An LED based spectrophotometric instrument

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ABSTRACT
The performance of an LED-based, dual-beam, spectrophotometer is discussed. The difficulty with producing an LED based instrument in the past has been the limited choice of LEDs, particularly in the blue/green region. Recent advances in LED technology have made such a device possible. The instrument discussed uses commercially available LEDs and other off-the-shelf electronic components which results in a low cost durable device. A mathematical model of the device is constructed, and the sources of deviations from this model are discussed.

Keywords: Spectrophotometer, Colorimeter, LED

1. INTRODUCTION
The availability of LEDs at wavelengths that span the visible spectrum make possible the construction of a spectrophotometer which uses LEDs as the sole illumination. The ColorMouse Too! is an example of a 45/0 LED based instrument. The device is shown in Figure 1.

The ColorMouse Too! is a dual beam instrument. One photo-detector measures light from the LEDs and a second photo-detector measures the diffuse reflectance of the LED light from the sample under measure. A ratio of these two measurements provides a measurement which is less sensitive to LED output variations compared to a single beam instrument.

In this paper, we will discuss the performance of this instrument. A mathematical model of the instrument is used to present theoretical performance levels. The model has proven useful in the determination of various error sources which are also discussed.

Figure 1. The ColorMouse Too!
2. MATHEMATICAL MODEL

Optical measuring instruments can be mathematically modeled with the vector space notation\textsuperscript{1,2,4} which has proven useful in solving difficult color reproduction problems. Examples of its use can be seen in color filter design,\textsuperscript{3,6,10,8,7} color sampling,\textsuperscript{5} and device profiling.\textsuperscript{9} For the optical measuring instrument, a vector space model facilitates an understanding of the physical processes taking place in the instrument and provides a way to determine the source of errors in the device.

In the vector space notation, the visible spectrum is mathematically uniformly sampled at $N$ points. The LED based instrument with $M$ spectrally unique LEDs can then be modeled as

$$m = GS^TDr + b + n$$

where $m$ is an $M \times 1$ vector representing the recorded values, each column of the $N \times M$ matrix $S$ contains the spectral power distribution of an LED, the $N \times N$ diagonal matrix $D$ represents the photo-detector spectral sensitivity, the $N \times 1$ vector $r$ represents the spectral reflectance of the sample being measured, the $M \times 1$ vector $b$ is a bias vector, the $M \times M$ diagonal matrix $G$ accounts for the gain settings in the device.

Other instruments can be modeled using a similar notation. For example, an instrument which has poly-chromatic illumination and achieves spectral separation with filters over multiple photo-detectors can be modeled as

$$m = GS_d^T Lr + b + n$$

where the diagonal matrix $L$ represents the spectral power distribution of the illumination, the $i$th column of the matrix $S_d$ contains the vector representing the spectral sensitivity of the $i$th detector combined with the filter transmittance. If the diagonal matrix $D_i$ represents the $i$th detector sensitivity and the transmittance of the filter over that detector is $f_i$, then the $i$th column of the matrix $S_d$ is given by

$$s_i = D_i f_i.$$  

If an instrument is to be designed as a colorimeter, then it is necessary to map the measured values $m$ into a CIE color space. The CIE tristimulus value for a reflectance sample $r$ under illuminant $L_v$ is given by

$$t = A^TL_v r,$$

where the columns of $A$ contain the sampled CIEXYZ color matching functions. The determination of a mapping from $m$ to $t$ is an optimization problem which can be posed as

$$\mathcal{F} = \arg(\min_{\gamma} E\{|\gamma(m) - L(t)|^2\})$$

where $L$ is a mapping from CIEXYZ to a perceptually uniform color space and $E\{}$ is the expected value operation.

Due to the nonlinear function $L$, this problem is usually solved by numerical methods. Alternatively, the mapping $L$ can be locally approximated by a linear function which will lead to a sub-optimal transformation that can be analytically determined.\textsuperscript{8} In this case, the analytical solution to the problem of mapping the LED based measurement values is given by

$$\mathcal{F}(m) = B_L m$$

where

$$\text{vec}(B_L) = \left[(M^T \otimes I_3) S_r (M \otimes I_3) + S_n \right],$$

$$S_r = E\{(rr^T) \otimes (J_L^T (t(r)) J_L (t(r)))\},$$

$$S_n = E\{K_n \otimes (J_L^T (t(r)) J_L (t(r)))\},$$

$$K_n = E\{nn^T\},$$

$I_3$ is the $3 \times 3$ identity matrix, $J_L (t(r))$ is the Jacobian matrix of the transformation $L$ at $t(r)$, $M^T = GS^T D$, vec() stacks the columns of a matrix into a vector, and $\otimes$ is the Kronecker product operator.
If the problem is solved with $L$ as the identity function and the mapping $F$ as a matrix, then another sub-optimal analytical solution to the optimization problem for the LED based instrument is given by

$$F(m) = B_A m$$

(4)

where

$$B_A = A^T L_n R_r M [M^T R_r M + K_n]^{-1}$$

and $R_r = E\{rr^T\}$.

