Group theoretical investigations of daylight spectra

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Abstract

Understanding the properties of spectral distributions of daylight and its dynamical changes at different sites with varying atmospheric conditions is an active research area. Results obtained in these studies are of interest in many fields such as color vision, meteorology, biology, photography, etc... Many efforts to measure and model daylight spectra originate in the 60s [1, 2, 3, 4, 5]. The SMARTS model [6] is one example of recent tools to compute clear sky spectral irradiance from a description of atmospheric conditions, time and solar geometries. In this paper we describe our investigation of daylight spectra based on the principal component analysis (PCA) of spectra. We will show that the structure of the space leads to the well-known Poincaré disk model of hyperbolic geometry. The natural group **SU(1,1)** operating on the disk is then used to model the PCA representations of measured daylight spectra sequences and spectra generated by the SMARTS model.

1. Introduction

In this paper, we will describe our investigations of sequences of spectral distributions. Daylight illumination spectra sequences are typical examples and their properties will be described in the experimental part.

The daylight spectra (either measured spectra or sequences of modelled spectra generated from simulation programs such as SMARTS) investigated in this paper are special examples of spectral distributions in general. By a spectral distribution we mean a non-negative function of a single variable. We approximate spectra by functions in a low dimensional space that describe daylight spectra with minimum approximation errors. The spectra, however, do not fill up the original vector space because of the non-negativity constraint. Instead they are all located in a convex conical region of the vector space. This region can be characterized by special isometry groups preserving the geometry. Using the conical structure of the space and the corresponding isometry groups, we can make optimal use of the non-negativity constraint. With the group theoretical description of spectral sequences, we can linearize problems involving these spectra leading to methods that are more powerful than techniques based on mere curve fitting. This group theoretical linearization is crucial in many subsequent applications such as: illumination invariants, optimization, forecast, tracking and segmentation.

In this paper we start with an investigation of the structure of the PCA space of spectra. We consider a spectrum as a non-negative one dimensional signal and then we present some theoretical results showing that the first eigenvector of spectral datasets is always non-negative. Under certain conditions (for example when all the spectra are positive or when the correlation matrix is irreducible) we show that this vector is strictly positive. From this we derive the conical geometry of the PCA space of spectra. A natural set of transformations of this cone are the Lorentz transformations.

It is well known that illumination spectra can be described by linear combinations of only few basis vectors [7, 4, 8, 9, 10, 11, 12]. Here we restrict us to the three dimensional conical space spanned by the three dimensional PCA basis. This three dimensional description is combined with a perspective projection onto a two dimensional disk on the complex plane. The resulting, projected coordinate sequences are then investigated using subgroups of the **SU(1,1)** group. The description of the coordinates of illumination spectra sequences on the disk using one-parameter subgroups of **SU(1,1)** can be considered as defining a group structure on the sequences and a linearization.

In the experimental part of the paper we will describe our experiments with two different sets of illumination spectra: a large database containing 21871 daylight spectra measured in Sweden, and sequences of daylight spectra generated by the simulation program SMARTS2 with changing parameters describing atmospheric conditions or the Sun position.

2. The conical model

2.1. Positivity of the first PCA basis

We will first describe a derivation of the conical structure of the spectra space using general results from matrix theory and functional analysis. We will also introduce the notations used in the rest of the paper. Denote by $I = [\lambda_{min}, \lambda_{max}]$ the closed interval of the wavelengths of interest. The Hilbert space of square integrable functions on this interval is $H(I)$. The scalar product of elements f, g in the Hilbert space will be written as $\langle f, g \rangle$. We define a spectrum as an element in the Hilbert space with non-negative function values everywhere: $s(\lambda)$ is a spectrum if $s(\lambda) \geq 0$ for all $\lambda \in I$. For illuminant spectra the function values could be the photon counts and for reflection spectra they could represent the probability that a photon of a certain wavelength is reflected from the surface point.

