

Impact of Instrumental Bandpass on Spectral Quantities

Michael Rodriguez

Keywords: spectral, colorimetry, bandpass, tristimulus, graphic arts

Abstract

Colorimetric quantities calculated from spectral measurement data are essential metrics for assessing color reproduction. ISO 13655, the standard for spectral measurement and calculation in graphic arts, has heretofore specified a nominal spectral bandpass of 10nm for these measurements but has not addressed errors that arise under this condition. A revision of ISO 13655 will now recommend a spectral bandpass of 5nm to minimize the impact of bandpass error on tristimulus calculations.

However, an alternative to using devices with narrower bandpass is to apply “bandpass correction”, a subject of much research over the last three decades. The goal of this paper is to illustrate the nature of bandpass errors on graphic arts reflectance data, to review the key approaches for bandpass correction and to present simulations showing the reduction in colorimetric error that can be achieved. It is concluded that available methods for bandpass correction are effective, and should be specified in standards for spectral measurement and calculation.

Introduction

Researchers have investigated practical methods for accurate calculation of tristimulus values from spectral measurement data since the 1980’s [Billmeyer and Fairman (1987), Fairman (1995)]. Although CIE guidelines have long recommended the acquisition of spectral data at a wavelength interval and bandwidth of 5nm or less, economics have constrained most of today’s field devices to 10nm or 20nm. For graphic arts reflectance data, where colorimetry is based on the CIE D50 reference illuminant and 1931 standard observer, bandpass errors may be modest, up to 1 dE76 for 10nm and 4 dE76 for 20nm, if bandpass correction is not applied. For this reason, and due to lack of universally accepted methods for bandpass correction, no recommendation on this issue was incorporated into ISO 13655 (ISO, 2009) when it was last revised.

Independent color consultant

In recent years however, tolerances for color reproduction have tightened and errors due to bandpass may contribute significantly to overall colorimetric uncertainty. Hence there is good reason to now address this issue. A revision to ISO 13655, now in preparation, will recommend the use of devices with 5nm interval and bandpass to better align with CIE S014-3 (CIE, 2012). This standard recommends that, while 5nm provides acceptable results in many applications, data taken at 10nm or 20nm should be corrected for bandpass error.

Instrumental bandpass causes a convolutional smoothing in data measurements when the bandpass function is wide compared to the transitions in the actual reflection spectrum of a specimen. The resulting spread of spectral power causes errors in the numerical integration used to calculate tristimulus values. In general, the errors cannot be eliminated entirely, but, under certain conditions, mathematical techniques for correction can be quite effective.

There are two general approaches for bandpass correction. In the first, a deconvolution filter is applied to the measured data in an attempt to restore spectral detail that was lost through instrumental bandpass. CIE TC2-60 recently published a technical report, CIE 214 (CIE, 2014), which provides a thorough review of this type of correction. A filter of this type is now defined in ASTM E2729 (ASTM, 2009) and specified in ASTM E308 (ASTM, 2013) for correction of 10nm or 20nm data prior to tristimulus calculation.

The second method is based on introducing compensation into spectral weighting tables that are used to calculate tristimulus values. Spectral weighting tables combine color matching functions and illuminant to simplify the numerical calculation of tristimulus values. ASTM E308 (ASTM, 2013) has provided a standard practice since 1985 for calculation of tristimulus values at 10nm and 20nm using such tables. Research has shown that colorimetric errors due to instrument bandpass can be mitigated by linear least squares optimization of the weighting tables. CIE TC1-71 has investigated such computational methods, which are appropriate when actual corrected spectral data are not needed for other purposes. Prior to 2010, ASTM E308 had recommended the use of such optimized weighting factors, known as “Tables 6”, for calculating tristimulus values from uncorrected spectral data. CIE TC1-71 will soon publish a report and recommendations on this methodology.

Simulations in this paper are presented to illustrate the effectiveness of bandpass correction with the aforementioned techniques. A database of graphic arts spectral data measured with a 1nm bandpass instrument will serve as a baseline from which test data at 10nm and 20nm are derived mathematically using a triangular bandpass filter. Bandpass correction using methods described above are presented to show that worst case errors can be reduced from 1 dE76 to less than 0.04 dE76 for 10nm data, and from 4 dE76 to less than 0.5 dE76 for 20nm data.

