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Investigation on color characterization methods for 3D printer

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Abstract

In this study, the third order polynomial regression (PR) and deep neural networks (DNN) were used to perform color characterization from CMYK to CIELAB color space, based on a dataset consisting of 2016 color samples which were produced using a Stratasys J750 3D color printer. Five output variables including CIE XYZ, the logarithm of CIE XYZ, CIELAB, spectra reflectance and the principal components of spectra were compared for the performance of printer color characterization. The 10-fold cross validation was used to evaluate the accuracy of the models developed using different approaches, and CIELAB color differences were calculated with D65 illuminant. In addition, the effect of different training data sizes on predictive accuracy was investigated. The results showed that the DNN method produced much smaller color differences than the PR method, but it is highly dependent on the amount of training data. In addition, the logarithm of CIE XYZ as the output provided higher accuracy than CIE XYZ.

Introduction

Technologies for full color 3D printing have been dramatically developed, including the PolyJet based on UV cured light from Stratasys, ColorJet Printing with powder binder from 3D Systems, UV-curable inkjet printing technology from Mimaki, MultiJet Fusion with powder fusion from Hewlett Packard, and LOM from Mcor [1]. It has been widely applied in various industrial applications due to its advantages in flexible design, low cost, and customization [2]. The accuracy and consistency of color reproduction in the 3D printing process is of vital importance for meeting modern aesthetic and practical needs.

In the digital printing process, reliable color reproduction is always highly desired and printer color characterization to make connection between device color input to printer (RGB or CMYK) and output device independent color space (CIE XYZ or CIELAB) is an essential step [3]. For conventional color printer, various mathematical models have been developed and acknowledged to be effective, such as 3D look-up tables [4], least-squares based polynomial function [5], empirical techniques based on principal component analysis [6], the artificial neural network [7], etc. Most of those models focused on simple color transformations between RGB and CIE XYZ or CIELAB color spaces. With the development of machine learning methods, it has become possible and workable to perform printer color characterization from complex subtractive CMYK color system to CIELAB color space [8-10].

Based on the FOGRA53 dataset consisting of 1617 color samples, Velastegui et al. compared the performance of four different machine learning approaches, Support-Vector Regression (SVR), Artificial Neural Network (ANN), Deep Neural Network (DNN), and Radial Basis Function (RBF) models, on color space transformation between CMYK and CIELAB color spaces [9]. It was found that all these four methods could achieve very high predictive accuracy, with 99.5% of the color-difference values obtained less than 3 units. When it comes to practical printing, the DNN-based transformation method reached lower color differences than other methods, and the average color difference is 4.65 CIELAB units.

For the applications in 3D color printing, Xiao et al. used a third-order polynomial regression to develop a printer color profile transforming between printer RGB and CIE XYZ color spaces, based on the digital Macbeth ColorCheckerDC chart consisting of 240 color patches [2]. By printing 14 skin color samples using a Z Corp Z510 color printer, the accuracy of the derived color characterization model was 4.50 CIELAB units. In addition, with the aim of improving color reproduction of dental prostheses, Liu et al. selected 96 color patches to develop a color profile for a 3D printer and the polynomial regression method with different orders were investigated on the performance of color characterization between CIE XYZ and printer RGB values [11]. With 18 tooth and gum shades printed to evaluate the 3D color reproduction system, it was found that the third-order polynomial regression yield smaller color differences than the quadratic polynomial, and the average color difference achieved was 6.54 CIELAB units.

Although the color management methods in graphic art industry have been applied in 3D color printing, as far as we know, the existing research on comparing the performance of different color characterization methods for 3D color printers is limited, and currently it still lacks a standard numerical model for predicting the color of 3D printed objects.

With all above issues into consideration, this study was conducted to comprehensively evaluate color characterization models for 3D printer. More specifically, the polynomial regression (PR) and deep neural networks (DNN) were utilized to perform printer color characterization, and the effect of the output variables and the amount of training data on color characterization accuracy were investigated in terms of CIELAB color differences.