A random function $s_\omega(\lambda) \in H(I)$ where ω is a stochastic variable in the probability space, represents elements in the spectra space. The correlation function is defined as the function $\Gamma(\lambda_1, \lambda_2) = E(s_\omega(\lambda_1) \cdot s_\omega(\lambda_2))$ where $E(\cdot)$ denotes the expectation with respect to the stochastic variable ω. This correlation function defines the correlation operator O_C that maps the function f to another function f_C given by:

$$O_C f(\lambda_2) = f_C(\lambda_2) = \langle \Gamma(\lambda_1, \lambda_2), f(\lambda_1) \rangle \qquad (1)$$

If the functions $s_\omega(\lambda)$ are positive then it can be shown that the correlation operator O_C is compact, self-adjoint, positive (mapping positive functions to positive functions) and positive definite. Applying the Krein-Rutman theory [13, pg. 2129], the following results can be derived:

- Since O_C is self-adjoint and positive, all of its eigenvalues are real and positive.
- The eigenfunction corresponding to the largest eigenvalue is also strictly positive.

Practically we often use finite dimensional vectors to describe spectra resulting in a correlation matrix instead of a correlation operator. In this case, the Perron-Frobenius theory [14, chapter 13] can be applied to derive the non-negativity of the first eigenvector. From Perron-Frobenius theory follows that there exists a non-negative eigenvector which is associated with the largest eigenvalue of a non-negative matrix. The correlation matrices of non-negative spectra sets have always non-negative entries, thus satisfy this condition. If the spectra are strictly positive, or if the correlation matrix is irreducible then this eigenvector is strictly positive. We observe that in all the investigated spectra databases, these two later constraints are always satisfied, i.e. we can always assume that the first eigenfunction/vector of the investigated database is strictly positive.

2.2. Conical structure of PCA spaces of spectra

The conical structure of the PCA coordinate space of spectra is a consequence of the fact that the first PCA basis function is strictly positive.

Given an orthonormal set of bounded basis functions $(b_k)_{k=0}^K$ where b_0 is strictly positive, we see that:

- A spectrum $s(\lambda)$ is characterized by its coordinates $(\sigma_k)_{k=0}^K$ with regard to this basis, i.e. $\sigma_k = \langle s, b_k \rangle$.
- The first coordinate σ_0 of the spectrum is always positive since it is a scalar product of a positive and a non-negative function[1].
- There exists a constant C such that the following holds for all spectra coordinates:

$$\left| \frac{\left\| (\sigma)_{k=1}^K \right\|}{\sigma_0} \right| < C \qquad (2)$$

Proof Since b_0 is positive, there exists a constant $C_1 > 0$ such that: $\sigma_0 = \langle s, b_0 \rangle > C_1 \langle s, 1 \rangle$. From the constraint on the bound of the basis functions, we can also see that $\sigma_k = \langle s, b_k \rangle \leq C_2 \langle s, 1 \rangle$ for some positive constant C_2. This leads to $\left\| (\sigma)_{k=1}^K \right\| \leq \sqrt{K} C_2 \langle s, 1 \rangle$. Therefore

$$\left| \frac{\left\| (\sigma)_{k=1}^K \right\|}{\sigma_0} \right| < \frac{\sqrt{K} C_2}{C_1} = C$$

In all of the spectra databases we have investigated we observe that Eq. 2 holds for $C = 1$, i.e. the coordinate space of spectra has a topology of a three dimensional unit cone.

From this follows that for all spectra in the set we have:

$$\sigma_0^2 - \sigma_1^2 - \sigma_2^2 > 0; \qquad \sigma_0 > 0 \qquad (3)$$

[1] We exclude the zero valued function $s(\lambda) = 0;\ \forall \lambda$ from the space of spectra.

where σ_k is the k-th coefficient in the expansion. A conical projection in the space of spectra coordinates is defined as the following perspective projection:

$$x = \sigma_1/\sigma_0; \qquad y = \sigma_2/\sigma_0 \tag{4}$$

A spectrum in this space is thus characterized by its σ_0 (related to the intensity) and the coordinate $z = x + iy$ (related to the chromaticity). The points $z = x + iy$ lie on the open unit disk of the complex plane. In the following we will use the terms "*intensity*" and "*chromaticity*" in the sense defined here. They are convenient terms but are, of course, different from their meaning in traditional color science.

