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Determination of Pigment Combinations for Textile Printing Using Artificial Neural Networks

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Abstract
This paper demonstrates the possibility of using counter-propagation neural networks to identify the combinations of dyes in textile printing paste formulations. An existing collection of 1430 printed samples produced with 10 dyes was used for neural network training. The reflectance values served as input data and the known concentrations of single dye or two dyes were used for printing each sample. Some variations of neural network parameters were tested to determine the best model, and a cross-validation method was used to estimate the generalization error. Also, some modifications of input and output data were made to improve the learning capabilities.

Key words: *neural network, colorimetry, colour combinations, textile printing.*

Introduction

Although computer colour matching is well established for dyeing, in textile printing many colour recipe predictions are still made visually by colourists. In one plant in Slovenia, an extensive library of printed samples, produced with combinations of two dyes of different ratios and concentrations, is used for visual matching. After selecting the closest sample, an experience-based adaptation of concentrations in this sample is made to match the colour requested. If a test print is not satisfactory, the concentration is corrected and a further test print is conducted. This trial-and-error procedure is time-consuming and expensive, therefore modern methods for its improvement were investigated.

The computer recipe prediction based on the Kubelka-Munk theory of radiation transfer is well known for dyeing processes. However, this method requires exact knowledge of dyeing theory and depends on precise fulfilling of dyeing conditions [1]. In textile printing it is very difficult to control all the process parameters; therefore other methods for recipe calculation have been investigated. One of these is the use of artificial neural networks (ANNs), which enable the relationship between reflectance values and concentrations to be mapped. Once the selected neural network is sufficiently trained with a set of known input (colour values) and output data (concentrations of each dye), it can predict the concentrations for an unknown set of coloured samples. One of the advantages of neural networks is their capability to establish relations between input and output data without explicit programming of Kubelka-Munk equations or analytical knowledge into the model.

Artificial neural networks have not been widely used in the textile industry. Some research projects were carried out in the areas of production planning [2, 3], quality control [4] and wastewater treatment [5]. Some work was also done in the field of colour science [6, 7]. The use of neural networks for colour recipe prediction was also investigated [8, 9]. Most of the researchers used error back-propagation networks to predict reflectance values (output) for known concentrations (input values). Kohonen and counter-propagation networks have not been used so often as they are more suitable for classifying, categorising or grouping data together [10, 11].

In this research programme an attempt was made to follow the colouration process in textile printing in a more general way. When a new colour is requested from a buyer or designer, colourists have to define the recipe (concentration of each dye in the printing paste). In the trial-and-error method previously described, it sometimes becomes evident that the combination of dyes selected is not appropriate for achieving the requested colour.

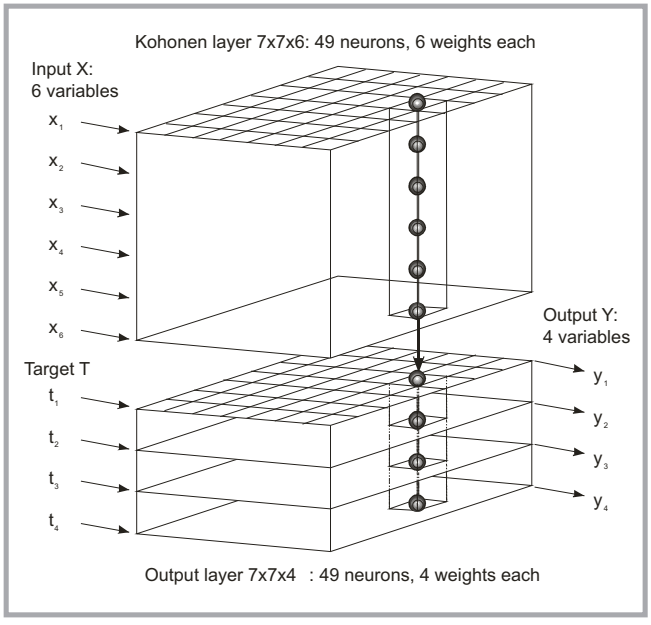

Figure 1. *Counter-propagation artificial neural network with 49 (7x7) neurons. In the scheme presented the input objects and targets are 6- and 4-dimensional, respectively.*