3. SIMULATED PERFORMANCE

With the model in the above section, it is possible to simulate the LED based unit and determine how well it should perform for a given signal-to-noise ratio (SNR) using the mapping methods discussed in the previous section. While the noise of the unit is a Poisson process we will use a Gaussian approximation. In addition, it is assumed that the noise is uncorrelated between channels (i.e. $K_n$ is a diagonal matrix).

To model the device, it is necessary to determine the model parameters. These parameters are the detector spectral sensitivity $D$, the LED spectral power distributions $S$, the gain matrix $G$, and the bias vector $b$. The detector spectral sensitivity was determined by measuring the response of the photo-detector using a chromatic source generator and a PhotoResearch PR-704 spectroradiometer. A plot of the sensitivity is shown in Figure 2. The $M = 8$ LEDs were measured using the PhotoResearch PR-704 spectroradiometer, providing the matrix $S$. The spectral power distribution of the LEDs are shown in Figure 3. Determination of the vector $b$ and the diagonal matrix $G$ were made by measuring a known black and white reference.

At this point, we have a model for the LED based instrument. To simulate the unit, two sets of spectral reflectances were measured with an X-Rite 938 spectrophotometer. The first set served as the training set while the second set served as the testing set. The training set consisted of 200 reflectance samples coming from a variety of processes including Pantone colors and other ink on paper samples. The testing set consisted of 12 BCRA ceramic tiles (a color standard from the Hemmendinger Color Laboratory) which are often used as a standard for quantifying instrument performance.

The training samples were used to determine an estimate for the correlation matrix $R_r$ and the matrix $S_r$ (cf. Eq. (3) and Eq. (5)). Using these estimates for $R_r$ and $S_r$, the matrix mappings given in Eq. (2) and Eq. (4)
Figure 3. Relative Spectral Power Distribution of LEDs.

were each determined for various SNRs. The function $\mathcal{L}$ was the mapping from CIEXYZ to CIELAB. SNR was defined as

$$SNR = 10 \log \frac{E\{m^Tm\}}{E\{n^Tn\}}$$

(6)

where $E\{m^Tm\}$ was estimated using the 200 testing samples.

The values $m_i = GS^TDr_i + b + n_i$ were computed for several noise levels, which provided the simulated recorded value for reflectance sample $r_i$. The ideal CIEXYZ value was also computed using

$$t_i = A^T L_e r_i.$$

The mappings which were optimal for the particular SNR were applied to the recorded values, giving the estimates

$$\hat{t}_\mathcal{L} = B_\mathcal{L} m_i,$$
$$\hat{t}_A = B_A m_i.$$

The CIELAB $\Delta E$ errors were computed between $t_i$ and the estimates. The results are given in Table 1.

Table 1. Modeled Performance of LED based instrument at various SNRs

<table>
<thead>
<tr>
<th>SNR</th>
<th>Transformation $B_\mathcal{L}$</th>
<th>Transformation $B_A$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>average $\Delta E$</td>
<td>max $\Delta E$</td>
</tr>
<tr>
<td>30</td>
<td>5.27</td>
<td>18.96</td>
</tr>
<tr>
<td>40</td>
<td>1.81</td>
<td>4.89</td>
</tr>
<tr>
<td>50</td>
<td>0.70</td>
<td>2.41</td>
</tr>
<tr>
<td>60</td>
<td>0.52</td>
<td>2.43</td>
</tr>
</tbody>
</table>

Note that the theoretical performance of this device is quite good for SNRs of 40dB and above. The question is how good is the device in reality, and what is the source of any discrepancies with the model.
4. ACTUAL PERFORMANCE & ERROR SOURCES

The usefulness of the model comes in comparing the actual measurements from the unit with the measurements predicted in the model. Discrepancies between the two can lead to the determination of various error sources.

By comparing the model values \( m_i \) to the actual measures from the instrument, a significant error source was traced to sample fluorescence. In particular, fluorescence was observed on the orange BCRA tile. The fluorescence in this case is from the blue region of the visible spectrum into the near infrared region of the spectrum. A device such as the X-rite 938 or GRETAG SPM60 which both have poly-chromatic illumination will not be affected by the small amount of fluorescence. The LED based instrument is greatly affected however, since the photo-detector has a large sensitivity in the IR region (cf. Figure 2). Hence the model values predicted for the orange BCRA sample and the blue LEDs were much smaller than what was observed from the actual instrument. The existence of fluorescence in the orange BCRA was verified by illuminating the orange BCRA tile with a blue light source, and measuring the reflecting radiation with the PR-704. The light source itself was also measured with the PR-704, along with the light reflected from the yellow BCRA tile for comparison. These tiles were also measured with a GRETAG SPM60 spectrophotometer. Figure 4 demonstrates the sample fluorescence. Note the energy appearing above 700nm for the orange BCRA tile when the blue LED illuminates the sample. This does not occur on the yellow sample. The problem of the unit being sensitive to IR radiation was solved by the inclusion of an IR filter in the optical path. These filters are stable, well-behaved, and inexpensive. This solution reduced the CIELAB \( \Delta E \) error on the orange BCRA tile from over 17 to a value under 5.