3. Group theoretical description of chromaticity sequences

Given a set/sequence of illumination spectra, we first compute the correlation matrix of the set. The three dimensional PCA basis is then constructed by selecting the three eigenvectors of this correlation matrix corresponding to the largest eigenvalues. In this projection space, spectra are represented by their three-dimensional coordinate vectors.

Next we characterize a spectra sequence by its sequence of projected points as shown in Eq. 4. From Eqs. 4, 3 we can see that those projected points are located on an open unit disk defined in the complex plane. The open unit disk is denoted by $\mathfrak{U}$ and defined as:

$$\mathfrak{U} = \{z \in \mathbb{C} : \ |z| < 1\} \tag{5}$$

It is known that the open unit disk is a two dimensional Poincaré model of hyperbolic geometry, and its isometry transformation group is **SU(1,1)**. An isometry transformation group of a geometry is a group operating which preserves the geometrical distances and angles. **SU(1,1)** is the group consisting of 2×2 complex matrices of the following form:

$$\mathbf{M} = \left\{ \begin{bmatrix} a & b \\ \overline{b} & \overline{a} \end{bmatrix} : a, b \in \mathbb{C}, |a|^2 - |b|^2 = 1 \right\} \tag{6}$$

An element $\mathbf{M} \in$ **SU(1,1)** acts as the fractional linear transformation on a point $z \in \mathfrak{U}$:

$$w = \mathbf{M}\langle z \rangle = \frac{az + b}{\overline{b}z + \overline{a}} \tag{7}$$

Special subgroups of **SU(1,1)**, known as one-parameter subgroups $\mathbf{M}(t)$ are given by group elements that are functions of the real values t, having the following properties:

$$\begin{aligned} \mathbf{M}(t_1 + t_2) &= \mathbf{M}(t_1)\mathbf{M}(t_2); \qquad \forall t_1, t_2 \in \mathbb{R} \\ \mathbf{M}(0) &= \mathbf{E} = \text{identity matrix} \end{aligned} \tag{8}$$

For a one-parameter subgroup $\mathbf{M}(t)$ we introduce its infinitesimal generator, represented by the matrix $\mathbf{X}$:

$$\mathbf{X} = \left.\frac{d\mathbf{M}(t)}{dt}\right|_{t=0} = \lim_{t \to 0} \frac{\mathbf{M}(t) - \mathbf{E}}{t} \tag{9}$$

The infinitesimal matrices $\mathbf{X}$ representing one-parameter subgroups $\mathbf{M}(t) \in$ **SU(1,1)** form the Lie algebra *su(1,1)*, which consists of 2×2 complex matrices of the form:

$$su(1,1) = \left\{ \begin{pmatrix} i\gamma & \beta \\ \beta & -i\gamma \end{pmatrix} : \qquad \gamma \in \mathbb{R}, \beta \in \mathbb{C} \right\} \tag{10}$$

The Lie algebra *su(1,1)* forms a three-dimensional vector space [15], spanned by the basis $(\mathbf{J}_k)$:

$$\mathbf{J}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \ \mathbf{J}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \ \mathbf{J}_3 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \tag{11}$$

Each infinitesimal matrix $\mathbf{X} \in$ *su(1,1)* of a one-parameter subgroup $\mathbf{M}(t) \in$ **SU(1,1)** has thus a coordinate vector specified by the three real numbers ξ_1, ξ_2 and ξ_3.