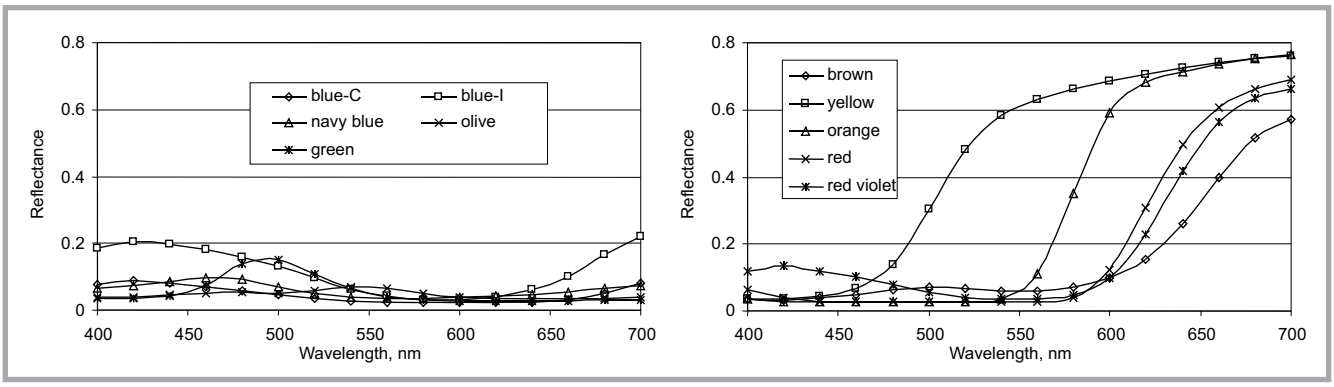

Figure 2. *Reflectance values of each dye at the maximum concentration.*

A new sample with different dyes is then selected and a new correction is made. Most colour recipes in the factory library used contain either one or two dyes, therefore the selection of dyes capable of achieving the required colour is very important. For this reason colour cards contain samples produced with a large number of different dyes, including dyes of similar hues. Selection of the sample which matches best requires a great deal of experience, as well as time to search through the whole colour card library.

The aim of the present work is to investigate the use of ANNs for assisting colourists to determine the correct combination of dyes for textile printing pastes. The use of counter propagation neural networks will be described and discussed. As only two dye combinations are preferred by the industry, research was conducted to comply with this demand.

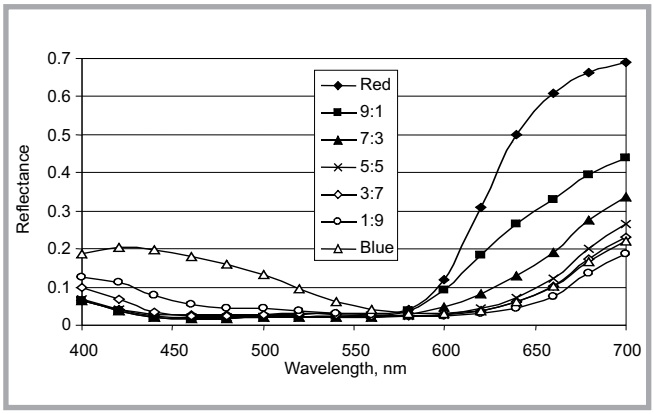

Figure 3. *Reflectance values of different ratios for the combination of the red and the blue dye.*

Theory

Counter-propagation artificial neural networks (CP-ANN) are based on Kohonen ANN [12], which represents a special form of artificial neural network consisting of a Kohonen layer and an output layer. Neurons are represented as columns and are arranged in a quadratic matrix. The length of the columns corresponds to the number of weights and consequently to the dimensions of the input vector X. The output layer has exactly the same number layout of neurons, as the Kohonen layer. The length of the columns in the output layers corresponds to the dimensions of the output vector Y (***Figure 1*** see page 93).

