The Inverse Problem of Spectral Reflection Prediction: Problems of Framework Selection

Dmitry A. Tarasov[1,a)], Oleg B. Milder[1,b)]

[1]*Ural Federal University, Mira str., 19, Ekaterinburg, RUSSIA 620002*

[a)]Corresponding author: datarasov@yandex.ru
[b)]milder@mail.ru

Abstract. Digital image processing requires substantial computations for characterization. It is since the reliable color reproduction can be achieved by establishing the correspondence between the spectral reflectance of the printed surface and the amounts of deposited inks. The processing is implemented by using different mathematical models. Most of the color prediction models engage some mathematical techniques to predict spectral reflectance for a mixture of colorants that are characterized by absorption and scattering during the light propagation. However, few attempts were made to make a model for prediction the colorants values based on an observing spectrum. This work is devoted to application of artificial neural network approach for solving the inverse problem of spectral reflection prediction. This task has been considered unsolvable as it involves solving a system of the linear differential equations, in which the number of unknowns exceeds the number of equations. Our attempt is based on the assumption that the prediction of the initial colorants from spectral data is possible by analogy with the work of the color perception system in humans. The aim of our study is to offer an approach to the framework selection. The model is built in Matlab and shows satisfactory prediction accuracy.

Keywords: Color reproduction, Spectral reflection prediction, Artificial neural networks, Framework, Training set.

INTRODUCTION

Digital printing has been growing in recent decades. A key issue with print quality is the color accuracy. The most promising method (for adjusting the color for a given set of source colorants and preset print parameters) is to use a spectral prediction model calibrated on a limited set of test samples.

The first color prediction models were proposed in the 20th century by Neugebauer [1], Yule and Nielsen [2] and later were expanded by Viggiano [3], Balasubramanyan [4], and others. Most color prediction models are somehow based on the Kubelka-Munk reflection theory [6]. However, this theory is not appropriate for colored or very dark print substrate when light absorption reaches a high level. Nevertheless, this is ideal for the case when the absorbent layer is much thinner than the total paper+ink thickness, and when the absorbing and scattering media are evenly distributed over the sheet. These models, as well as the numerous ones created on their basis, are designed to map between the vector of dyes and the vector of the spectral reflection coefficients of the sample. This describes the direct problem of color prediction. All these models are based on a combination of the spectral reflectivity of the solid tones. In addition, to improve the accuracy of prediction, the spectral reflection coefficients of certain halftones were added to the models. To date, the most applicable model is the modified Neugbauer–Yule–Nielsen spectral model, in which the Yule–Nielsen approach is applied to the Neugebauer spectral equations [7].

The current color prediction models taking into account the physical dot gain might predict the reflection spectra depending on the surface coverage of the 3–4 inks [8]. The criterion for estimating the performance of the model is to minimize the metric difference between the measured and predicted reflection spectrum for each overlap condition. The most applicable difference metric is the color difference CIE Lab dE (or ΔE) [9].

Obviously, the direct color prediction problem is well developed and continues to evolve. However, attention to the solution of the inverse problem, on the contrary, is extremely low, since it is likely to be considered unsolvable.

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The inverse problem of color prediction in the case of standard process printing (CMYK) is to indicate which fractions of the tones of the primary colorants lead to the observed reflection spectrum. Thus, a set of 36 monochromatic reflection coefficients must be associated with 4 tonal values. For definiteness, in the future both monochromatic reflection coefficients (ρ) and tonal values (TV) will be calculated in fractions, and moreover, $\forall\rho(\lambda) \in (0; 1)$ and $TV \in [0; 1]$. The inverse problem is incorrect: firstly, because of the excess of the black channel, secondly, because nonideality (in terms of A. Hübl) of the reflection coefficients of basic colorants. Indeed, within the framework of the deterministic approach, there is no solution to such a problem. Therefore, a paradigm changing is needed.