Given a start point $z(0)$ on the unit disk together with a one-parameter subgroup $\mathbf{M}(t)$ we define an **SU(1,1)** curve as the following function of t:

$$z(t) = \mathbf{M}(t)\langle z(0) \rangle = e^{t\mathbf{X}}\langle z(0) \rangle; \qquad t \in \mathbb{R}, \ z(t) \in \mathfrak{U} \tag{12}$$

The **SU(1,1)** curves are straight lines in the three dimensional Lie algebra space *su(1,1)*, thus the estimation of input chromaticity sequences using **SU(1,1)** curves can be considered as the linearization. The Lie algebra **SU(1,1)** provides a powerful tool to linearize problems involving chromaticity sequences. We developed several methods [16] to compute the group parameters of **SU(1,1)** curves from input data sequences. These methods are used to study the properties of sequences of daylight spectra.

4. Experiments

We investigated two different types of daylight spectra:

- A database of 21871 daylight spectra measured at the same location (Norrköping, Sweden) from June 16th, 1992 to July 7th, 1993; between 5:10 and 19:01 (Local time); in 5nm steps from 380nm to 780nm, and
- Daylight spectra sequences generated by the simulation program SMARTS2 [6]. The SMARTS model accepts as its input the Sun position and atmospheric parameters including: Ångström beta, precipitable water, ozone, and surface pressure. The wavelength range of the generated spectra was 380nm to 780nm in 1nm steps. In a series of experiments, sequences

of spectra were generated by changing a single parameter in its allowed range while keeping the others fixed to the default values. In another experiment a large set of simulated daylight spectra with all the feasible combinations of parameters were also created to simulate the investigated space of daylight spectra.

Fig. 1 shows one result obtained from the study of the measured spectra. It shows the analysis of a sequence of daylight spectra measured at 10/March/1993 and shows that such sequences in general create non-linear curves on the disk and that these sequences can be adequately be described by **SU(1,1)** curves. Usually the variations in such sequences are very small and the sequence shown in Figure 1 is an atypical example where we have a large variation and even a gap between two subsequences (for some unknown reason). Even for this relatively complicated sequence we find a very good description by the one-parameter curve.

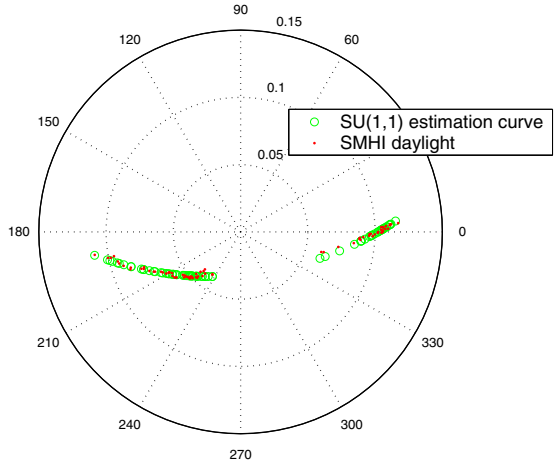

Figure 1: ***SU(1,1)*** *curve estimating the chromaticity of a sequence daylights measured at 10/March/1993*

Figs. 4, 5, 6 show the results of the **SU(1,1)** estimations of SMARTS2 spectra sequences. The chromaticity sequences are generated by SMARTS2 simulation program by changing a single atmospheric or the Sun position parameter at time while keeping other parameters fixed to the default values for Norrköping condition[2].

Fig. 5 and Fig. 6 show the same set of chromaticity points of the daylight spectra generated with different values of the Ångström beta and Precipitable water parameters varying within the allowable ranges [0.0032:0.03:0.30] and [0.0:0.5:5.0] respectively. They can be seen as the images of a grid in the (Ångström beta, precipitable water) plane under the SMARTS2 mapping. The chromaticity sequences corresponding to a single parameter (Beta or Water) changes are then created by grouping all chromaticity points having the same setting value of the other parameter. Fig. 5 shows **SU(1,1)** curves accounting for Ångström beta parameter changes with different settings of precipitable water. Here we choose the value of the precipitable water parameter as constant and estimate the one-parameter group as the Ångström beta varies. In Fig. 6 we show the **SU(1,1)** curves accounting for precipitable water parameter changes with different settings of Ångström beta. The group coordinates characterizing these estimated **SU(1,1)** curves are not constant but forming a linear function of different settings of the other parameter[3]. Figs. 2, 3 show the computed group coordinates of estimated **SU(1,1)** curves varying as functions of the other parameter's settings.

