Non-negative matrix factorization using genetic algorithm for spectral colors

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SUMMARY   In this paper we introduce novel methods for non-negative matrix factorization (NMF) using a genetic algorithm. The methods find the optimal basis functions for the spectral colors in both spectral and color spaces. We show that one of the proposed algorithms works as well as the standard NMF algorithm in spectral space. Further, this algorithm is modified to obtain a functionality to work in color space which the standard NMF is currently not capable to provide. The modification involves optimization in color space reducing the approximation error by a factor of 6 for Macbeth ColorChecker colors. The algorithm can be used in digital camera design. In addition, we propose an algorithm based on multiobjective optimization in both spectral and color space which can be used in digital image archiving.
key words: Genetic algorithm, spectral colors, Macbeth ColorChecker, non-negative matrix factorization

1. Introduction

Non-negative Matrix Factorization (NMF) gives a representation of the latent data structure and reduces the dimensionality of the data. There are at least two good physical reasons to use the technique for spectrometry and imaging: Firstly, optical sensors generate non-negative signals, that may require non-negative decomposition, and, secondly, the optical color filters can be physically implemented only with non-negative spectral characteristics [1]. In multispectral imaging, for example, the technique may be used to calculate the digital camera spectral band characteristics and is particularly attractive for spectral reflectance estimation using the Wiener method [2].

NMF solves the problem of non-negative data decomposition [3–6]. NMF was used in spectral unmixing for non-resolved space object characterization [3]. NMF and a related technique called non-negative tensor factorization (NTF) were used to define the optimal non-negative representation of spectral colors for different sets including the Macbeth ColorChecker (MCC) and Munsell color set [1], [7]. NMF method represents the measured spectra by a

few non-negative basis functions. NMF determines non-negative factors W and Z implementing non-negative factorization of the given matrix X as follows: $X \approx WZ$. If the size of V is the number of wavelengths times the number of spectra then the columns of W are the basis functions found minimizing the error of approximation while Z is a matrix of weights.

Here we mainly study three band systems which are most popular in camera industry. If the three spectral responses of the color sensor of a camera are equal to the color matching functions of the Standard Observer then color is reproduced correctly. This is not achieved, yet. The reason is that for display and printer control the transformed matching curves are used [8]. Therefore a further study for color image acquisition in digital cameras optimized for color matching functions is required. This can be based on the NMF approach. For example, the basis functions found by NMF optimized in spectral space give rough representation of shapes, wavelength subranges and the location of the modes for color matching functions (Fig. 1). However, the published results [1], [7] only reported about spectral optimization that is rather rough while the accurate approximation of colors is required.

In this paper we propose the genetic algorithm (GA) as an optimization technique for solving the NMF task. Our purpose is to find non-negative basis functions to obtain accurate color reproduction for the given spectral dataset. The following three novel algorithms are developed: non-negative matrix factorization in the spectral space, non-negative matrix factorization regarding the color space, and optimization in both spectral and color spaces. The first algorithm optimized in spectral space achieves similar performance as the standard NMF. Then, this algorithm is modified to obtain a new functionality to work in color space which the standard NMF is currently not capable to provide. The modification involves optimization in color space and gives much more accurate result.

The paper is arranged as follows: The methodology is considered in Section 2, the algorithms are discussed in Section 3, experimental results are given in Section 4, and conclusions are given in Section 5.

2. Methodology

The GA is known as a search technique for large spaces and is superior to other optimization methods when require-

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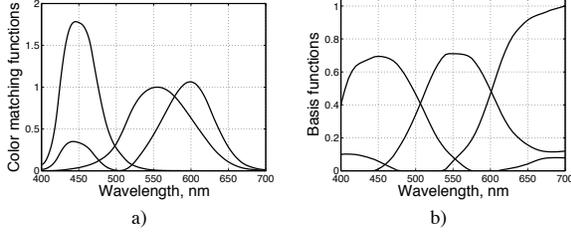
Fig. 1 Spectral curves. a) The CIE 1931 color matching functions of Standard Observer. b) The normalized basis functions calculated using standard NMF and optimized in a spectral space.

Fig. 2 Diagram.

ments for function features like smoothness, continuity and differentiability are violated [9]. In addition, the GA concept is easy to understand and implement, works in noisy environments and supports multiobjective optimization.

The GA contains a population of individuals and assesses the fitness of individuals for each generation. We consider matrices $X \in \mathbb{R}^{d \times n}$, $W \in \mathbb{R}^{d \times r}$ and $Z \in \mathbb{R}^{r \times n}$, where d is the number of wavelengths, n is the number of spectral colors, and r is the maximum number of basis functions or the rank of factorization. The number of basis functions can be less or equal to the rank of factorization. We use the GA to define the best subset of variables according to the fitness function:

$$\min_{W,Z} \frac{1}{2} \sum_{i=1}^{n} \|x_i - W z_i\|^2$$

$$\text{subject to } W \geq 0; \ z_i \geq 0,$$

(1)

where x_i and z_i are the columns of the matrices X and Z, respectively.

