Manifold Analysis of Spectral Munsell Colors

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Abstract. The spectra of color can represent a color in the most accurate way, but the dimension of the spectral data is too high to process. This paper aims to analyze the spectral reflectance curves of 1269 Munsell standard color samples with some influential algorithms in manifold learning. Experimental results reveal that the intrinsic dimension of the embedded manifold in the spectral Munsell color space is 3 and the 3-dimensional structure of this manifold looks like a cone, consistent with the development and structure of the Munsell color system.

Keywords: Spectral Color, Munsell Color System, Manifold Learning, Manifold Analysis, Intrinsic Dimensionality.

1 Introduction

Spectral color has been studied for over 20 years. But there are few studies [1,2,3] focusing on the number of basic factors required to describe spectral color. They usually take the number of dimensions as an input, and then utilize dimension reduction techniques, such as Principal Component Analysis (PCA), Singular Value Decomposition (SVD), and so on, to investigate the characteristic spectra of spectral color.

Several researchers [4,5,6] investigated the configuration of color space derived from spectral data. The spectral dataset studied by Lenz and Meer [4] includes not only 1269 color chips from the Munsell system but also 1513 color chips from the NCS system. A hyperbolic coordinate system is defined in that work to represent the spectral data because the coordinate vectors lie in a cone. Romney and Indow [6] analyze the reflectance spectra of 1269 color chips from the Munsell system and present a set of nested cone-like structures, each made up of a single Munsell chroma. The narrow tips of each cone-like structure are found at the lowest value levels.

High-dimensional color spectra can be essentially represented by a small number of dimensions, corresponding to a low-dimensional embedded manifold in geometry. Determining the intrinsic dimension and the geometric structure of such manifold is useful and challenging. With the manifold learning techniques popular [7], this paper mainly studies the intrinsic dimension and extracts the geometric structure of the manifold embedding in the spectral Munsell color space.

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2 Manifold Analysis

2.1 Intrinsic Dimensionality Estimation

The approaches to intrinsic dimensionality estimation can be divided into two groups, the neighborhood-based [8,9,10] and the elbow [11,12] techniques.

The Neighborhood-Based Techniques. Three typical methods are briefly introduced in this section, which estimate the intrinsic dimension based on the nearest neighbors.

The geodesic minimal spanning tree (GMST) method [8] proceeds as follows: First, a complete geodesic graph between all pairs of data points is constructed. Then, a geodesic minimal spanning tree is obtained by pruning the complete geodesic graph down to a subgraph that still connects all points with the minimum overall length. The intrinsic dimension are then estimated from the GMST length function using the linear least squares.

Although similar to the GMST method, the k-nearest neighbor (k-NN) graph method [9] does not require estimation of geodesic distances on the manifold. The k-NN method first constructs the Euclidean k-NN graph over all points, and then uses its growth rate to estimate the intrinsic dimension by simple linear least squares.

The MLE algorithm in [10] applies the principle of maximum likelihood to the distances between close neighbors. The maximum likelihood estimator estimates the number of data points covered by a hypersphere with a growing radius. It models the number of data points inside the hypersphere as a Poisson process. Then the intrinsic dimensionality d around point x_i with k nearest neighbors is estimated by:

$$d_k(x_i) = \left(\frac{1}{k-1} \sum_{j=1}^{k-1} log \frac{R_k(x_i)}{R_j(x_i)} \right)^{-1},$$

where $R_k(x_i)$ represents the radius of the smallest hypersphere with center x_i covering k neighboring points.

The Elbow Techniques. The classical multidimensional scaling (MDS) [11] and Isomap [12] methods are influential in the field of manifold learning. They are also capable of detecting the underlying intrinsic dimensionality of high-dimensional data sets by the elbow technique. Since residual variance decreases as the dimensionality is increased, the intrinsic dimensionality can be estimated by looking for the "elbow" at which this curve ceases to decrease significantly with added dimensions.

2.2 Manifold Learning

In general, manifold learning algorithms can be categorized into two families: global and local methods. The following discusses 6 different methods, which are tested for extracting the implicit manifold in spectral Munsell colors in the following experiments.

Global Methods. Global methods attempt to preserve global properties of the data lying on manifolds. Two of the well-known examples of this family of algorithms are MDS [11] and Isomap [12].