Further comparison of the model predicted values with those observed from the instrument revealed additional errors on certain BCRA samples, in particular the orange, yellow, and red samples. Figure 5 illustrates this error, where the model predicted values are denoted by x’s and the actual values are denoted by o’s. These values in the figure are centered at the peak wavelengths of their respective LEDs. Note that the model is predicting more light than the actual device is “seeing” (i.e. the x’s are above the o’s).

It is believed that this discrepancy may be due to lateral diffusion error which is related to how the illumination spot size compares to the view the detector has of the sample. Altering the size of the spot illumination and reducing the amount of light scattered in the device improved the amount to which the model and the instrument agreed. After these optical changes, and remeasuring the same sample we obtain the model/instrument agreement shown in Figure 6. Correction of the optical problem has led to performance given in Table 2.

Errors can also occur due to noise and unit drift. To quantify the significance of these error sources in the actual instrument, a series of repeated measurements were performed on a black sample and on a white sample. The black
Figure 5. Model vs Instrument when measuring yellow BCRA Tile

Figure 6. Model vs Instrument when measuring yellow BCRA Tile after optical changes
sample had an average reflectance of 0.5% and the white sample had an average reflectance of 75%. Eight hundred measurements were performed, which is greater than the set of samples in the large IT8 target used for profiling a four-color (cmyk) printer.

A time dependent model for the $\Delta E$ error can be expressed as

$$\Delta E(t) = \Delta E_0 + d_{\Delta E}(t) + n_{\Delta E}(t)$$

(7)

where $\Delta E(t)$ is the $\Delta E$ error at time $t$, $n_{\Delta E}(t)$ is the error caused by additive noise, $d_{\Delta E}(t)$ is the error caused by unit drift, and $\Delta E_0$ is the noise free $\Delta E$ error at time $t = 0$. Figures 7-12 display the $\Delta E$ error as a function of time where the error is split into a drift and noise component using a 10 tap FIR filter.

The standard deviation on the noise induced portion of the $\Delta E$ error was 0.09 for the black sample and 0.01 for the white sample. It is noted that the signal in Figure 9 is nonstationary. The cause of this may be due to temperature changes in the unit, which is also the source of the unit drift. It is clear from these measurements that unit drift is more significant than the Poisson and thermal noise in the unit. However, in terms of $\Delta E$ error, the drift over such a large number of measurements is not excessive.

Finally, it is useful to relate the actual noise levels in the unit with an SNR value which will allow a comparison of the results of Table 1 with Table 2. Using the repeated measurements from the black and white sample it is possible to compute an SNR using Eq. 6 where $E\{m^T m\}$ is replaced by the power in the black or white LED measurements (e.g. replace $E\{m^T m\}$ with $m_w^T m_w$ where $m_w$ is the LED measurements for the white sample; the SNR will be dependent upon the sample under measure). In this case, each LED is modeled in a fashion similar to that given in Eq. 7 and due to the short number of measurements over which the BCRA samples are measured, the noise power of the term $n$ (cf. Eq. 1 ) is equated to the power of the nondrift noise sources (i.e. the drift is negligible over the 12 BCRA measurements). In this case, the SNR is computed as 38dB on the black sample and as 73dB on the white sample. The transformations used to compute the data in Table 2 assumed a SNR level of 60dB (i.e. $K_n$ was adjusted accordingly in both transformations).
Figure 7. $\Delta E(t)$ for white sample

Figure 8. $d\Delta E(t)$ for white sample
Figure 9. $abs(n_{\Delta E}(t))$ for white sample

Figure 10. $\Delta E(t)$ for black sample
Figure 11. $d_{\Delta E}(t)$ for black sample

Figure 12. $abs(n_{\Delta E}(t))$ for black sample
5. CONCLUSION

The performance of a low-cost LED-based colorimeter/spectrophotometer was discussed. The actual performance was compared to a mathematical model of the device which was of assistance in determining error sources. The current performance level is approaching that achieved by costlier and more sophisticated instruments. The cost/performance ratio of the instrument is such that it is an ideal solution for applications requiring accurate and repeatable color measurements.

REFERENCES