Table 1. *Dyes selected for neural network training.*

Dye	Maximum amount of dye in the printing paste, g/kg
Yellow	100
Orange	80
Red	50
Red Violet	100
Blue-C	80
Blue-I	50
Navy blue	80
Green	80
Olive	60
Brown	100

While the Kohonen ANN, also called a self-organising map, serves for unsupervised learning, CP-ANN enables supervised types of problems to be solved, i.e. one trains such a network with a set of known input and output vectors, $\{\mathbf{X}_s, \mathbf{T}_s\}$. Each step of the counter-propagation learning strategy consists of four acts [13]:

1. The input vector $X_s = (x_{s1}, x_{s2}, \ldots x_{sn})$ enters the Kohonen layer and locates the most excited neuron W_e^K on the basis of the weights that are most similar to the input variables (Eqation 1);

$$\text{neuron } e \longleftarrow \min\left\{\sum_{i=1}^{m}\left(x_{si} - w_{ji}\right)^2\right\} \quad (1)$$

2. All the weights w_{ei} in the most excited neuron W_e^K, and in a specific neighbourhood of it are corrected according to Equation 2;

$$w_{ij}^{K(new)} = w_{ij}^{K(old)} + \\ +\eta(n_t)\alpha(r_e - r_j; n_t)x\left(x_{sj} - w_{ij}^{K(old)}\right) \quad (2)$$

3. The position e of the most excited neuron W_e^K 'points out' the neuron W_e^o, having exactly the same position e in the output layer. To this neuron W_e^o in the output layer the target vector $T_s = (t_1, t_2, \ldots t_m)$, associated with the X_s, is "input";
4. All weights of the neuron W_e^o, and its neighbouring neurons in the output layer are corrected according to Equation 3,

$$w_{ij}^{o(new)} = w_{ij}^{o(old)} + \\ +\eta(n_t)\alpha(r_e - r_j; n_t)x\left(t_{sj} - w_{ij}^{o(old)}\right) \quad (3)$$

where

K = index indicating the Kohonen layer;
o = index indicating the output layer;
e = position of the most excited neuron;
n_t = number of iteration steps;
$\eta(n_t)$ = function monotonically decreasing between the two predefined values α_{max} and α_{min}; with an increasing number of iteration steps

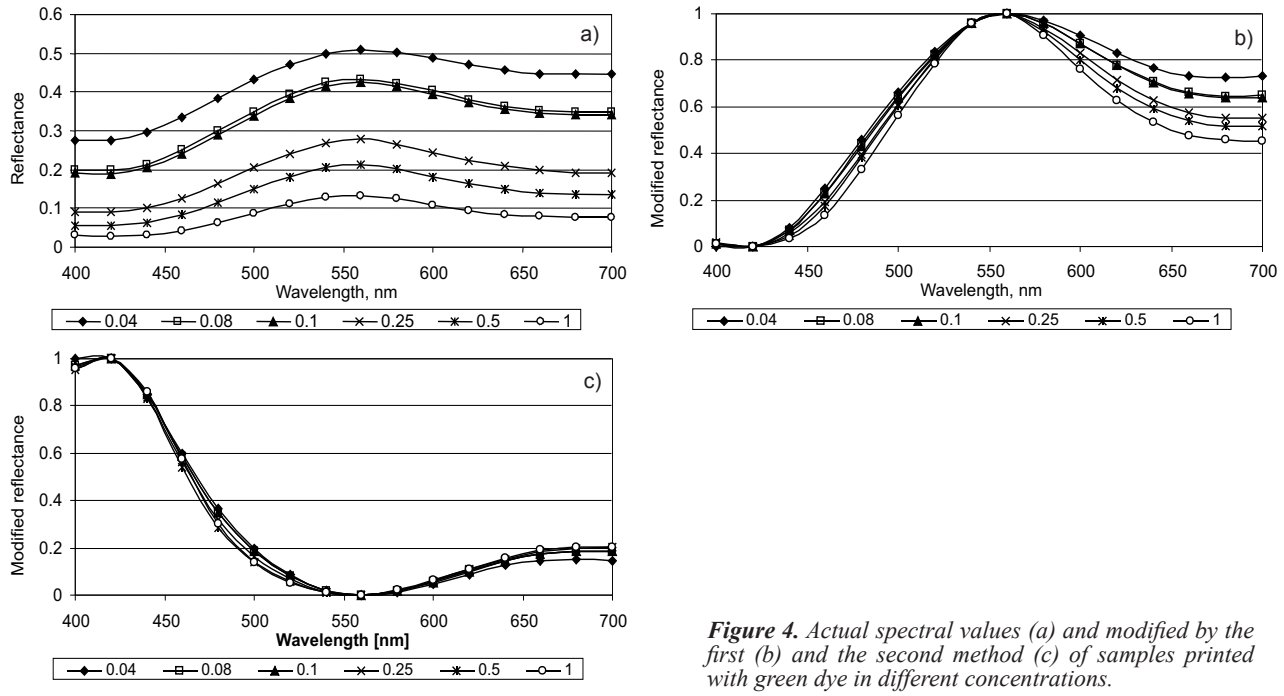

Figure 4. *Actual spectral values (a) and modified by the first (b) and the second method (c) of samples printed with green dye in different concentrations.*