The classical multidimensional scaling (MDS) maps the high-dimensional data to a low-dimensional representation while retaining the pairwise distances between the data points as much as possible. The quality of the mapping is expressed in the cost function, a measure of the error between the pairwise distances in the low-dimensional and high-dimensional representation of the data. The coordinate vectors for points in the low-dimensional Euclidean space are chosen to minimize the cost function, which can be achieved through eigen-decomposition of matrices.

Different from MDS that is based on Euclidean distances, Isomap attempts to preserve pairwise geodesic distances between data points. Geodesic distance is the distance between two points measured over the manifold. The geodesic distances between the data points are computed by constructing a k-nearest neighbor graph. The shortest path between two points in the graph forms a good estimate of the geodesic distance between these two points. Then, the low-dimensional representations are obtained by applying MDS to the pairwise geodesic distance matrix.

Local Methods. Local methods attempt to retain global properties of the data by preserving local properties obtained from neighborhoods around data points. Locally Linear Embedding (LLE) [13], Hessian LLE [14], Local Tangent Space Alignment (LTSA) [15] and Maximum Variance Unfolding (MVU) [16] fall under this category of algorithms.

In LLE, the local properties of the data manifold are constructed by describing the data points as a linear combination of their nearest neighbors. The local linearity assumption in LLE implies that the reconstruction weights of the data points are invariant to translation, rotation, and scaling. In the low-dimensional representations of the data, LLE attempts to retain the reconstruction weights in the linear combinations as well as possible.

Hessian LLE is a variant of LLE that minimizes the 'curviness' of the high-dimensional manifold when mapping it into a low-dimensional space. This is done by an eigen-analysis of a matrix which describes the 'curviness' of the manifold around the data points.

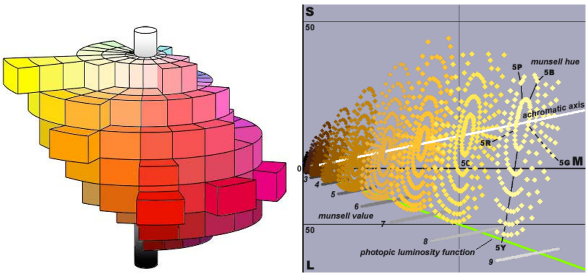
Local Tangent Space Analysis (LTSA) is a technique that describes local properties of the high-dimensional data using the local tangent space of each point. LTSA is based on the observation that, if local linearity of the manifold is assumed, there exists a linear mapping from a high-dimensional point to its local tangent space, and that there exists a linear mapping from the corresponding low-dimensional point to the same local tangent space. The manifold embedding can be found through aligning the tangent spaces between the high- and low-dimensional spaces.

The idea behind MVU is that local nonlinear techniques for dimensionality reduction aim to preserve local properties of the data, but not necessarily aim to completely 'unfold' a data manifold. When a manifold is properly unfolded, the variance over the points is maximized. MVU performs the unfolding based on the low-dimensional data representation computed by LLE, thereby improving the low-dimensional representation.

3 Experimental Results

3.1 Spectral Munsell Data

This study is based on the 1269 color chips of the Munsell color book [17]. In colorimetry, the Munsell system consists of three independent dimensions which can be represented in three dimensions in Fig.1 as an irregular color solid: hue, chroma, and value. Each horizontal circle is divided into five principal hues: Red, Yellow, Green, Blue, and Purple, along with 5 intermediate hues (e.g., YR) halfway between adjacent principal hues. Chroma, measured radially from the center of each slice, represents the 'purity' of a color (related to saturation), with lower chroma being less pure. Value varies vertically along the color solid, from black (value 0) at the bottom, to white (value 10) at the top. Neutral grays lie along the vertical axis between black and white.



(a) Original development (b) Ideal structure

Fig. 1. Development and structure of Munsell colors

The spectral Munsell dataset is downloaded from the website[1]. The color spectra are measured on Munsell colors matt with a spectrophotometer from 380 nm to 800 nm at 1 nm resolution. Different from the study in [6], where the spectral data is reduced to a segment (430–660 nm), we investigate the whole Munsell color spectra, with 421 spectral values of 1 nm spectral interval for each Munsell chip.