Methodology

Dataset

The dataset was generated using a Stratasys J750 3D printer with different CMYK densities. It consists of 2016 color samples with each sample represented in CMYK color space and spectral reflectance data ranging from 400 nm to 700 nm with intervals of 10 nm. A X-Rite i1PRO3 spectrophotometer was employed to take color measurement. The corresponding CIE XYZ and CIELAB values were calculated from the spectral reflectance with the CIE1931 standard observer and CIE D65 illuminant. Figure 1 shows the distributions of the 2016 color samples in a^*b^* and L^*C^* plane, which refers to the colors that the 3D printer can produce. In addition, the color distributions generate a color gamut of the 3D printer, with colors ranging from -84.90 to 74.49 for the a^* redness-greenness value, 5.77 to 93.53 for the

L^* lightness, and -48.20 to 113.17 for the b^* yellowness-blueness scale.

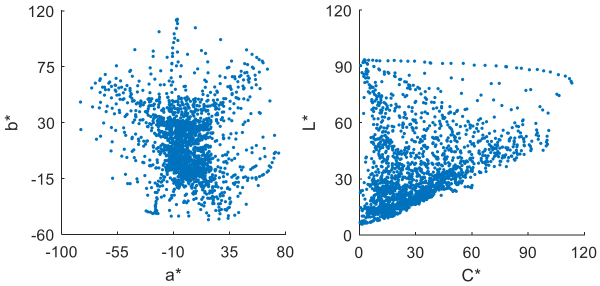

***Figure 1.** Color distributions of the 2016 printed samples in a^*b^* and L^*C^* plane*

Color Characterization

A forward color characterization process was performed to transform from the printer input vectors P to the output vectors C, and the relationship is expressed as Equation (1), where M indicates the color characterization model developed.

$$C = MP \tag{1}$$

Input and Output Vectors

The 3D printer's CMYK combinations served as the input vectors. Regarding the device-independent color space as the output, the spectral reflectance data (r), CIE XYZ tristimulus values and CIELAB values were considered. To compare the performance of different output variables, five types of data were employed for printer color characterization:

- CIE XYZ,
- log(XYZ): the logarithm to CIE XYZ,
- CIELAB,
- r: spectral reflectance data,
- PCA(r): principal components of spectral data.

CIE XYZ and CIELAB color spaces have been widely used for color characterization in most studies. The logarithm of CIE XYZ was selected because it was found that the logarithmic function applied to CIE XYZ values yielded better performance for 2D printer color reproduction. In addition, the use of spectral reflectance data as the output is beneficial for spectral reconstruction from device-dependent color space, which is critical for practical applications since spectral data contain essential information that cannot be obtained from CIE XYZ and CIELAB values. By applying Principal Component Analysis (PCA), it is possible to reduce the dimension of the spectral data and derive the basis function that are sufficient to describe the spectral reflectance [12]. Marimont and Wandell [13] stated that the principal components are usually 5-10 for providing an accurate estimation for natural objects. In the present study, the principal components of the spectral reflectance of the 2016 color samples were finally determined as 6.

Polynomial Regression

The 3rd-order polynomial regression was applied to the input CMYK vectors, making it expanded from $n \times 4$ to $n \times 35$ dimensions, given the number of the training data is n. By performing matrix operations in MATLAB, the color characterization model M was determined based on the Equation (1). A 35×3 matrix was derived for the output variables of CIE XYZ and CIELAB values which were in $n \times 3$ dimensions. When the spectral data r and PCA(r) were served as the output values, the corresponding color characterization matrix determined was in 35×31 and 35×6 dimensions, respectively.

Deep Neural Networks

The architecture of the deep neural networks used in this study contained multiple hidden layers to distribute different neurons and process the information sequentially layer by layer. The first input layer was the predictor variables CMYK, then followed by four fully connected layers (Fc) with a swisher layer in between, and the final regression layer was the output predictions, such as CIE XYZ, CIELAB, spectral reflectance.

The numbers of the neurons in the four fully connected layers were given in Table 1. For the CIEXYZ and CIELAB-based color characterization, the numbers of the neurons in the four Fc layers were 21-77-21-3, respectively. For the spectra-based color characterization, the numbers in the four Fc layers were defined as 22-66-33-31, considering the higher dimensions of the spectral data. The parameters were the same for the principal components of spectral data (PCA(r)), except for the number in the last layer which was 6, consistent to the dimensions of the output. Typically, there is no universal method for determining the optimal number of neurons in each layer of a neural network.