Recently, it has been showed that Artificial Neural Networks (ANNs) are able to provide an alternative approach to mapping between colorant concentrations and spectral reflectance; and they are even able to provide transformations between color spaces [10, 11]. The feed forward multi-layer perceptrons have shown satisfactory results in the colorant-to-reflectance mapping, as well as in the similar issues [12]. There are a number of attempts to apply the ANNs for the forward problems of color prediction [13–23]. The ANNs have brought ample opportunities into the issues under consideration. A three-layer network (only one hidden layer) is able to solve the color-prediction problem. However, the number of neurons, the learning method etc. are determined empirically and depend on particular conditions of problem being solved. We expand this approach to the inverse problem. This work is an attempt to offer the network selection algorithm in an inverse problem of the spectral reflection prediction.

APPROACH AND EXPERIMENTAL

In the experiment, we have studied two issues. First, the influence of amount of the neurons in the hidden layer onto the model error. Second, those regarding the training set volume. For the experiment, we use the 4-color (CMYK) electrophotographic printer Konica-Minolta C6000L. Print mode: 1200×1200 dpi, round dot. Substrate was the coated paper 135 g/m^2. The measurement tools are: spectrophotometer X-Rite iOne iSis + X-Rite ProfileMaker package. Charts generation is made in the ArgyllCMS package. For the ANN development, we use the Matlab 16 package.

Since monochromatic reflection coefficients ($\rho(\lambda)$) are mathematically equal and the division of the visible spectrum into zones is arbitrary, we believe that there is no reason to introduce a more complex neural network structure, for example, a network of deep learning. So, the applied ANN type is a multilayer perceptron with one hidden layer, the amount of hidden neurons varied from 1 to 15 (net framework: 36×N×4, $N \in [1; 15]$). The training set for the networks was also altered. The network has 36 inputs, which correspond to the spectral zones from 380 to 730 nm with 10 nm step, and 4 outputs (CMYK fractions). The training techniques are the Levenberg–Marquardt method with the Bayesian regularization.

The training sample sets are regular grids in the colorants recipe space. The number of grid nodes per each formal CMYK direction is considered by the dimension of the cube. The points are also located in the centers of the main cells. Such an organization of the training sample is similar to a crystallographic body-centered cubic lattice (bcc) and, therefore, has been called “the bodycube” (bc). The number of samples of the training set is fully determined by the bodycubic dimension. In the experiment, we used training sets of dimensions from 3 to 6. Their main features are shown in Table 1.

$$TS = R^4 + (R - 1)^4, \tag{1}$$

where TS is a complete amount of samples in the training set, R is a dimension of a particular bodycube (bc$R$).

TABLE 1. ANN training sets configurations

Training set	**bc6**	**bc5**	**bc4**	**bc3**
Number of patches	1921	881	337	97
Dimension, *R*	6	5	4	3
Step of the main grid, tone fraction	0.20	0.25	0.33	0.50

Training sets were synthesized in Matlab, their graphical images were obtained using the PM MeasureTool for the automatic spectrophotometer X-Rite iSis. We also created a validation set to assess the prediction performance

of the network. This set contains more than 2700 randomly chosen recipes. The measured spectral reflection coefficients for both training and validation sets were converted into the spectral density $D_i(\lambda) = -log_{10}\rho_i(\lambda)$, were λ is the wavelength in the range (380–730) nm, i is the counter of patches to print.. This is required because optical density depends on the amount of applicable ink (toner) directly whilst spectral reflection coefficients and ink amount are linked with inverse relationship.

In order to evaluate the statistical behavior of the errors in the experiment, we passed multiple trainings. In total, 51 cycles of training were carried out for each network configuration in combination with each training set, such, 3060 trainings were passed. For each of the training sets depending on the bc$R$ size, complete cycle of 765 (15 neurons × 51 trains) experiments took time from a half an hour to several hours. The validation set did not take part in the training. Its purpose was to evaluate the model's prediction error that was assessed by the "taxi cab" metric between a printed and a predicted recipe. Obviously, this is the only reasonable metric as the common dE is not applicable. Moreover, we even cannot apply the Euclidean metric because the recipes space is not Cartesian.