Nature of instrumental bandpass

A common monochromator architecture used in spectrometers is illustrated in Figure 1. Reflected light from a sample at A enters at slit B, is focused on dispersive element D, and finally imaged upon an exit slit F. Rotation of the grating allows sequential collection of energy from various portions of the light spectrum at the exit slit. It is now common to use a photodetector array at F to capture all spectral components at once. The capture width of each photodetector element is analogous to the slit width.

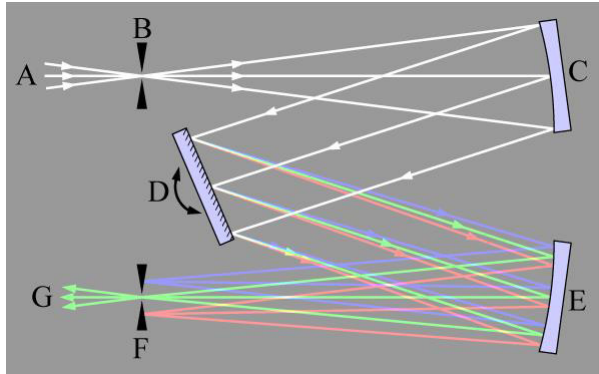


Figure 1. Basic architecture of a Czerny monochromator

The necessity of using spatial slits of a finite width for signal to noise requirements limits the accuracy with which spectral components at various wavelengths can be characterized. The result is that the spectral measurements will portray a smoothed profile in comparison to the true spectrum. As explained in CIE 214 (CIE, 2014), this smoothing can be characterized as a convolutional filtering of the actual spectrum. This is typically modeled as a triangular bandpass function for the case of equal sized entrance and exit slit widths with ideal optics and unity magnification. For non-equal slits, the function shape would be trapezoidal. In practice, imperfections and design details yield a bandpass function that is never perfectly triangular or trapezoidal. However, as further discussed in CIE 214, a triangular bandpass model serves as a good baseline for most spectral devices, giving results that deviate only slightly from more detailed models of bandpass functions.

The impact on spectral measurement with this model is illustrated in Figure 2 where a triangular bandpass function with a 20nm FWHM (full width half magnitude) bandwidth, when convolved with a 1nm spectrum, produces measured samples that give a smoothed characterization of a steep transition.

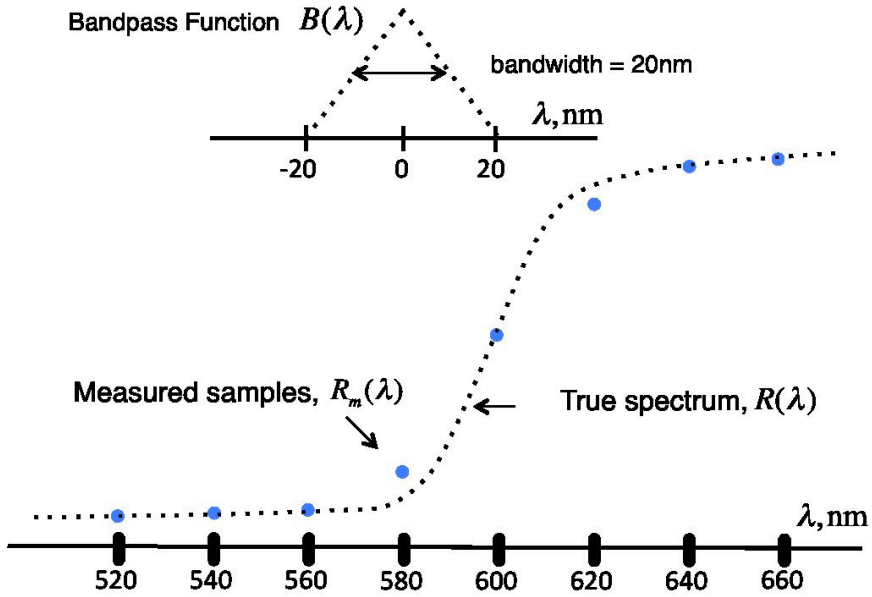


Figure 2: Illustration of smoothing of spectral detail due to instrumental bandpass. Actual 1nm spectrum (small black dots), when convolved with bandpass function, yields measured samples (solid blue dots).