The networks transforming from the input to the output variables were trained in MATLAB with the optimization method of Adam. Five attempts were made with the maximum epochs number of 2000 and the learning rate of 0.01. Based on the optimal results of the 5 attempts, another neural network was trained to achieve better results, with the maximum epoch number of 4000 and the learning rate of 0.01 for CIELAB predictions and 20000 and 0.001 for spectral estimation, respectively.

Table 1 The number of the neurons in the four fully connected layers

Output variables	Number of neurons
CIE XYZ	21-77-21-3
log(XYZ)	21-77-21-3
CIELAB	21-77-21-3
r	22-66-33-31
PCA(r)	22-66-33-6

Model Performance Validation

The process of color characterization is illustrated in Figure 2. The 10-fold cross validation was applied to evaluate the accuracy of the color characterization models developed using different approaches, which means that the fitting procedure was performed 10 times with each fit consisting of 90% (1814 color samples) of the total dataset and the remaining 10% (202 color samples) used for validation. For each implementation of the color characterization, the 1814 training data were randomly selected from the entire dataset, so the training data were not exactly same for the 10 repetitions.

Additionally, in order to explore the effect of the amount of training data on color characterization accuracy, particularly for the method of deep neural networks, different percentages of the entire dataset, ranging from 5% to 95% (101-1915 samples), were randomly selected as the training data, and the remaining color samples were considered as the testing data. The validation procedure was performed 10 times for each training dataset to achieve reliable results, when the percentage equaled to 90%, it was the case of 10-fold cross validation.

The accuracy of each color characterization model was quantified by calculating the CIELAB color-difference values between the predictions and the measurements of the 202 testing data under D65 illuminant. Moreover, to assess the accuracy of the spectral data estimated by each model, the root-mean-square error ($RMSE$) was calculated with the raw measured spectral reflectance.

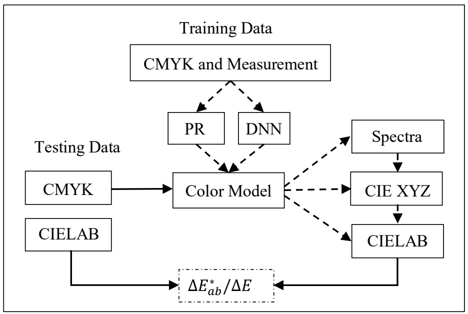

Figure 2. Process of color characterization using different approaches and the validation procedure

Results and Discussion

Evaluation of the Color Characterization Models

The printer color characterization was implemented using different approaches, and each model was evaluated using the 10-fold cross validation. The average CIELAB color differences of ten repetitions were given in Table 2 and Figure 3, with the mean, median, maximum and the standard deviation presented. Regarding the results achieved using the 3rd polynomial regression, the best accuracy was produced using CIELAB as the output, with the average color difference of 4.69 units, followed by the logarithm of CIE XYZ (5.74 units). For the results of the other three types of output variables, the average color differences reached were larger than 11 CIELAB units. As for the results produced using the deep neutral network, the smallest color difference achieved was 1.49 units for the model using the logarithm of CIE XYZ as the output. All the average color differences attained using the DNN method were smaller than 2.69 CIELAB units.

Table 2 The mean, median and maximum CIELAB color differences and standard deviations achieved using different approaches

Method	Output	Mean	Median	Max	SD
3rd PR	Lab	4.69	3.95	22.72	2.99
	XYZ	12.44	10.26	60.46	9.62
	log(XYZ)	5.74	4.94	20.63	3.71
	r	11.74	9.86	45.16	8.25
	PCA(r)	12.05	9.75	46.34	8.35
DNN	Lab	1.59	1.27	9.25	1.03
	XYZ	2.69	2.13	18.53	2.81
	log(XYZ)	1.49	1.26	5.52	0.97
	r	2.34	1.93	11.19	1.37
	PCA(r)	1.84	1.62	7.82	1.06

It can be clearly seen from Figure 3 that the method of deep neural networks gave much better performance than the 3rd polynomial regression, producing significant smaller CIELAB color differences for the five output variables. Even the maximum value (5.52 units) achieved using the logarithm of CIE XYZ values was close to the best result (5.74 units) obtained using the 3rd polynomial regression. In comparison, the method of the 3rd polynomial regression gave greater color differences, particularly for the cases of using CIE XYZ, spectral data (r) and principal components of spectral data (PCA(r)) as the output, and the maximum values achieved were approximately larger than 20 CIELAB units which are not acceptable in color reproduction.