RESULTS AND DISCUSSION

As a result of the experiment, we took the distribution of the prediction errors for each training set depending on hidden neurons amount (Fig. 1). The statistical behavior of the errors is indicated as the SD bars at plots. As it may be seen from the graphs, for the small training sets (bc3 and bc4), the mean prediction error is quite high (about 0.5 tone fraction, *i.e.* on the average about 0.1–0.15 per color channel) and almost do not depend on the number of hidden neurons in the model. For bc3, the best error is achieved at 6–7 hidden neurons and for bc4 do at 6 ones. The description of the behavior of the standard deviation deserves special attention. For two considered cases, the opposite SD behavior is observed. A weakly manifested minimum of the average prediction error corresponds to the minimum SD for bc3, whilst a more expressed minimum of the average error corresponds to the maximum SD for bc4. In general, it is impossible to point out any dependence of the error on the number of neurons for these two cases.

In the cases of a relatively amplified volume of training samples, the dependence of the average error on the number of hidden neurons becomes more expressed. The more hidden neurons, the less the mean prediction error is. However, this impression is in many ways deceptive, since SD also grows sharply after 7–8 hidden neurons. This can be interpreted as a decrease in the stability of the obtained prediction, *i.e.* the recipes with extremely high prediction errors start to appear. Thus, for the bc5 and bc6, the number of neurons should not be increased by more than 8.

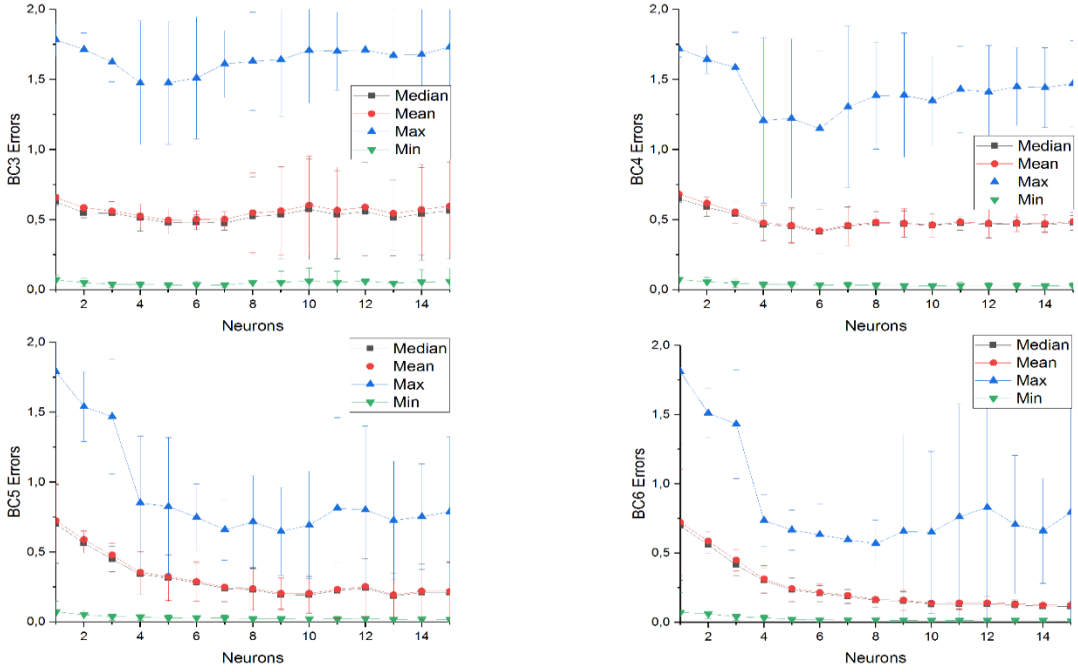

FIGURE 1. Errors with SD for different training sets.

CONCLUSION

This work is an attempt to solve the inverse color prediction problem by mean of the artificial neural network. We predict the initial colorants (CMYK) formulation by the spectral data. This problem was previously considered unresolvable. We prepared an experiment based on the electrophotographic digital printing system. The numerical experiment consisted of sequential training of a set of neural networks with varying configuration using altering training sets. We studied the influence of amount of the neurons in the hidden layer on the model error, as well as those regarding the training set volume.

As it is seen from the results, the training sample should contain not less than 1000 patches, and the number of hidden neurons should be 6–8. The less number of neurons leads to raise in the mean prediction error, whilst the more neurons are equal to a high SD of errors that correspond to the model instability.

The further experiments will touch the dependence of the error on the total ink coverage and number of colorants acting in a particular recipe.

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