Impact of bandpass on colorimetric accuracy

The smoothing of spectral detail has an impact on tristimulus calculation for an example illustrated in Figure 3. Samples of the spectral reflectance of a solid spot color, Pantone 806, are shown both at 1nm and 20nm interval and bandpass. The 20nm samples have a transition near 600nm that is less steep compared to the 1nm spectrum. This shift of spectral power results in errors in XYZ values calculated from numerical integration.

Tristimulus values were calculated for 1nm data per CIE S 014-3 (CIE, 2012) using the following numerical integration,

$$V = k \sum_{\lambda=380nm}^{780nm} R^1(\lambda) W_r^1(\lambda) \Delta\lambda \quad \text{for } V = X, Y, X \quad \text{and } \Delta\lambda = 1 \quad (1)$$

$R^1(\lambda)$ represents the 1nm data samples and $W_r^1(\lambda)$ represents the tristimulus weighting factors at 1nm, i.e. the product of the CIE 1931 observer color matching functions and the D50 illuminant at 1nm intervals. Tristimulus values for 20nm data are calculated using the following numerical integration,

$$V = k \sum_{\lambda=380nm}^{780nm} R_m^{20}(\lambda) W_r^{20}(\lambda) \Delta\lambda \quad \text{for } V = X, Y, X \quad \text{and } \Delta\lambda = 20 \quad (2)$$

$R^{20}(\lambda)$ represents the 20nm data samples and $W_r^{20}(\lambda)$ represents the 20nm spectral weighting factors found in Table 5.10 in ASTM E308 (ASTM, 2013), which defines the standard practice for tristimulus calculation at bandpass wider than 5nm. The weight tables in this standard have been derived to give results equivalent to interpolating data to 1nm and using 1nm weights to calculate tristimulus values.

Tristimulus values calculated as described above for the example in Figure 3 lead to CIELAB values of (60.3, 89.3, -11.3) for 1nm data and (60.7, 86.4, -9.3) for 20nm data. The differences between spectral plots appear modest on visual inspection, but there is a CIELAB colorimetric difference of 3.8 dE76. As suggested earlier, errors of this magnitude may add significant uncertainty to the tolerance requirements in modern color reproduction applications.