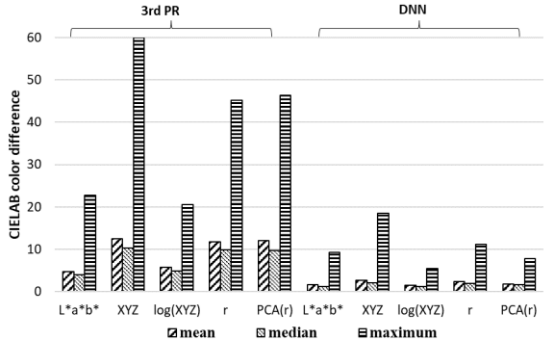

Figure 3. CIELAB color differences of 10-fold cross validation for each model under D65 illuminant

Considering the color-difference perceptibility and acceptability in industrial applications [14], the color differences of the testing data were classified into three groups: $\Delta E \leq 3$, $3 < \Delta E \leq 6$, and $\Delta E > 6$, which were correspondingly defined as "Hardly perceptible", "Perceptual, but acceptable" and "Not acceptable" [9]. Figure 4 illustrates the CIELAB color difference distributions in the three ΔE groups. It shows that over nearly 70% of color differences predicted using the deep neural networks method were less than or equal to 3 CIELAB units. In contrast, only a minority (less than 35%) of the CIELAB color differences estimated using the 3rd polynomial regression method were in this group. When CIE XYZ, spectra and the principal components of spectra were used as the output, over 70% of CIELAB color differences were larger than 6 units.

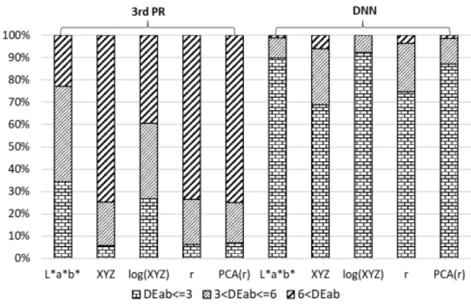

Figure 4. Examples of spectral estimation using the DNN method.

One interesting finding is that the logarithm of CIE XYZ gave higher accuracy than CIE XYZ as the output of printer color characterization, reducing nearly 7 CIELAB units for the PR method and about 1 unit for the DNN method. This is possibly because of the similarity between a logarithmic function and a power law function which was applied to the calculation from CIE XYZ to CIELAB values. In this study, the prediction results of the models using CIELAB and the logarithm of CIE XYZ as the output were better the other three variables, and the CIELAB-based model achieved the smallest color difference for the PR method, and the logarithm of CIE XYZ produced the best accuracy for the DNN method.

Regarding the results based on the spectral data by using the 3rd polynomial regression, it failed to achieve acceptable performance, with an average color-difference value of 11.74 CIELAB units. The same to the results produced using the principal components of spectral data, which resulted in over 70% of color differences greater than 6 CIELAB units. In comparison, the method of deep neural networks gave a significantly better performance on spectral estimation, approximately 25% of color differences larger than 3 CIELAB units.

To quantify the error in spectral estimation, the average RMSE values of the 202 testing data between the predicted and the measured spectral data were calculated, where the RMSE values obtained using the deep neural networks method were 0.51% and 0.48% for the spectra r and PCA(r), respectively, which were smaller than the values of 2.06% and 2.18% achieved using the polynomial regression method. It is indicated that the 3rd polynomial regression method cannot accurately predict the spectral data from printer CMYK values. This is probably due to the high dimensions and complex features of the spectral reflectance. In such cases, the DNN method is preferred because it has better self-learning capabilities for complex patterns and provide higher accuracy

Effect of Different Training Data Sizes

The accuracy of color characterization is not only determined by the method utilized, but also relies on the quality and amount of the training data. In the present study, the effect of different training data sizes on performing color characterization was investigated by quantifying the CIELAB color differences. Figure 5 demonstrates the predictive accuracy by using different training data sizes of 101 (5%) to 1915 (95%) samples, and (a) is the results for the PR method, (b) is for the DNN method.

