

Optimal colorant design for spectral colour reproduction

*Ali Alsam and Jon Y. Hardeberg
The Norwegian Color Research Laboratory
Dept of Computer Science and Media Technology
Gjøvik University College*

Abstract

The gamut of a colour space is defined by a number of extreme points. The best inks to achieve an accurate spectral reproduction of a given target are those which span the target's spectral gamut. Using a modified non-negative matrix factorization (NMF) algorithm we derive m colorants and their spectral curves such that they are the extreme points of the targets gamut. Using the spectral Neugebauer printing model where eight colorants are assumed we compare our new method with existing techniques. Comparison with a set of optimal rotated principal vectors as well as the classical NMF clearly shows that the performance of the new method is superior.

1. Introduction

The rapid development of digital imaging devices is accompanied by the user-expectation that the quality of the reproduced image is very high. To satisfy this expectation, digital images need to be captured and reproduced with high colour fidelity, i.e. they need to be as truthful as possible to the original. There are two measures to assess colour fidelity, the first is the degree to which an image and its reproduction appear to be identical to a human observer, while the second is the degree to which the spectral data of the image is accurately reproduced in the print.

Due to metamerism, which is the phenomenon that many spectrally different surfaces integrate to exactly the same CIEXYZ response, it is possible to produce a large number of spectrally different prints which appear identical both to each other and to the original image. These images are metameric to each other and satisfy the first colour fidelity measure defined above. Conventional printing, where three to four inks are normally used, is based on the idea that it is sufficient to produce a metameric match of the original image. The main problem with this approach is that the colour of the reproduced image appears to be identical to the original only under certain conditions such as fixed illumination and observer. If the illumination source changes then the reproduced image will no longer appear

to be identical to the original and hence violates our first condition for high colour fidelity quality.

In order for a printed image to be identical to the original under any viewing conditions, it needs to be an exact spectral reproduction of the original. Moreover, if two images are an exact spectral copy of each other then any change in the spectral power distribution of illumination source will affect them equally. Hence an observer will not perceive any differences between the two. Unfortunately, unlike conventional metameric printing, which requires three inks, achieving a spectral match is a challenging process where a larger number of spectrally different inks is needed.

This paper is concerned with the question of how many inks are needed to accurately reproduce a spectral image and which spectral properties these inks should have. Due to practical considerations relating to cost and complexity the number of inks used should be kept to a minimum. Hence the question which we need to answer is which few inks should we use in printing a specific target. From the statistical studies in¹⁻⁴ and others all of which show that a very large number of reflectances can be well described using six to eight basis functions, we might think that the best colorants are related to the basis functions needed to adequately describe the data. Indeed the authors in⁵ proposed a rotated version of the first six basis functions of the spectral data to be used as the best possible colorants.

This paper follows on from the idea presented in⁵, in that we agree with the authors that the properties of the selected inks should be derived from the original spectral image. Though, to optimize the selection of the colorants we combine the selection procedure with the Neugebauer printing model which is considered as the basic physical model for printing systems^{6,7}. The spectral Neugebauer equations state that an arbitrary reflectance can be estimated as a convex sum⁸ of the colorants and their associated combinations. This basic definition indicates that it is not possible to achieve an errorless spectral reproduction of a reflectance unless it is known to be inside the gamut defined by the set of colorants. Hence to minimise the errors in the printing process we choose the colorants such

that the gamut they define encompasses as many as possible of the reflectances which we wish to reproduce.

2. Theory

2.1. Kubelka-Munk Model

The Kubelka-Munk theory is a general theory for predicting the reflectance of single colorants and their combined mixtures. Before we introduce an expression for the reflectance of a mixture of inks we need to define a few basic properties of colorants. The reflectance of an infinitely thick surface is defined as:

$$R_{\infty}(\lambda) = 1 + \frac{K(\lambda)}{S(\lambda)} - \sqrt{\left(\frac{K(\lambda)}{S(\lambda)}\right)^2 + 2\left(\frac{K(\lambda)}{S(\lambda)}\right)} \quad (1)$$

A colorant is infinitely thick, i.e. has reflectance R_{∞} if an increase in the thickness of the colorant layer does not result in a change in its reflectance. $K(\lambda)$ and $S(\lambda)$ in Equation (1) are the spectral absorption and spectral scattering coefficients, respectively.