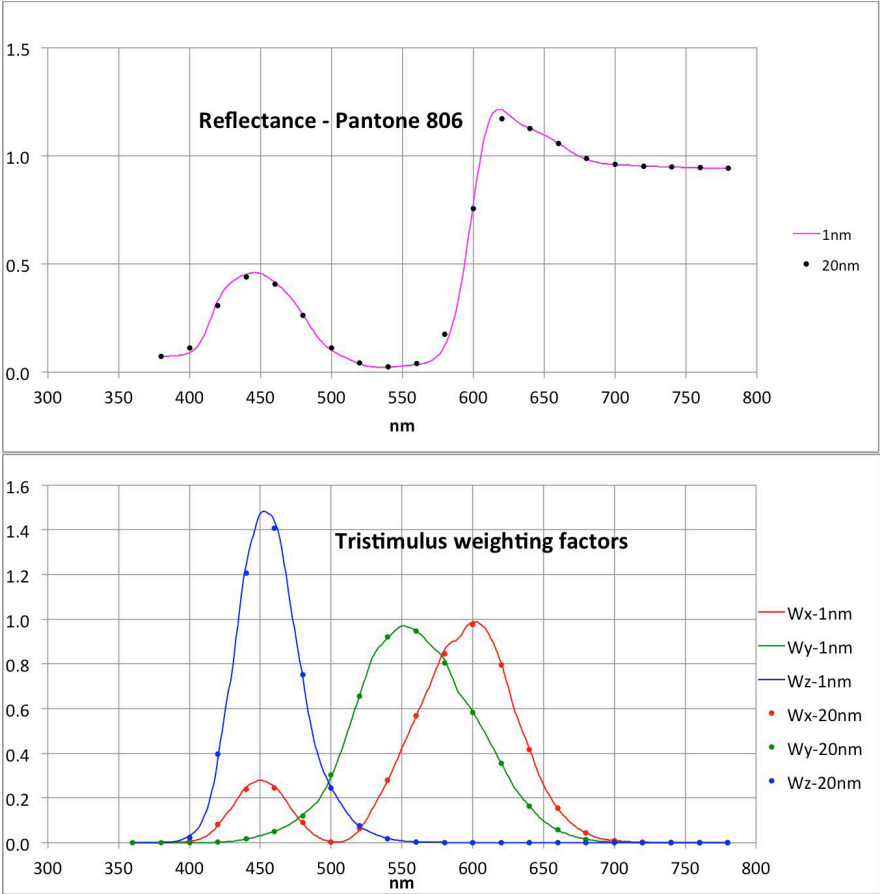


Figure 3. Impact of spectral bandpass error on tristimulus calculations. For D50 illuminant and tristimulus calculations per CIE S014-3 for 1nm data and ASTM E308 for 20nm data, the CIELAB error is 3.8 dE76.

Bandpass correction strategies

As implied in Figure 2, spectral measurements can be modeled as a convolutional distortion $B(\lambda)$ of reflectance $R(\lambda)$,

$$R_m(\lambda) = B(\lambda) * R(\lambda) \quad \text{Eq (3)}$$

where $*$ represents the convolution function. A linear filtering strategy may be used to determine a function $D(\lambda)$ that, when convolved with measurements, yields a corrected spectrum $R_c(\lambda)$ that approximates the true spectrum,

$$R_c(\lambda) = D(\lambda) * R_m(\lambda) = D(\lambda) * B(\lambda) * R(\lambda) \approx R(\lambda) \quad \text{Eq (4)}$$

The goal is to find a “deconvolution” filter $D(\lambda)$ such that $D(\lambda) * B(\lambda)$ is close to a convolutional identity function, e.g. a unit impulse. This intuitively means that $D(\lambda)$ will be a sharpening filter that compensates for the smoothing effect of the bandpass function.

The development of bandpass deconvolution for spectral measurement data originated with Stearns and Stearns (1985). This work assumed a triangular bandpass function and a spectrum that can be modeled by quadratic curves, a reasonable assumption for graphic arts reflection data. Refinements by Ohno (2005), Gardner (2006), and Fariman (2009) have led to ASTM E2729 (ASTM, 2009), the standard practice for bandpass correction. This method is specified in ASTM E308 (ASTM, 2013) for calculating tristimulus values with 10nm and 20nm data. The methodology has been further analyzed and formalized by CIE TC2-60 and published in technical report CIE 214 (CIE, 2014). In this report the method is termed “weighted-mean bandpass correction” to distinguish it from other algorithms for used for deconvolution.

Figure 4 illustrates the essence of the method. A deconvolution filter such as the one pictured and taken from ASTM E2729 tends to sharpen spectral transitions, effectively reversing the smoothing cause by the instrumental bandpass. The correction will generally not be perfect but can be effective in reducing errors in tristimulus calculations as will be seen in simulations later in this paper.

An alternative strategy for bandpass correction focuses more directly on the reduction of colorimetric error caused by instrument bandpass. Insight for this method is gleaned by considering the general formula for calculating tristimulus values from measurements in Eq (2) and inserting the effect of bandpass from Eq (3) to give,

$$V = k \sum [B(\lambda) * R(\lambda)] W_V(\lambda) \Delta\lambda \quad \text{for } V = X, Y, Z \quad (5)$$

Linearity of the convolution process within the numerical tristimulus integration allows an alternate representation of Eq (5) as,

$$V = k \sum R(\lambda) [B(\lambda) * W_r(\lambda)] \Delta\lambda \quad \text{for } V = X, Y, Z \quad (6)$$

This reformulation indicates that, from the point of view of tristimulus calculations,