$r_e - r_j$= topological distance of neuron W_j from the position of the most excited neuron W_e^K (number of neurons between both);

$\alpha(r_e - r_j;n_t)$ = neighbourhood function defining the percentage of actual correction (between 0.0 and 1.0) of the weight in each neuron; its value decreases with topological distance and an increase in the number of iteration steps.

The larger the distance $r_e - r_j$, the smaller the correction of weights is. At the beginning of the learning phase, the correction encompasses the weights of all neurons in the network. During the learning process, the number of neighbouring neurons in which the weights are corrected decreases, and in the last epoch only the weights of the central neuron are corrected. One epoch represents the input of all vectors of the learning set into the network.

After the training is completed, the Kohonen layer acts as a pointer device, determining the position of the neuron in the output layer, in which the answer is stored. Similar input vectors are stored close together and very different inputs are topologically separated. Since, during the learning phase, the answers are distributed over the entire output layer; each output neuron has an answer even if a corresponding neuron in the Kohonen layer was never selected as a central neuron.

Experimental

A colour library with 1430 printed viscose samples, produced with 10 different vat dyes, served as a base for this experiment. Each sample was printed with either a single dye or a combination of two dyes. For single dye printings eight different concentrations were used: the maximum amount of dye in the printing paste, as recommended by the producer (e.g. 100 g/kg for yellow, 80 g/kg for orange etc.), were 50%, 25%, 10%, 8%, 4%, 2% and 1% of the maximal quantity. Combinations of two dyes were produced by first mixing two 100% single dyes in five different ratios for each dye (1:9, 3:7, 5:5, 7:3, 9:1), and then the mixture was diluted to produce five additional concentrations of each ratio (50%, 25%, 10%, 8%, 4%). ***Table 1*** shows the selected dyes and their maximum amounts in the printing paste (here referred to as 100%).

Each sample was measured with a Datacolor SF 600 Plus spectrophotometer. The measuring geometry was d/8 and aperture 9-mm. ***Figure 2*** shows the reflectance values of each single dye at maximum concentration.

Figure 3 shows the reflectance values of different ratios in combination of a red and a blue dye at the maximum concentration.

The resulting database contained records for 1430 samples (10 single dyes × 8 samples + 45 combinations × 30 samples), each represented by 16 input values (reflectance values in the region of 400 - 700 nm in 20 nm steps) and 10 output values. The output values consisted only of ones (1) and zeros (0), indicating whether a dye is present in the colour combination or not. Thus, for each record only one or two output values can be "1", while all others must be "0".

For more efficient training the records were randomised, because the input sorted by any property (dye type or concentration ratio) produces a biased training sequence, which will consequently lead to a biased prediction and biased grouping of data.

The shape of the spectral curve is more important than the absolute value of the amplitudes for the determination of the dyes in the colour combination. Therefore the spectral values were modified to diminish the influence of dye concentration on the spectral curve. Several different modifications were tested, and the two showing the best improvement were investigated further. The first one (min-max) set the lowest spectral value of each sample to zero (0%) and the highest value to one (100%) and correspondingly adjusted all other values according to Equation 4:

Table 2. *Ten typical prediction results from the 30x30 counter-propagation network giving examples of all four cases.*

	Sample ID		Yellow	Orange	Red	Red Violet	Blue-C	Blue-I	Navy Blue	Green	Olive	Brown
Case 1	405	**Target**		**1**					**1**			
		Prediction		1.000					1.000			
	1270	**Target**								**1**	**1**	
		Prediction	0.001				0.001	0.001	0.001	0.995	0.999	
	1115	**Target**						**1**			**1**	
		Prediction						0.666	0.333		1.000	
	473	**Target**		**1**							**1**	
		Prediction		1.000						0.498	0.502	
Case 2	1264	**Target**								**1**	**1**	
		Prediction	0.004	0.002	0.001			0.001	0.002	0.494	0.996	0.001
	157	**Target**	**1**						**1**			
		Prediction	0.336			0.334	0.328		0.337	0.334	0.329	
Case 3	1072	**Target**						**1**	**1**			
		Prediction					0.503	0.497	0.998		0.002	
	544	**Target**			**1**		**1**					
		Prediction		0.004	0.498	0.497	0.501	0.499				0.002
Case 4	1011	**Target**					**1**				**1**	
		Prediction	0.502				0.496	0.504		0.002	0.496	0.001
	19	**Target**	**1**	**1**								
		Prediction	0.328	0.328							0.672	0.672

