Simulating effects of unknown correlations in spectral data on uncertainties of TOC derived from multispectral measurements

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Uncertainty of spectrally derived quantities

- Quantities such as Color Coordinates $x$ and $y$, color temperature $CCT$, and amount of ozone $TOC$ are calculated using measured spectra.
- Uncertainties of spectral irradiance values at different wavelengths are correlated, but mostly we do not know how.
- New approach: form spectral functions that simulate different scenarios that the correlations may have.
- Monte Carlo analysis with the functions gives uncertainty values.
- Two steps:
  - First develop methods for $x$, $y$ and $CCT$ (more familiar, possibility to compare).
  - Extend to TOC.
- Progress with colorimetry.
Preliminary work with FEL lamps

- Analyse uncertainties of color coordinates of Aalto spectral irradiance lamps
- $x$, $y$ derived from spectrum as integrals

- Form a distorted spectrum
  \[ E_e(\lambda) = (1 + \epsilon \delta(\lambda) u_E(\lambda)) E(\lambda) \]
  - $u_E(\lambda)$ is the relative uncertainty of $E(\lambda)$
  - $\delta(\lambda)$ is an error function with $\sigma = 1$.
  - $\epsilon \sim N(0,1)$ is a Monte Carlo variable
- The error function is formed as sum of cosines

\[
X = \int_{\lambda_1}^{\lambda_2} E(\lambda) \tilde{x} d\lambda, \\
Y = \int_{\lambda_1}^{\lambda_2} E(\lambda) \tilde{y} d\lambda, \\
Z = \int_{\lambda_1}^{\lambda_2} E(\lambda) \tilde{z} d\lambda, \\
x = X/(X + Y + Z), \text{ and} \\
y = X/(X + Y + Z),
\]
Error function from orthogonal base-functions in $[\lambda_1, \lambda_2]$

- The error function is formed as
  \[ \delta(\lambda) = \gamma_1 f_1(\lambda) + \gamma_2 f_2(\lambda) + \gamma_3 f_3(\lambda) + \gamma_4 f_4(\lambda) \]
- $\gamma_1 - \gamma_N$ are Monte Carlo variables.
- To get standard uncertainties, it must be that $\gamma_1^2 + \gamma_2^2 + \gamma_3^2 + \gamma_4^2 = 1$
- This can be accomplished by taking a random point in $N$-dimensional spherical coordinate system, and using its $x, y, z, \ldots$ coordinates as the weights
- The base functions have been chosen so that their RMS-value is 1 in $[\lambda_1, \lambda_2]$
- \[ E_e(\lambda) = (1 + \varepsilon \delta(\lambda) u_E(\lambda)) E(\lambda) \]

\[
\begin{align*}
  f_1(\lambda) &= \frac{2}{\sqrt{\pi}} \sin \left( 1 \left( 2\pi \frac{\lambda - \lambda_1}{\lambda_2 - \lambda_1} + \phi \right) \right) \\
  f_2(\lambda) &= \frac{2}{\sqrt{\pi}} \sin \left( 2 \left( 2\pi \frac{\lambda - \lambda_1}{\lambda_2 - \lambda_1} + \phi \right) \right) \\
  f_3(\lambda) &= \frac{2}{\sqrt{\pi}} \sin \left( 4 \left( 2\pi \frac{\lambda - \lambda_1}{\lambda_2 - \lambda_1} + \phi \right) \right) \\
  f_4(\lambda) &= \frac{2}{\sqrt{\pi}} \sin \left( 8 \left( 2\pi \frac{\lambda - \lambda_1}{\lambda_2 - \lambda_1} + \phi \right) \right)
\end{align*}
\]
Preliminary results

- Simulation of uncertainties of colorimetric properties of Aalto lamps
- With 10 000 runs
- Individual base functions give maxima at $f_1$ – $f_2$ and reduce to negligible at $\sim f_5$
- Cumulative uncertainties sound reasonable

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Plan for further work

• Half wave, quarter wave, and full correlation should be considered as well and added to the model
• Simulations give maksimum uncertainties and conditions leading to them
  – How will the maxima convert to standard uncertainties?
  – How should the components to include be selected?
    • Go through all scenarios?
    • Select the most likely base functions?
• Compare with earlier work of Jim Gardner of CSIRO
• After knowing that the model works, apply to Ozone measurements
  – How should the base functions then be selected? The wavelength range 290 – 320 is significantly narrow, there can not be many sign changes.