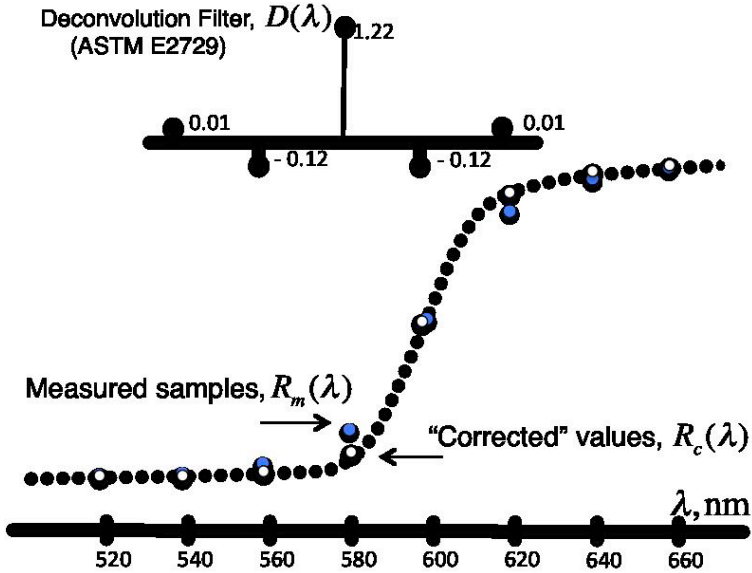


Figure 4. Bandpass correction via deconvolution. A 5-point sharpening filter, as specified in ASTM E2729, is convolved with measurement data (solid blue dots), to produce corrected values (open white dots).

the impact of bandpass can be modeled as an equivalent distortion of the tristimulus weighting factors. Thus, as an alternative to deconvolution of measurement data, one may introduce compensation into the tristimulus weights to counteract the impact of bandpass on colorimetric error.

This approach, which has been termed “optimized tristimulus weights”, was originally developed by Venable (1988). Rather than correct the measured spectral data, the goal is simply to reduce error in tristimulus values by introducing compensation into the weighting factors used in the numerical integration. This has the advantage of including the illuminant in the optimization. However it has the disadvantage of not providing a corrected spectrum. The methodology has been refined, formalized and published by Li (2008, 2014, 2015) as part of the work of CIE TC 1-71. A CIE report is expected in the near future.

The mathematics of this optimization is beyond the scope of this paper, but is fully detailed in Li (2015). In essence, a least squares method is used to find weights that, when smoothed by the triangular bandpass function, best approximate the nominal weights for tristimulus calculation. It is observed that this optimization produces

weights with a “sharpened” spectral profile compared to nominal weights, analogous to what occurs in the deconvolution method with reflectance data.

Figure 5 illustrates the concept. Though subtle to see in the plots, the optimized weighting factors are “sharpened” compared to the nominal weighting factors as seen in Figure 4. This is a result of the least squares optimization providing compensating for bandpass smoothing as modeled in Eq (6).

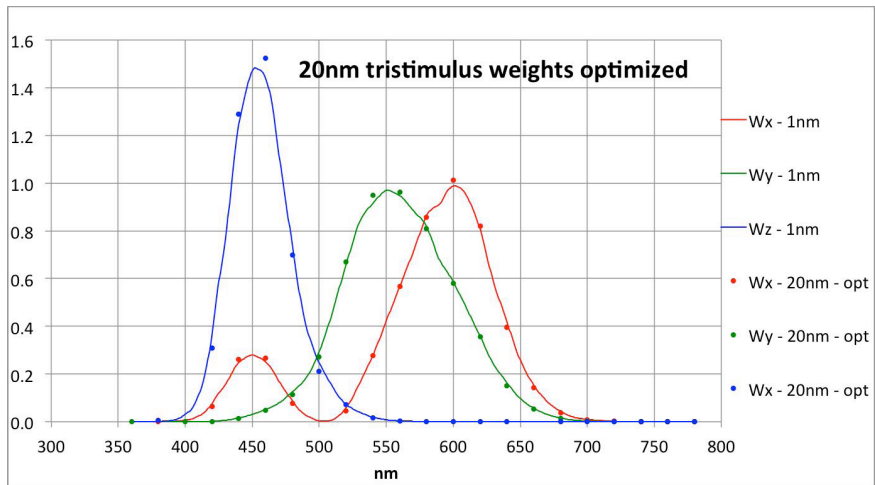


Figure 5: Illustration of tristimulus weights optimized for 20nm bandpass using the method described in Li (2015). It can be seen that the weights are sharpened, in comparison to the 1nm weights, to compensate for the spectral data smoothing caused by bandpass.