$$R_{j,c} = \frac{R_j - R_{\min}}{R_{\max} - R_{\min}} \quad (4)$$

where:

$R_{j,c}$ corrected reflectance value
R_j actual reflectance value
R_{max} maximal reflectance value for each sample
R_{min} minimal reflectance value for each sample
j index of reflectance values (j = *1 to 16*) for wavelength from 400 nm to 700 nm in 20 nm steps.

In the second method each reflectance value was transformed to its K/S value, and then the same modification as above (min-max) was applied. The equation for the Kubelka Munk transformation is:

$$K/S_j = \frac{(1 - R_j)^2}{2 \cdot R_j} \quad (5)$$

Figure shows the spectra of six samples (yellow and olive mixture 50 : 50 in six different concentrations) with actual spectral values (a), including values corrected by the first (b), and second method (c).

All three data types were examined in the modelling process and in the cross-validation procedures. Additionally, several different parameters were tested during the modelling process. The dimension of the Kohonen network varied from 15 x 15 to 30 x 30 neurons and the number of epochs from 300 to 1200. A maximal correction factor was tried with values between 0.2 and 0.9. The initialisation of weights was always done with the same random sequence seed, providing the same initial random weight values for each repetition of the learning process.

Among several different dimensions and parameters, the best result (yielding the smallest RMSE value between the 10-bit binary targets and the actual network outputs) was achieved with the network having of 900 (= 30 x 30 neurons), trained with 1200 epochs, and using the maximal correction factor of 0.5, which was linearly diminished towards the minimal value of 0.01 during the training.

Results

The final result of the training process with all 1430 colour combinations is the coefficient indicating the possibility of each of the 10 dyes to be either present or absent in the colour combination of the input sample. The order of dyes is shown in ***Table 2***. The output for each reflectance spectrum of a two-dye printed sample was a 10-dimensional vector (p_1, p_2, … p_{10}) with the values of the components p_i between "0" and "1". Each output p_i is associated with one specific dye.

The output values, p_i, actually achieved, usually being close to the target values of zero or one, are proportional to the possibility of each dye being present in the colour combination of the selected input sample. The predictions obtained for two-dye samples can be divided into four classes:

1. Both constituent dyes have the highest among the ten outputs, with values higher than 0.5,
2. Both constituent dyes have the highest values, but one or both is lower than 0.5,
3. One constituent dye output is not among the two highest ones,
4. Outputs for both constituent dyes are not among the two highest ones.

The first two outcomes are considered as correct predictions, while the last two are regarded as being partially or completely incorrect. To illustrate this, the outputs for actual predictions in all four possible cases of ten samples are listed in ***Table 2***. For the sake of legibility all output zeros are suppressed by blanks, and the layout is slightly modified from the original computer output.

A complete overview of the correctness of the predicted results of 1350 two-dye samples using the 30 × 30 counter-propagation network is given in ***Table 3***, which shows the numbers and percentages of outcomes for each category and for each modification type (min - max and K/S + min - max, respectively). The best predictions for the modified data were achieved using K/S + min - max modification, yielding 83.8% of predictions, in which both the dyes actually implemented in the sample-print were predicted correctly.

A large majority of the cases that fall into category 1 predicted the correct dyes with values of p_i higher than 0.9 and all other dyes with possibilities lower than 0.1 (e.g. sample IDs 405, 1270 in ***Table 2***). There were also several predictions where the possibilities for two, or even three dyes were very close to each other (e.g. sample IDs 544, 1011). Close inspection of the reflectance spectra of the samples that produced the "semi-correct" decisions suggests that the reflectance values of two or three selected dyes were, in most cases, so similar that it was almost impossible to unambiguously select the two correct dyes for the colour combination. Furthermore, it was apparent that the specified colour sample could be achieved with several different combinations of dyes, which is known to

be true in practice. In order to obtain a detailed insight into the properties of the complete system, all 212 partially-incorrect predictions (case 3) were inspected, the results of which are shown in ***Table 4***. The table contains the frequency distributions of incorrectly predicted dyes for each target dye in the study.