The ratio between the absorption and spectral scattering coefficient can be obtained by inverting Equation (1), i.e.

$$\frac{K(\lambda)}{S(\lambda)} = \frac{(1 - R_{\infty}(\lambda))}{2R_{\infty}(\lambda)} \quad (2)$$

For a mixture of colorants the absorption coefficient $K(\lambda)$ can be defined as:

$$K(\lambda) = K_p(\lambda) + \sum_{i=1}^{n_k} \zeta_i k_i(\lambda) \quad (3)$$

where $K_p(\lambda)$ is the absorption coefficient of the paper, n_k is the number of inks used and ζ_i is the concentration of colorant i .

The reflectance of a transparent colorant can be written as:

$$R(\lambda) = R_p(\lambda) \exp[-2XK(\lambda)] \quad (4)$$

where X is the thickness of the colorant layer. Inverting Equation (4) we get:

$$K(\lambda) = -0.5 \ln \left[\frac{R(\lambda)}{R_p(\lambda)} \right] \quad (5)$$

where \ln is the natural logarithm.

Finally, using Equations (4) and (3) we can write the reflectance of a mixture of colorants as:

$$R(\lambda) = R_p(\lambda) \exp \left[-2X \left(K_p(\lambda) + \sum_{i=1}^{n_k} \zeta_i k_i(\lambda) \right) \right] \quad (6)$$

2.2. Neugebauer Printing Model

The Neugebauer printing model is an attempt to mathematically account for halftone printing⁹. Neugebauer recognized that given two concentration levels for a colorant, i.e. full concentration and zero then there are

$$N = 2^{n_k}, \quad (7)$$

colorant combinations. Hence if the number of inks is $n_k = 3$ then the number of combinations $N = 2^3 = 8$. The ink combinations are known as the Neugebauer primaries and can be calculated using the Kubelka-Munk or the Beer-Bouguer¹⁰ models. Given these primaries, we can use the Neugebauer equation to model an arbitrary reflectance as:

$$R(\lambda) = \sum_{i=1}^N w_i P_i \quad (8)$$

where, w_i is the i th area coverage of the i th Neugebauer primary with reflectance P_i . By default all w_i have to be positive numbers defined in the range $0 \leq w_i \leq 1$. Furthermore, the sum of all w_i has to be equal to one. Given these properties, we can rewrite the classical Neugebauer equation as:

$$R(\lambda) = \sum_{i=1}^N w_i P_i \text{ subject to } \sum_{i=1}^N w_i = 1 \quad (9)$$

In the parlance of convex optimization⁸ Equation (9) states that a given reflectance is a strict convex combination of the Neugebauer primaries.

3. Selecting Colorants

To aid our discussion we divide the Neugebauer primaries into two basic types. The first includes the actual colorants of the printer while the second is any combination of these as defined by the Kubelka-Munk model described previously. In the remaining sections of this paper our focus is directed towards deriving an optimal set of the first type, i.e. a set of vectors which when used as colorants result in the best possible reproduction of the spectral data.

3.1. Rotated PCAs as colorants

In this section we assume that the best colorants are a rotated version of the first few principal basis functions spanning the space of the spectral data to be reproduced. The principal vectors describing the space of general reflectance are characterized by having both negative and positive values and are often bipolar⁵. See Figure 1 where a set of eight basis functions are shown. Using a limited number

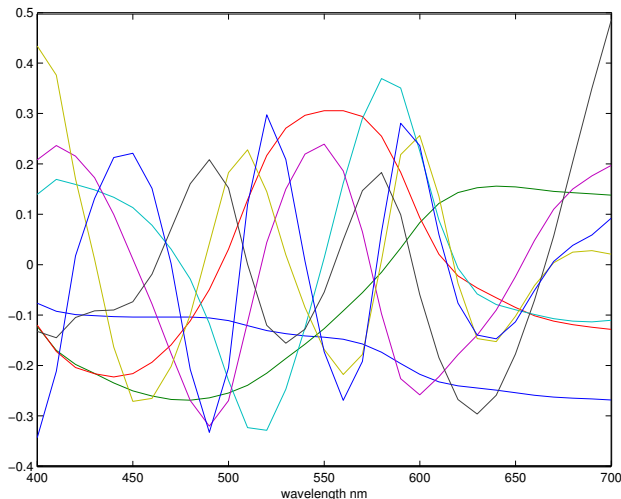


Figure 1: The first eight PCA basis functions obtained from the spectral data of the Esser calibration target.

of PCA basis functions we can approximate a set of spectral vectors as:

$$R \approx B\sigma \quad (10)$$

where R is an $n \times m$ matrix whose columns are the m spectral vectors to be reproduced, B is an $n \times f$ matrix encompassing the first f PCA basis vectors describing the space of R and σ are linear weights.