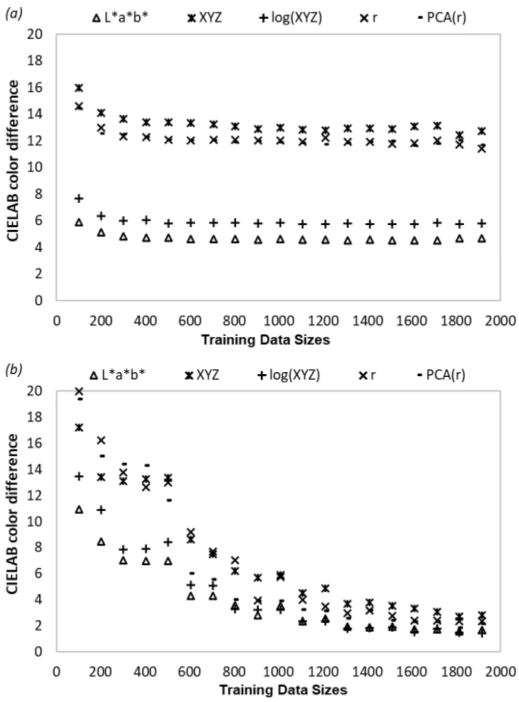

Figure 5. *The average CIELAB color differences achieved using different training data sizes for the PR (a) and the DNN method (b).*

From Figure 5(a), it showed that different training data sizes have little effect on the predicted results for the PR method. The largest color difference was produced when the size of the training data was 101 (5% of the entire dataset), and then the values decreased as the number of the training data increased to 302 color samples (15%), which indicates that more training data resulted in improved performance. However, once the size of the training data exceeded 302, the color differences obtained using the PR method remained stable, approximately 13 CIELAB units for the outputs of CIEXYZ, spectra and PCA(r) and 5 CIELAB units for CIELAB and the logarithm of CIE XYZ, regardless of further increases in the training data size.

In comparison, the color differences calculated using the DNN method, as shown in Figure 5(b), decreased dramatically from about 20 to 3 CIELAB units as the number in the training dataset increased from 101 to 1310 (5%-65%). Afterwards, the color-difference values changed very little with increasing training data. It is evident that the results achieved using the DNN method were affected significantly by the training data size, and a larger training dataset including diverse and representative samples can provide a higher accuracy of color characterization.

Although the DNN method provided accurate prediction results, it highly relied on the training data size. The optimal number of training data was at least 1310 (65% of the dataset) for achieving consistent smaller color differences in this study, which suggested that the amount of the training data is preferred to be greater than that of the testing data. In addition, the process of training a network was time-consuming, the larger the training data size, the more time it takes. Specifically, it took about 200 minutes to complete a 10-fold cross validation based on a common laptop with the Intel® Core™ i5-1035G1 CPU processor. The time was reduced to approximately 40 minutes by using a high-performance desktop PC with the intel® XEON® Silver 4214 CPU processor. In contrast, the PR method only took less than 1 second to give the results of a 10-fold cross validation. Therefore, it is generally compromised between prediction accuracy and processing time.

Conclusion

Based on a large database consisting of 2016 color samples, the method of deep neural networks yielded color differences less than 3 CIELAB units in the color characterization for a 3D printer, outperforming the 3rd polynomial regression method which produced color differences of 4.69-12.44 CIELAB units. Among the five output variables, CIELAB and the logarithm of CIE XYZ exhibited obvious advantages than others, with smaller color differences produced. In addition, it was evident that the size of training data had significant effect on the DNN method. Its predictive accuracy was not supreme and robust until the number of training data reached exceed 1310 in this study. In contrast, the results achieved using the PR method dropped slightly and stayed almost the same as the amount of training data increased.

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