The dyes in ***Table 4*** are arranged in spectral order, from blue (short wavelength) to red (long wavelength); hence, visually similar dyes are grouped together. Diagonal fields contain the number of correct predicted dyes in these "semi-correct" combinations. Therefore, the sum of the numbers on the diagonal, as well the sums of all rows and all columns, respectively, (without the diagonal figures) are equal to all inspected outputs, i.e., to 212. Each row of the numbers shows how many times the particular dye has been erroneously predicted by the dye in the corresponding column.

One can see that most of the wrongly predicted dyes are "substituted" by dyes close to the main diagonal, i.e. by a dye similar in hue to the actual one: for example, Blue substituted by Navy Blue; Orange by Red; Red by Red-Violet, etc. As the reflectance values of these dyes are similar (***Figure 2***) it is clear that such exchanges or mistakes can easily happen and will probably always persist. In a way, the similarity of reflectance spectra between two similar dyes presents the physical limitation of any system, even for a trained human eye. Numerical predictions reveal that the correct dye is usually predicted with a very high possibility (near 1), while the incorrect one is often spread among several similar dyes (e.g. sample ID 1072 in ***Table 2***). It is interesting to note that dyes Blue-I and Red produced the largest and smallest proportion of incorrect predictions, respectively.

The number of predictions with both incorrect dyes is 0.5%, which illustrates the great capabilities of neural network modelling. Even with the data which were not normalised, less than 2.5% of predictions were completely wrong. Considering only the combinations of two dyes, the neural network model made incorrect predictions for both dyes in only 7 cases out of 1350. These predictions are presented in ***Table 5***. The predictions are sorted by increasing maximal the value of the wrong prediction. Possibilities for the target (should-be-predicted) dyes are printed in bold, and dyes whose predictions were among the two highest ones in italics.

Table 3. *Statistical survey of prediction results for all three types of input data.*

No	Class	Without modification		Modification Min = 0; Max = 1		Modification K/S + Min - Max	
		Number	Percent	Number	Percent	Number	Percent
1	Both correct and > 0.5	732	54.2	956	70.8	1069	79.2
2	Both correct ≤ 0.5	158	11.7	83	6.1	62	4.6
1+2	Correct decisions	890	65.9	1039	77.0	1131	83.8
3	Only one correct	427	31.6	301	22.3	212	15.7
4	Both incorrect	33	2.4	10	0.7	7	0.5

Table 4. *Predicted dyes for the two-colour combinations yielding only one of the two dyes correctly.*

Frequency of the wrongly predicted dyes		Predicted dye										Total minus diagonal
		Blue-C	Blue-I	Navy Blue	Olive	Green	Brown	Yellow	Orange	Red	Red Violet	
Actual dye in the sample	Blue-C	***13***	31	7	1		1				4	44
	Blue-I	25	***12***	6	3				1		1	36
	Navy Blue	7	8	***28***					1		1	17
	Olive	1	6		***17***		2	4	2		2	17
	Green		1	2	7	***27***					2	12
	Brown	2	1			1	***20***	5	6		6	21
	Yellow	2			3		7	***18***	2		5	19
	Orange				10	1	3	2	***14***	3	3	22
	Red		1				1		3	***46***		5
	Red Violet	1	2	1		1	11	1	2		***17***	19
Total minus diagonal		38	50	16	24	3	25	17	12	3	24	***212***

Table 5. *Predicted coefficients of possibilities for completely incorrect predictions as obtained by the data normalised according to K/S+min-max modification.*

ID	Yellow	Orange	Red	Red Violet	Blue C	Blue I	Navy Blue	Green	Olive	Brown
95	*0.493*				*0.497*	**0.503**		0.002	**0.504**	0.001
1011	**0.502**				*0.496*	**0.504**		0.002	*0.496*	0.001
1336	**0.504**	0.001	**0.503**						*0.496*	*0.496*
955	0.002	0.001		0.001	*0.499*	**0.505**	*0.492*		0.001	**0.500**
498	**0.502**	*0.494*	**0.506**							*0.498*
1048	0.002	0.001			*0.498*	**0.506**			**0.502**	*0.490*
19	*0.328*	*0.328*							**0.672**	**0.672**