Evidently, the basis functions in Figure 1 don't correspond to natural, physically realizable surfaces and inks. To transform these basis functions such that they are a closer representation of physical ink spectra the authors in⁵ used a "constrained-rotation engine". The description of such a "constrained-rotation engine" given in⁵, does not infer that the rotation is optimal. To calculate the colorants based on the assumption made in⁵ that the best colorants are a rotated version of the first principal components with an added optimality criterion, we used the rigid varimax rotation described in^{11,12}. Using a rigid rotation results in a new set of basis function, which are strictly orthogonal but different to the original principal components the rotated basis function are mostly positive. The relation between the original and rotated basis functions is:

$$\hat{B} = BT \quad (11)$$

where \hat{B} are the rotated basis vectors and T is an $f \times f$ rigid rotation matrix. The rotated basis functions obtained from the varimax rotation based on the PCA vectors in Figure 1 are plotted in Figure 2. We see in Figure 2 that the resultant rotated vectors \hat{B} have negative values, which contradicts the natural properties of colorants spectra. Imposing a positivity constraint on the output of the varimax rotation enables us to solve for strictly positive functions which are

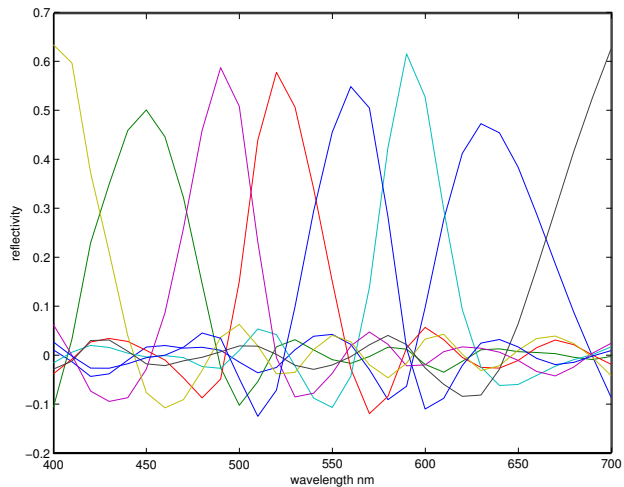


Figure 2: The rotated eight PCA basis functions obtained using the varimax rotation.

as close as possible to the original basis vectors. Mathematically, we can represent the positivity constraint as a minimization problem of the form:

$$\min \|B\alpha - \hat{b}\|^2 \text{ subject to } B\alpha \geq 0 \quad (12)$$

where B are the original basis functions, α are linear weights and \hat{b} is the i th rotated basis as described in Equation (11).

Figure (3) shows the rotated version of the basis functions with the added positivity constraint.

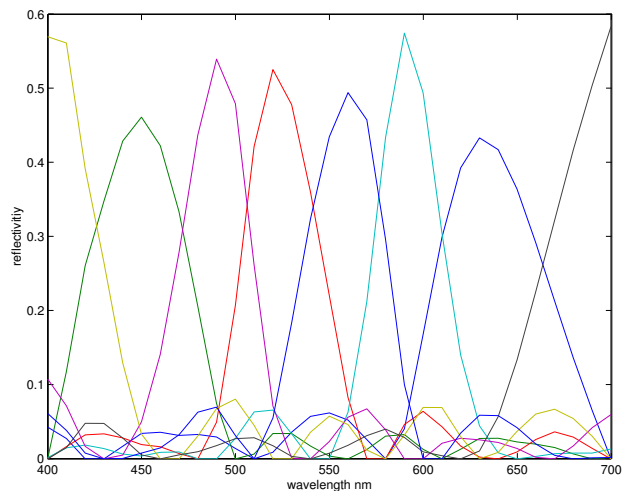


Figure 3: The rotated eight PCA basis functions obtained using the varimax rotation with an added positivity constraint.

3.2. Non-Negative Matrix Factorisation

In Section 3.1 we had to solve for the basis function, find an optimal rotation, and finally, solve for feasible all positive colorants. We might thus wonder if it is possible to factorise the colour signal matrix into a set of optimal basis functions and associated weights as in Equation (10), with the added constraint that the basis functions are strictly positive. In¹³ Buchsbaum and Bloch used a technique called non-negative matrix factorisation (NMF) to solve for such a non-negative basis set.