[1] http://spectral.joensuu.fi/

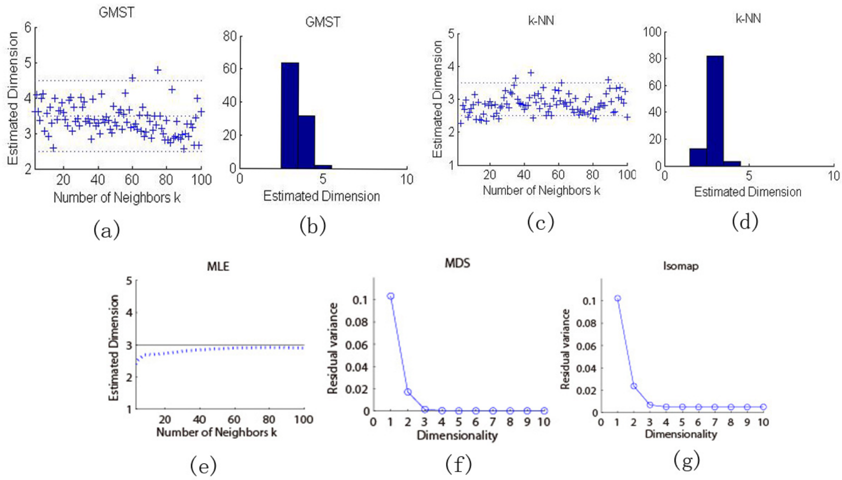


Fig. 2. Intrinsic dimensionality obtained with 5 different methods. (a) and (b): GMST, (c) and (d): k-NN, (d): MLE, (e): MDS, (f): Isomap.

3.2 Intrinsic Dimensionality Estimation of Spectral Munsell Colors

To estimate the intrinsic dimensionality of Munsell colors, we apply five methods discussed in 2.1 to the spectral Munsell data and yield the results shown in Fig.2.

In the first three algorithms, in order to eliminate the influence of the number of neighbors k and gain the most convincing results, we vary this parameter k from 3 to 100, as shown in Fig.2(a-e). In GMST and k-NN, since the estimation does not vary smoothly when the number of neighbors increases, we show both the scatter diagram in panels (a) and (c) and histogram in panels (b) and (d). The histogram of the GMST in panel (b) show that the intrinsic dimensionality falls between 3 and 4 with much more possibility to be 3. The k-NN method is more stable when the number of neighbors increases. Most of the estimation lies between 2.5 and 3.5 in panel (c), which indicates the intrinsic dimension of the spectral Munsell dataset should be 3. The MLE method also gives the estimation of 3 clearly for this spectral dataset.

In addition, the curves in panels (f) and (g), respectively representing the residual variances of MDS and Isomap, cease to decrease significantly at the dimensionality of 3, which is essentially the elbow point.

From the above tests, we draw the conclusion that the embedded manifold of spectral Munsell colors has an intrinsic dimension of 3, consistent with the development of the Munsell color system [17]. In colorimetry, the Munsell color system is a color space that specifies colors based on three color dimensions: hue, value (lightness), and chroma (color purity).

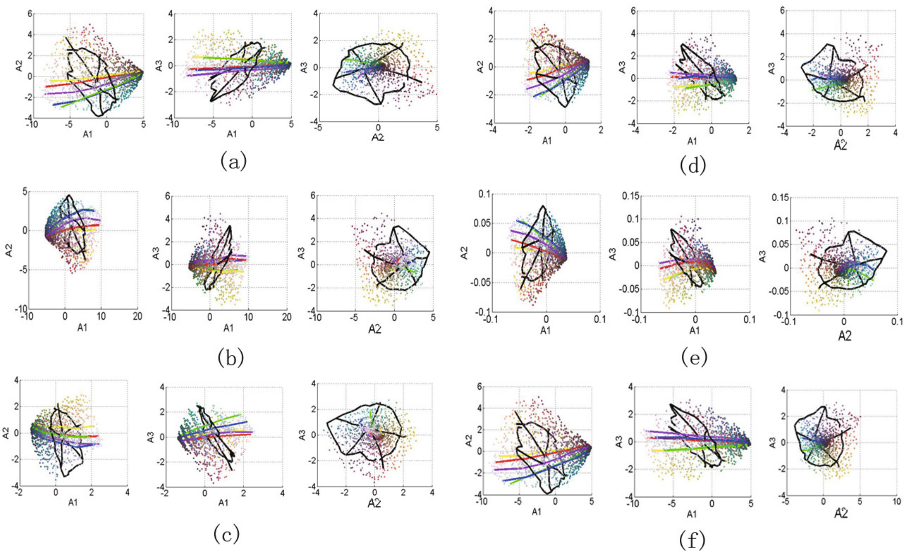


Fig. 3. Comparison of manifold embeddings obtained with 6 different manifold learning methods. (a): MDS, (b): Isomap, (c): LLE, (d): Hessian LLE, (e): LTSA, (f): MVU.