Simulations of bandpass correction

Past simulations by researchers have used various graphic arts databases as well as different observers and illuminants in performing simulations for bandpass correction. Simulations in this study included only one database, a collection of 1124 Pantone spot color spectral data that represents the range of colors encountered in commercial print. Also, the tristimulus calculations in this study used only the CIE 1931 observer and the D50 illuminant in order to provide the framework most familiar in graphic arts print applications. The following CIELAB dE76 error statistics compare tristimulus calculations at 1nm, as specified in CIE S014-3 (2012), to calculations at 5m, 10nm and 20nm as specified in ASTM E308 (2013). The data interval and bandpass of 1nm data was widened to 5, 10, or 20nm using a triangular function as is specified in Annex E of ISO 13655 (ISO, 2009). Table 1 illustrates colorimetric error reduction achieved for these data using deconvolutional and tristimulus weight optimization methods described in the previous section.

Bandpass	Bandpass correction - 1124 Pantone samples		
	dE76 avg/max relative to 1nm calculations, 360-780nm		
	No Correction XYZ per ASTM E308	ASTM 2729 Correction XYZ per ASTM E308	Optimum weights XYZ per Li (2015)
5nm	0.06 / 0.24	0.005 / 0.008	0.0001 / 0.0002
10nm	0.27 / 1.01	0.010 / 0.039	0.002 / 0.004
20nm	1.15 / 4.31	0.151 / 0.533	0.032 / 0.140

Table 1. Reduction of colorimetric error using bandpass correction for 5nm, 10nm and 20nm data compared to original 1nm data.

While beyond the scope of this study, it should be noted that for illuminants such as fluorescents, which have extremely narrow spectral spikes, bandpass correction may not be as effective as shown in the above table. This is because small residual spectral errors that are inevitable in any bandpass correction strategy can be amplified greatly by narrow spikes in the weighting factors used in tristimulus calculations.

Discussion

In Table 1 note that, for 5nm data with no bandpass correction, errors are quite small, less than 0.25 dE76. While not entirely negligible, this level of error tends to confirm the adequacy of 5nm bandpass for graphic arts reflectance data as has been suggested in CIE recommendations. However, the simulations indicate that even these small levels of error can be reduced with bandpass correction.

For the calculations performed with on 10nm and 20nm data with no bandpass correction, CIELAB colorimetric errors range up to 1.0 dE76 for and 4.3 dE76 respectively. The simple 5-point deconvolution filter specified in ASTM E2729 reduces these maximum errors to about 0.04 dE76 and 0.53 dE76 respectively, an order of magnitude improvement. This level of improvement is consistent with other reported studies using this deconvolution methodology for bandpass correction.

The results also suggest that the method of optimized weights achieves slightly better error reduction than the deconvolution method. This has been confirmed in a range of simulations performed in Li (2015) that include several databases and a variety of combinations illuminants and observer functions. This observation can be expected since the algorithm is aimed directly at reducing colorimetric error and includes the assumed bandpass function as well as the illuminant spectrum in the optimization process. The advantage of this slightly smaller residual error is offset by the fact that the method does not provide a corrected reflectance spectrum, as does the deconvolution method.

It is anticipated that new developments in both deconvolution and weight optimization methods will provide customization of the algorithms to incorporate detailed models of the bandpass function. This can be useful since many spectral devices do not have a perfectly triangular bandpass function due to instrument design and manufacturing details.

Most modern portable spectrophotometers for graphic arts provide 10nm to 20nm physical bandpass. The simulations presented here indicate it is possible to eliminate much of the colorimetric error introduced at those conditions of instrumental bandpass. It would seem that universal adoption of bandpass correction could provide significant improvement in accuracy and inter-instrument agreement for this industry.

Conclusion

A consideration of practical limitations in spectral data measurement illustrates how instrumental bandpass can smooth spectral detail and lead to error in the calculation of tristimulus values. Two methods for bandpass correction are reviewed: deconvolution of raw spectral measurement data, and the optimization of spectral weighting functions used for tristimulus calculation. Simulations are presented indicating that errors may be significantly reduced for typical graphic arts reflectance data without having to resort to narrower bandwidth instrumentation. Bandpass correction should be specified in standards for spectral measurement since it could contribute to inter-instrument agreement for devices having bandpass wider than the CIE recommended maximum of 5nm.

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Acknowledgements

The author thanks Danny Rich (Sun Chemical), John Seymour (QuadTech), Changjiun Li (University of Science and Technology Liaoning, Anshan, China) and James Gardner (Thornleigh, Australia) for technical support.