The method is due to Lee and Seung¹⁴, who introduced an algorithm to factorise a strictly positive matrix such that the bases and the weights are constrained to be non-negative. Given our non-negative spectral matrix R , we write:

$$R \approx WH \quad (13)$$

where W is an $(n \times r)$ matrix of non-negative basis vectors and H is an $(r \times m)$ matrix of positive weights.

In terms of the Euclidian distance the problem we are trying to solve is:

$$\min_{W, H} \|R - WH\|^2 \text{ subject to } W, H \geq 0 \quad (14)$$

To solve the minimization in Equation (14) we need to iteratively update W and H until we converge to the best factorization. An example of such an iterative procedure is discussed in¹⁴.

3.3. A modified NMF

The minimization in Equation (14) factorizes R into two matrices one containing all positive basis functions and another containing the corresponding positive weights. Hence if we were to carry out this factorization for a set of spectral vectors then the resultant basis vectors W will be optimized to represent the data set. In this sense the columns of W are the best colorants to be used in the Neugebauer model described in Equation (8). Unfortunately, the weights encompassed in matrix H do not necessarily sum to one as is required in Equation (9). Hence we might wonder if it is possible to modify the non-negative matrix factorization algorithm proposed in¹⁴ such that all the elements in the resultant weight matrix H are strictly positive and the sum of each column is exactly one. To see how we might proceed we note that the i th column vector in the data matrix R can be written as a linear combination of the basis vectors in W and the corresponding weights, where those are the elements of the i th column of H , i.e.:

$$r \approx Wh \quad (15)$$

Hence to incorporate the added constraint, we can cast Equation (14) as a minimization problem of the form:

$$\min_h \|r - Wh\|^2 \text{ subject to } h_i \geq 0 \text{ and } \sum_{i=1}^r h_i = 1 \quad (16)$$

The result of the minimization described in Equation (16) is a weight's matrix H whose elements are all positive. Moreover, the sum of each of its columns is exactly one.

4. Implementation

From the minimizations described in Equations (14) and (16), we note that the procedure of factorizing a matrix R into two matrices W and H involves an optimization problem in terms of the two solution matrices, i.e. W and H . In this section we present a brief description of the factorization algorithm used by the authors.

1. Starting from a set of all positive spectra R ,
2. Let W^0 be an $n \times r$ arbitrary positive matrix.
3. Solve the minimization problem in Equation (16) for H , i.e. $\min_h \|r - W^0 h\|^2$ subject to the constraints described in (16)
4. Calculate W^{i+1} using a gradient descent update rule¹⁵ that reduces the squared distance $\|R - WH\|^2$. In this paper we used the following update rule:

$$W^{i+1} = W^i + \mu(R(H^i)^T - W^i H^i (H^i)^T) \quad (17)$$
 where μ is a small positive value.
5. set any negative value in W to zero.
6. If an element in w is greater than 1, divide w by the maximum value.
7. Iterate until $\|R - WH\|^2$ is smaller than a user defined tolerance.

5. Results

To test the modified non-negative matrix factorization and compare its performance with that of the rotated principal vectors and the conventional NMF, we used the algorithm to select a set of eight basis functions. Further, we assumed that the retained basis vectors are the available colorants and calculate the Neugebauer primaries using the Kubelka-Munk model. Hence we obtained $2^8 = 256$ primaries. Using the same procedure we calculated the Neugebauer primaries based on the rotated PCAs and the NMF. The calculations of the basis function for all the techniques were

based on a set of 264 reflectances obtained from the Esser calibration target.

The estimated basis functions obtained from the classical and modified NMF are shown in Figures (4) and (5). The rotated principal vectors for the same data set are those shown in Figure (2).

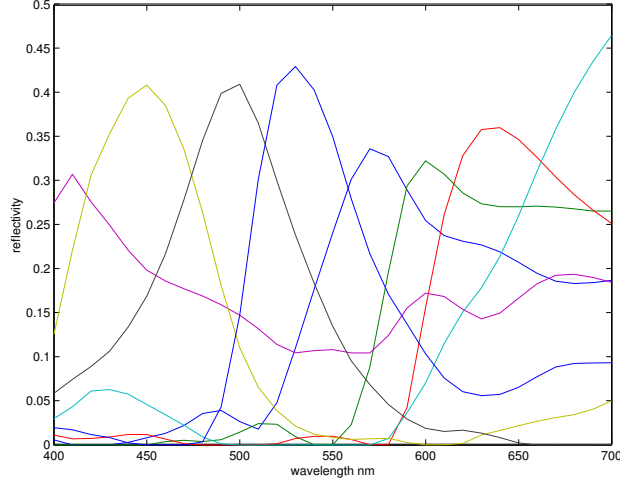


Figure 4: The best eight non-negative basis functions obtained from the spectral data of the Esser calibration target.