Another example is shown in Fig. 4 where we generated different daylight spectra by varying the zenith angle within the range $[3 : 2 : 85°]$ with all other parameters set to default values. This corresponds to a sequence of daylight spectra with different positions of the Sun, and can also be considered as time sequences of daylight spectra[4]. The same **SU(1,1)** curve can be used to estimate both sequences of equally spaced zenith angle changes and equally spaced time changes, but the group parameters t describing the locations of points on curve are different for each sequence.

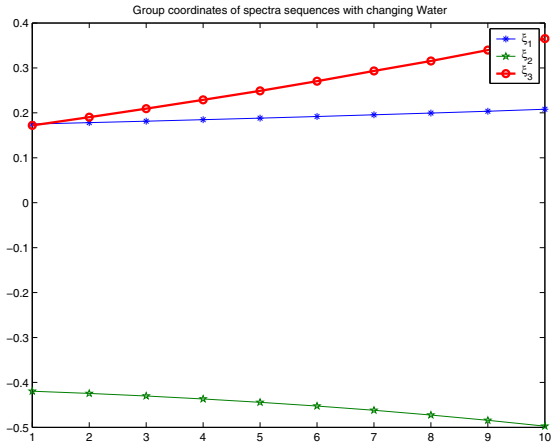

Figure 2: *Group coordinates of Water changing curves as functions of Beta settings*

In all the experiments described above, we found that **SU(1,1)** curves provide good estimation for all SMARTS2

[2] i.e. if not mention otherwise SPR=1013mb, Altitude=0, Ozone=0.334cm, Precipitable water=1.4cm, Ångström alpha=1.3, Ångström beta=0.045, Aerosol asymmetry factor=0.64, Longtitude=16.15, Latitude=58.58, Broadband albedo=10%, Wavelength range=380:780nm

[3] i.e. Ångström beta settings for Water changing curves and Precipitable water settings for Beta changing curves

[4] Zenith angle is a non-linear function of time of the day

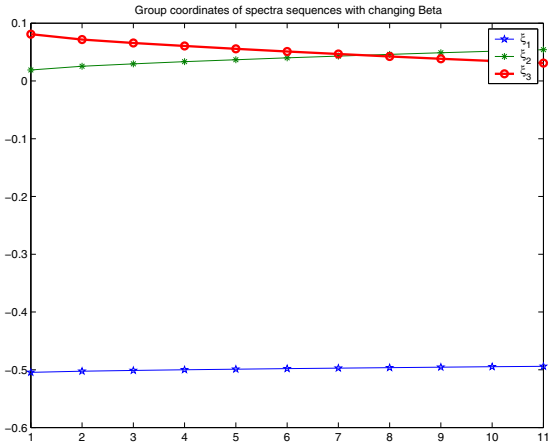

Figure 3: *Group coordinates of Beta changing curves as functions of Water settings*

spectra sequences generated by changing any single parameter. The method also provides good approximations when the remaining parameters are set to other reasonable values different from the default values.

