Update to Evaluation of Reference Materials for Standardization of Spectrophotometers

John Seymour
John the Math Guy, LLC
Warning!
This presentation contains mathematical material which may not be suitable for people with math phobia.
Statement of the problem
I’m trying to keep the math simple.
Statement of the goal
Standardization

*Standardization* is the process of adjusting measurements taken from one device to better match measurements taken from another.
Standardization, first step
Cast (in order of appearance)

Golden instrument

Silver instrument

Standardization set

Wicked smart standardization algorithms
The focus of this paper
How well do wicked smart standardization algorithms work on certain potential standardization sets?
Why do instruments disagree?

- Repeatability
- Black level
- Rejection of scattered light
- White level
- Measurement geometry
- Nonlinearity
- Aperture size
- Wavelength alignment
- Bandwidth difference
- Fluorescence
Why do instruments disagree?

- Repeatability
- Black level
- Rejection of scattered light
- White level
- Measurement geometry
- Nonlinearity
- Aperture size
- Wavelength alignment
- Bandwidth difference
- Fluorescence
Why do instruments disagree?

- Repeatability
- Black level
- Rejection of scattered light
- White level
- Measurement geometry
- Nonlinearity
- Aperture size
- Wavelength alignment
- Bandwidth difference
- Fluorescence
Why do instruments disagree?

- Black level
- White level
- Nonlinearity
- Wavelength alignment
- Bandwidth difference
Potential standardization formula

- Black level
- White level
- Nonlinearity
- Wavelength alignment
- Bandwidth difference

\[ R_c(\lambda) = R_m(\lambda) + \beta_1(\lambda) + \beta_2(\lambda)R_m(\lambda) \]

Measurement to correct

Black level correction

White level correction
Potential standardization formula

- Black level  \( \beta_1(\lambda) \)
- White level  \( \beta_2(\lambda)R_m(\lambda) \)
- Nonlinearity  \( \beta_5(\lambda) \left( (1 - R_m(\lambda))R_m(\lambda) \right) \)
- Wavelength alignment  \( \beta_3(\lambda) \frac{dR_m(\lambda)}{d\lambda} \)
- Bandwidth difference  \( \beta_4(\lambda) \frac{d^2R_m(\lambda)}{d\lambda^2} \)
## Five mathematical models

<table>
<thead>
<tr>
<th></th>
<th>Model #1</th>
<th>Model #2</th>
<th>Model #3</th>
<th>Model #4</th>
<th>Model #5</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Black level</strong></td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td><strong>White level</strong></td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td><strong>Nonlin</strong></td>
<td></td>
<td></td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td><strong>Wavelength shift</strong></td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td><strong>Bandpass</strong></td>
<td></td>
<td>X</td>
<td></td>
<td></td>
<td>X</td>
</tr>
</tbody>
</table>
Potential standardization sets

ChromaChecker

Lucideon Print Standards
Uses for reference materials

- Verify spectro hasn’t changed
- Assess inter-instrument agreement?
- Standardize one instrument to another???
Requirements for a standardization set

- Durable
- Fade resistant
- Opaque
- Similar surface to samples to measure
- Multiple reflectance values
One example – not so good
Requirements for a standardization set

- Durable
- Fade resistant
- Opaque
- Similar surface to samples to measure
- Multiple reflectance values
- Lots of transitions at all wavelengths
Looks pretty good, right??

Not much going on here

Not so good for wavelength stuff here
Derivatives show less variety
Less tiles, but perhaps enough variety?
Derivatives have a bit more variety
How can we quantify the amount of variety that a set of samples has?
Linear algebra

\[
\begin{bmatrix} 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}
\]

No solution. \( x + y \) would have to be equal to both 3 and 4.
Linear algebra

\[
\begin{bmatrix}
3.0 \\
4.0
\end{bmatrix}
= 
\begin{bmatrix}
1.00 & 1.00 \\
1.00 & 1.01
\end{bmatrix}
\begin{bmatrix}
x \\
y
\end{bmatrix}
\]

Solution: \( x = -97 \) and \( y = 100 \)

Changing this by 0.01 meant the equation could be solved.
Linear algebra

\[
\begin{bmatrix}
3.0 \\
4.0
\end{bmatrix}
= \begin{bmatrix}
1.00 & 1.00 \\
1.00 & 1.01
\end{bmatrix}
\begin{bmatrix}
x \\
y
\end{bmatrix}
\]

Solution: \( x = -97 \) and \( y = 100 \)

The equation can be solved, but the solution is very sensitive.

\[
\begin{bmatrix}
3.01 \\
3.99
\end{bmatrix}
= \begin{bmatrix}
1.00 & 1.00 \\
1.00 & 1.01
\end{bmatrix}
\begin{bmatrix}
x \\
y
\end{bmatrix}
\]

Solution: \( x = -94.99 \) and \( y = 98 \)

The equation is numerically instable.
Quick look back

We expect there might be some numerical instability in this region.
Numerical stability of the ChromaChecker set
Numerical stability of the ChromaChecker set

- The magnification is huge
- Small measurement errors will go berserk
- Models including bandwidth are worst
- Wavelengths above 600 nm are worst
Is the Lucideon set any better?
First conclusion

- Neither set can be used to standardize one instrument to another if bandwidth is part of the model.
- Is there a possible set?
- Additional sets tested: Behr paint ramps, BCRA tiles, Munsell Color Checker, Pantone primaries, Sherwin-Williams paints
Best of set found

Error magnification is still a deal-breaker
First conclusion, amended

- It is unlikely to find a standardization set that will allow standardization for instrument bandwidth.
Can we standardize with models that don’t include the bandwidth correction?
Standardization sets without bandwidth correction

ChromaChecker (full set) Error Magnification

Safe region

My proposed cut-off

Lucideon Error Magnification

Safe region
Second conclusion

- If we use mathematical models that include
  - *black level*,
  - *white level*,
  - *wavelength shift*, and
  - *nonlinearity*,
- the two potential standardization sets will *only* work for a range of wavelengths.
Is there any hope?
A set that could work for standardization

- A combination of the Lucideon set and the Munsell Color Checker is numerically stable.
- Munsell is not durable.
- There is hope that a durable and stable standardization set can be made.
Thank you for braving the math!

John Seymour
John the Math Guy
john@johnthemathguy.com