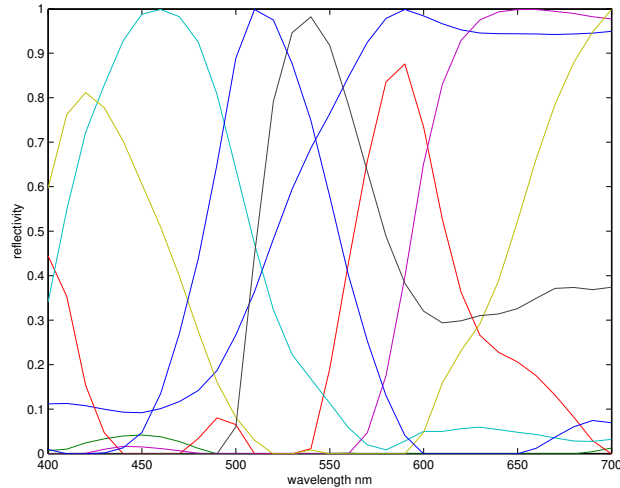


Figure 5: The best eight non-negative basis functions obtained using the new method. The basis functions are based on the spectral data of the Esser calibration target.

Using the basis functions from each method and the associated Neugebauer primaries we were able to assess the performance of the bases as colorants to reproduce the spectral data of the Esser calibration target¹⁶. This chart was chosen due to its high dimensionality. Knowing that

we are interested in a spectral match we used the spectral Neugebauer model described in Equation (9). Thus, for each method, namely, the rotated PCAs, NMF, and the modified NMF we obtained a set of 264 reflectance estimates.

Two metrics were used as a measure of the goodness of reproducing the Esser calibration target with the estimated colorants, these are the relative means squares error defined as:

$$E = \frac{\|r - \hat{r}\|^2}{\|r\|^2} \quad (18)$$

where r is the actual measured reflectance and \hat{r} is the estimate. The resultant error for the three methods were sorted in decreasing order and plotted in Figure (6). As is evi-

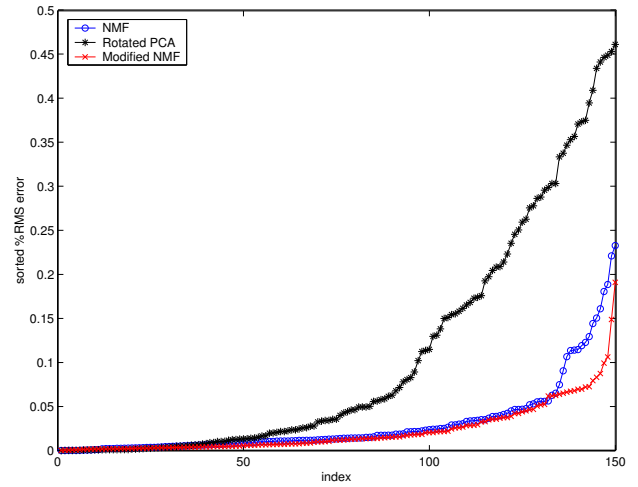


Figure 6: The relative mean square error for the rotated PCA, the classical and modified non-negative matrix factorization.

dent in Figure (6) the performance of both the classical and modified NMF algorithms is clearly superior to that of the rotated PCAs. Further, the colorants chosen by the modified non-negative matrix factorization technique improve the maximum error level of the classical NMF.

To assess the goodness of the methods in a perceptual space as well as its robustness under varying illumination conditions we calculated the perceptual difference ΔE_{ab}^* for all the surfaces under six different illuminants. The results for the rotated PCAs, the classical, and modified NMF are tabulated in Tables 1, 2, and 3, respectively. Clearly, the performance of the non-negative matrix factorization is much better than that of the rotated PCAs. Further, the modified non-negative matrix factorization algorithm proposed in this paper, is superior to that of the classical NMF. We especially note that the difference in the maximum ΔE_{ab}^* error which is around one half that achieved with the classical technique under all illuminants.