3.3 Manifold Embedding in Spectral Munsell Color Space

In this study, we utilize the above-mentioned 6 different methods to learn 3-dimensional manifolds. The obtained configurations in the 3-dimensional space are shown in Fig.3, where each point represents one certain sample from 1269 Munsell color chips. The RGB color values at each point are calculated under illuminant 'C'. The manifolds learned by different algorithms are similar and the structure looks like a cone: the right subfigures in each panel are viewed from the top of cone, and the left and middle ones are viewed from the other two sides. We also notice that the distribution of the manifold embedding of spectral Munsell colors are basically in accord with the 3-dimensional representation of Munsell color system: the points with similar colors are distributed on the close areas; the points with dissimilar hues are on the faraway positions, e.g., blue and red points are on the opposite side.

In addition, we also draw a few auxiliary lines to reveal the configuration more clearly:

1. Link the points sharing the same chroma (chroma=2) and the same hue (hue=5R, 5Y, 5G, 5B, 5P) together, which turns out to be five straight lines. These lines are almost parallel with the A1 axis, which implies that the A1 axis is supposed to be closely related to the value dimension in the Munsell color system.

2. Link the points sharing the same value (value=7), and the same hue (hue=5R, 5Y, 5G, 5B, 5P) together, which turns out to be five black straight lines. Clearly, the points of the same value seem to lie in the same plane.

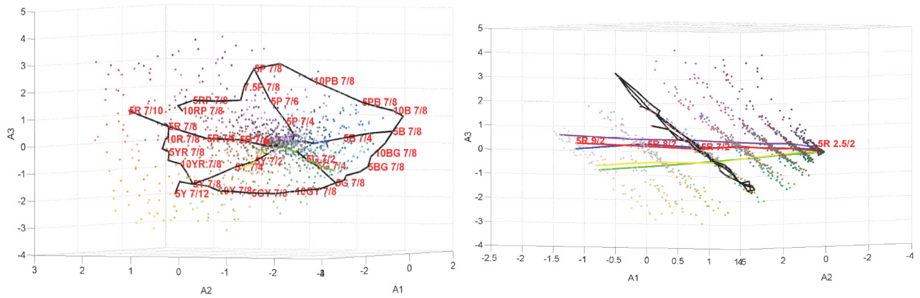


Fig. 4. 3-dimensional manifold embedding of spectral Munsell colors displayed in two different views. The Munsell color notations are plotted for some samples.

3. Link the points sharing the same value (value = 7), and the same chroma (chroma = 8) together, which turns out to be a distorted black circle. This circle gives us a general picture of this "value" plane.

In order to further explore the configuration of the color manifold, we marked some points in the 3-dimensional embedded manifold learned by Hessian LLE (k=50), as shown in Fig.4. From the left panel, the distribution regularity of points is easily recognized: the near points have similar Munsell color notations. At the distorted circle formed by the points with value=7 and chroma=8, the hue varies sequentially from 5R to 10R, 5YR, 10YR, 5Y, and so on. The points of Munsell color notations 5R 7/8, 5Y 7/8, 5G 7/8, 5B 7/8, 5P 7/8 are all approximately in the middle of each color zone. In addition, the five straight lines are drawn by linking points with the same value and hue, where the chroma varies sequentially. The lower chroma lies inside, closer to the center. Moreover, the points of 5R 7/10 and 5Y 7/12 are outside the distorted circle, which agrees with the prior knowledge that the maximum chroma of red and yellow is larger than that of other hues. In right panel, points of the same value form a separate plane and all planes are approximately parallel, with the low-value plane on the narrow tip of this cone-like structure. The corresponding value of each plane is 2.5, 3, 4, 5, 6, 7, 8, 8.5, and 9, respectively, which is consistent with the original description of the Munsell color system in Fig.1(b).

4 Conclusion

Through the above-mentioned experiments conducted with manifold learning techniques, we conclude that there exists a 3-dimensional manifold embedded in the spectral Munsell color space and the geometric structure of this manifold looks like a cone, which agrees with the original development of the Munsell color system.

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