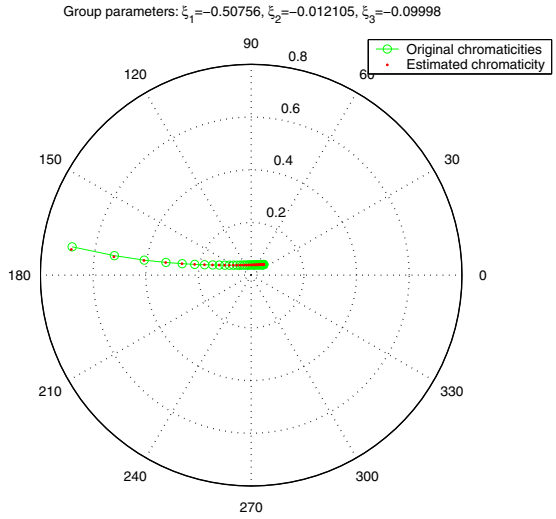

Figure 4: ***SU(1,1)*** *curve estimating sequence of spectra with changing Sun position (zenith angle)*

5. Discussions and Conclusions

We described a framework to investigate sequences of gradually changing spectra. This framework is not restricted to the analysis of illumination spectra with PCA description, but also covers all color spaces having conical properties (where the conical structures investigated in the Krein-Rutman theory are very general, they are for example independent of a metric in the vector space under consid-

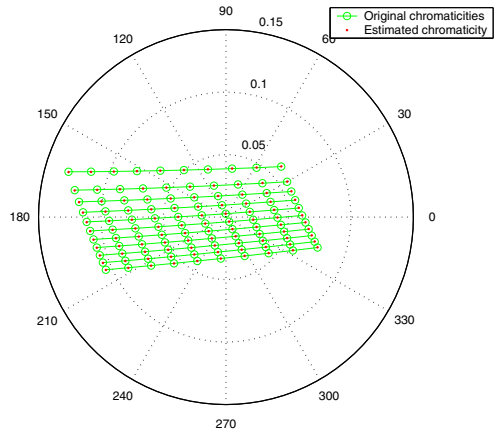

Figure 5: ***SU(1,1)*** *curves estimating sequences of spectra with changing Ångström beta, different settings of precipitable water*

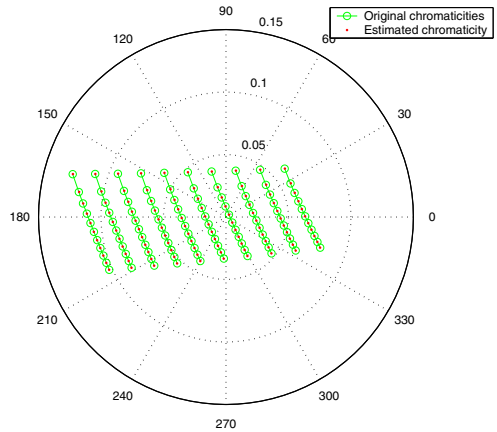

Figure 6: ***SU(1,1)*** *curves estimating sequences of spectra with changing precipitable water, different settings of Ångström beta*

eration). In the experiments described in this paper, we only concentrated on the changing daylight illumination sequences as the input data of interest (see also [17, 18]).

The success of the framework in investigating number of different daylight databases, including the measured and artificially generated by simulation software, demonstrate the applicability of this framework. The existence of a group structure in the dataset and the corresponding linearity properties can be used in subsequent processing steps.

One application where the group structure of the changing illumination spectra sequences can be used is the computation of illumination invariants. This follows from the observation that one-parameter transformation groups define curves in the data space and invariants are simply functions that are constant on these curves. One parameter groups define thus differential equations and invariants are simply solutions of these differential equations. These

group invariants can be easily and systematically derived by solving the partial differential equations. Nowadays this can be done automatically using symbolic math programs like Maple. For more information on the connection between the group theoretical structure and differential equations the reader may consult [19, 20]

Optimization problems involving gradually changing spectra can also benefit from the group theoretical structure of the space of spectra since the linearity of the chromaticity sequences allows the use of fast Newton-type methods to solve the problem.

Compression is another application, where one does not only compress the spectra with the lower dimensional PCA coordinate vectors, but also describes the whole sequence of changing spectra by just a few parameters.

Although we do not derive the relationship between group parameters and the parameters of the real physical processes, we still can expect the usefulness of the framework in many different applications.

Acknowledgements

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