Table 1: The mean, median, and maximum absolute ΔE achieved by assuming that the colorants are a rotated version of the first eight PCA basis vectors.

Rotated PCA	ΔE	ΔE	ΔE	ΔE	ΔE	ΔE
illuminant	D50	D65	F2	F7	F11	A
mean	14.03	13.98	14.87	14.27	14.86	13.93
median	2.77	2.51	2.95	2.55	3.53	2.37
max	97.43	98.11	104.04	99.93	103.39	94.26

Table 2: The mean, median, and maximum absolute ΔE achieved by assuming that the colorants are the first eight NMF basis vectors.

NMF	ΔE	ΔE	ΔE	ΔE	ΔE	ΔE
illuminant	D50	D65	F2	F7	F11	A
mean	3.03	3.11	3.11	3.21	3.63	2.77
median	0.12	0.10	0.18	0.14	0.44	0.13
max	53.89	56.04	53.39	56.41	58.70	46.91

Table 3: The mean, median, and maximum absolute ΔE achieved by assuming that the colorants are the first eight modified NMF basis vectors.

Modified NMF	ΔE	ΔE	ΔE	ΔE	ΔE	ΔE
illuminant	D50	D65	F2	F7	F11	A
mean	1.18	1.19	1.40	1.27	1.54	1.21
median	0.06	0.06	0.18	0.16	0.38	0.06
max	20.42	21.37	21.86	21.57	23.22	19.82

6. Conclusions

In this paper we presented a new method which we call a modified non-negative matrix factorization. Using this method we selected a set of colorants to reproduce a colour target. By comparing the selected colorants with those achieved using other methods we found that the performance of the new techniques is clearly superior to the existing techniques.

References

[1] L. T. Maloney and B. A. Wandell. Color constancy: a method for recording surface spectral reflectance. *Journal of the Optical Society of America A*, **3**(1), 29–33 (1986).

[2] Yinlong Sun, F. David Fracchia, and Mark S. Drew. A composite model for representing spectral functions. *Technical report*, (1998).

[3] J. Parkkinen, J. Hallikainen, and T. Jaaskelainen. Characteristic spectra of munsell colors. *Journal of the Optical Society of America A*, **6**(2), 318–322 (1989).

[4] Jon Y. Hardeberg. On the spectral dimensionality of object colors. In *Proceedings of CGIV'2002, First*

European Conference on Colour in Graphics, Imaging, and Vision, pp. 480–485, Poitiers, France (2002).

[5] D. Tzeng and R. Berns. Spectral-based ink selection for multiple-ink printing I. Colorant estimation of original object. In *Proceedings of IS&T/SID's 6th Color Imaging Conference: Color Science, Systems, and Applications*, pp. 106–111 (1998).

[6] Marc Mahy and Paul Delabastita. Inversion of the neugebauer equations. *Color Research and Application*, **21**(6), 401–411 (December 1996).

[7] H. E. J. Neugebauer. Die theoretischen grundlagen des mehrfarbendruckes. *Zeitschrift fur wissenschaftliche Photographie Photophysik und Photochemie*, **36**(4), 73–89 (1937).

[8] Joseph O'Rourke. *Computational Geometry in C, 2nd Edition*. Cambridge University Press (1998).

[9] Henry R. Kang. *Color Technology for Electronic Imaging Devices*. SPIE Optical Engineering Press (1997).

[10] G. Wyszecki and W. S. Stiles. *Color Science: Concepts and Methods, Quantitative Data and Formulae*. John Wiley & Sons, 2 nd edn (1982).

[11] H. F. Kaiser. The varimax criterion for analytic rotation in factor analysis. *Psychometrika* **23**, , 187–200 (1958).

[12] Richard A. Reymont and K.G. Joreskog. *Applied Factor Analysis in the Natural Sciences*. Cambridge University Press (1993).

[13] G. Buchsbaum and O. Bloch. Color categories revealed by non-negative matrix factorization of munsell color spectra. *Journal of Vision Research*, **42**, 559–563 (2002).

[14] Daniel D. Lee and H. Sebastian Seung. Algorithms for non-negative matrix factorization. In *Advances in Neural Information Processing Systems 13*, (2001).

[15] J. Kivinen and Manfred K. Warmuth. Additive versus exponentiated gradient updates for linear prediction. *Journal of Information and Computation*, vol. **132**, no. **1**, , 1–64 (1997).

[16] Esser Charts. <http://www.esser-test-charts.com/>.