In the first six of the seven cases, the predicted possibility for the correct dyes was almost as high as the possibility for the incorrect dye (e.g. 0.496 against 0.504 for sample ID 1011). This suggests that such a colour combination could easily be achieved by a combination of different pairs of dyes: e.g. Yellow and Blue I instead of Olive and Blue C, both of which produce a green shade. This kind of error occurs more frequently with unsaturated colours compared to the combination of two complementary dyes. In only one case (below the dashed line) the possibilities for incorrect dyes were considerably higher than for correct ones; only this case can be regarded as a severe error.

Validation of the method

Once the best model was determined and the results analysed, the k-fold cross-validation method was used to estimate the generalisation error [14, 15]. K-fold cross-validation represents the method where data are divided in k subsets of (approximately) equal size. The neural network is trained k times, each time leaving out one of the subsets to be used for testing purposes. At the end of the cross-

Table 6. *Correlations between the actual and predicted dyes in the samples of the full and the cross-validation model for each colour.*

Colour	Full model	C-V model
Yellow	0.940	0.835
Orange	0.943	0.861
Red	0.986	0.958
Red Violet	0.944	0.852
Blue C	0.865	0.581
Blue I	0.874	0.549
Navy Blue	0.949	0.814
Green	0.978	0.927
Olive	0.918	0.790
Brown	0.920	0.811

validation procedure, all data are used once for testing purposes (prediction) and k-1 times for net training. A special case of this method is called 'leave-one-out cross-validation, where each time only one record is omitted from a training set. This method requires as many repetitions of the learning process as there are objects (records) in the data set.

Generating 1430 models for the large data set used in this study would have been very time-consuming. Instead, the 1430 object data set was divided into 30 subsets: 20 containing 48 records and 10 with 47 records, respectively. In each subset we put one randomly selected record from each of the 45 two-dye combinations and, additionally, 2 or 3 records from the 80 single dye records (3 and 2 records in the 48-member and 47-member subsets, respectively). In the cross-validation procedure the net was trained 30 times; each time the training set consisted of 29 subsets, one subset being omitted from the training process. Predictions for this subset were calculated. Correlations with targets were calculated for the full model and cross-validation model. An in-house program was adapted for cross-validation of the counter-propagation neural networks [16]. The results of the cross-validation obtained by the data normalised according to K/S+min-max modification are showed in ***Table 6***.

The highest correlation values for the full model are as high as 0.986 for the Red colour and as low as 0.865 for the Blue C, which is quite good. Understandably, the correlation values of the cross-validation models are lower compared to those of the full model, but one has to take into account that each cross-validation model was trained with sample 48 or 47 left out of the training set. Additionally, it is important to realise that the full training set is based on a minimal experimental design for such a large dye-space and any truncation of data makes the training set much less representative in the regions of omitted data. One should also realise that the correlation values depend on the similarity of colours, namely the smallest correlation values (worst predictions), which are obtained for both blue colours, where the possibility of error is even larger for the visual colouristic evaluation. Samples printed with one of these two dyes (Blue-C or Blue-I) in combination are very close to each other. Therefore, in the cross-validation procedure where a sample printed with, for example, Blue-C dye in the combination is left out in the training phase, the neural network was able to easily assign this sample to any similar combination containing Blue-I in the testing procedure.

Conclusions

In the present work the efficacy of artificial neural networks to aid colourists in determining the dyes appropriate for achieving the required colour has been demonstrated. Although the initial effort of training a neural network and finding the optimal parameters is greater compared to other methods, the advantage of the neural network approach is that once the training phase is completed, determination of new unknown samples is very simple and fast. Further improvement could be done by transforming reflectance values in a way to completely eliminate the influence of different dye concentrations.

The next step of research in this area will be the determination of the quantity of a dye in printing paste for achieving the required colour. Once the correct combination of two constituent dyes is defined, one can use the error back-propagation neural network method to interpolate the concentration of each dye to reproduce the target sample much more precisely and easily. Also, when correct dyes are selected, the possibility of metamerism is very low because the reflectance curve of the target is closely matched.

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