on other datasets. Table 2 shows it did not produce a Δ E2000 that exceeds 0.4. As expected, most RMS statistics in Table 2 are worse than those in Table 1. It is interesting to note that in one case, the Agfa dataset, the Munsell PQR transform actually produces a lower number of high RMS errors although mean and maximum are better in Table 1. Also interesting is the fact that in all cases the max Δ E2000 in Table 2 is smaller than the corresponding one in Table 1. Such negative interactions between RMS spectra and colorimetry have been noted before.⁷



Figure 3. Roland CMYKOG. L*a*b* left, PQR right.



Figure 4. Munsell dataset. L*a*b* left, PQR right.



Figure 5. Munsell using Roland CMYKOG transformation. L*a*b* left, PQR right.

From the curves (Figures 1&2) it can be observed that the Reconstitution matrices for the different data sets are consistent with each other with respect to XYZ+, and P. The Q and R curves show greater differences.

From the scatter plots (Compare figures 4 and 5) it can be observed that using different LabPQR transforms result in different PQR encodings for the same Lab encodings.

Spectral Gamut Visualization

Imagine that a list of every possible device count combination (i.e., CMYKOG) is obtained with the corresponding LabPQR coordinate that represents the spectra for each device count combination. Then collect together all PQR coordinates for points that have exactly the same Lab value. A plot of these PQR coordinates corresponds to the spectral gamut of a Lab color. It is as if the Lab Coordinate is magnified to reveal spectral PQR sub-gamut volumes (Figure 6). This mimics the concept of metamerism. It follows that PQR can be used to describe the metameric black¹¹ aspect of a spectrum.



Figure 6. Spectral Gamut Visualization/Mapping

Spectral Gamut Mapping using LabPQR

With a visualization of a spectral gamut in mind, spectral gamut mapping can be considered. Colorimetric gamut mapping techniques can be extended rather easily by thinking of Lab coordinates as PQR volumes rather than as points. From Figure 6 there are three cases that need to be considered in terms of spectral gamut mapping:

- 1. If a desired color's LabPQR is in the output space then the spectrum can be exactly reproduced. No gamut mapping is necessary.
- 2. If a desired LabPQR is not in the output space, but the Lab coordinate is in the output space, it can at least be represented colorimetrically under at least one illuminant. One possible way of performing spectral gamut mapping would be to find the closest PQR value that is within the spectral gamut. Since PQR corresponds to spectral error minimizing distance in PQR minimizes spectral error.
- 3. If the color is outside the colorimetric gamut then conventional gamut mapping techniques can be employed only using Lab coordinates.

Conclusions

Spectral Colorimetry is presented with definitions of color transforms for LabPQR. Several example transformations were demonstrated and observations were made. One of the key observations is that LabPQR provides a fairly accurate representation of the smooth reflectance spectra of the devices being characterized. It also transcends metamerism, and provides a convenient medium for performing Gamut Mapping since by definition it bridges colorimetry and spectral reflectance.

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Biography

Maxim Derhak received his B.S. in Computer Science from the University of Utah in 1991. For the past 14 years he has worked with Onyx Graphics helping to pioneer the development of short run large format image reproduction using electrostatic and ink jet technologies. He is currently a Senior Software Architect and representative for Onyx Graphics in the International Color Consortium. He is currently acting as chair for the ICC Architecture Working Group. He is working on his M.S. in Imaging Science in the distance learning program at RIT. This paper is the result of his masters project.