On the other hand, GA provides an elegant way to select the best variables for color representation minimizing the color difference. The representation of individuals in this case is illustrated in Fig. 2. The individuals or chromosomes are presented by real valued vectors which live in the genotype space. The problem specific solutions are located in the visual phenotype space as colors. The mapping between the spaces is made using encoding and decoding. The encoding is usually not used while decoding the real valued vectors (spectra) helps to evaluate individuals according to their fitness function. From the spectral color viewpoint the genotype space corresponds to the physical spectral space, while the phenotype space relates to the physiological color space. The decoding is identical to the spectrum-to-color conversion, used in spectral imaging [10]. Thus, the real valued vectors/chromosomes are spectra and the problem specific solutions achieve color difference minimization.

Let $f()$ be a decoding function, i.e. a spectrum-to-color conversion function, then $\left\|\Delta E_{abi}^*\right\|^2 = \|f(x_i) - f(W z_i)\|^2$, where ΔE_{ab}^* is a CIELAB color difference:
$\Delta E_{ab}^* = \sqrt{(L_x^* - L_{Wz}^*)^2 + (a_x^* - a_{Wz}^*)^2 + (b_x^* - b_{Wz}^*)^2}$. We denote $|L_x^* \ a_x^* \ b_x^*|^T = f(x)$ and $|L_{Wz}^* \ a_{Wz}^* \ b_{Wz}^*|^T = f(W z)$.

In this case the fitness function in color space is as follows:

$$\min_{W,Z} \frac{1}{2} \sum_{i=1}^{n} \|f(x_i) - f(W z_i)\|^2$$

$$\text{subject to } W \geq 0; \ z_i \geq 0.$$

(2)
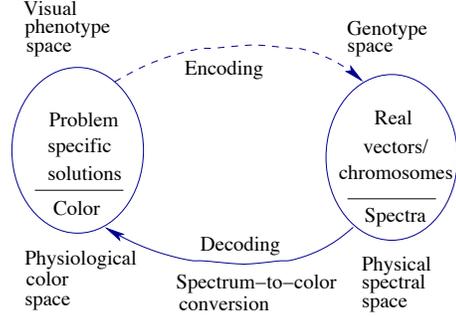
3. Algorithms

Three algorithms based on fitness functions are considered. The first algorithm is for the basis functions optimized in the spectral space (GA-NMF-S). The second algorithm is for the basis functions optimized in the color space (GA-NMF-C). The third algorithm uses multiobjective optimization for both the spectral and color spaces (GA-NMF-M). The pseudo-code for all these algorithms is as follows:

$t := 0$;
initialize P(t);
evaluate P(t);
while *not terminate* **do**
 $P'(t) := $ *select-mates(P(t))*;
 $P''(t) := $ *crossover(P'(t), pc)*;
 $P'''(t) := $ *mutate(P''(t), pm)*;
 $P''''(t)) := $ *smooth(P'''(t), ps)*;
 evaluate(P''''(t));
 $P(t) := P''''(t)$;
 $t := t + 1$;
end
Algorithm 1: GA-NMF-*i* algorithm, $i = $ S,C,M.

We denote by $P(t)$ a population consisting of individuals, and pc, pm and ps the probabilities for operations: *crossover*, *mutate*, and *smooth*, respectively. We use two kinds of populations to define the columns of W, i.e. basis functions, and the rows of Z. For both populations the sequence of procedures presented in Algorithm 1 is the same and, apart of the operation *mutate*, all procedures are identical.

3.1 Initialization

The presented Algorithm 1 is similar to general GA except for the initialization and the operation *smooth*. The initialization is important because it may affect the algorithm performance. In our earlier study we used a random initialization of W with Gaussian functions [11]. These functions

were utilized because of a priori knowledge that the resultant basis functions should be bell shaped and to provide the diversity of population that is is needed for evolution. For this purpose the Gaussians are more desirable than, for example, piecewise linear functions. However, the random initialization of GA, and the standard NMF as well, leads to variations in results. To avoid the random initialization and to improve performance of the standard NMF the non-negative singular value decomposition (SVD) for initialization and SVD-NMF algorithm were proposed [12]. We adopted this approach for GA-NMF and modified our operation *initialization*. For that we use singular value decomposition:

$$X = USV^T,$$

where S is the diagonal matrix of singular values, $S = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$, $\sigma_1 > \sigma_2 > \ldots, \sigma_n$, the columns of matrices U and V are the left singular vectors and the right singular vectors of S, respectively, and T is transpose.

Let us assume the rank r of factorization is less than n, $r < n$, and compute a fraction ($< 90\%$) of the total data variance to be retained. The retained variance in percents is as follows:

$$\frac{\sum_{i=1}^{r} \sigma_i}{\sum_{i=1}^{n} \sigma_i} 100\% < 90\%.$$

Then, we define the matrices $U_r = (u_1, u_2, \ldots, u_r)$ and $S_r = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_r)$ consisting of the first r^{th} vectors and the first r^{th} singular values of matrices U and S, respectively.

Finally, we initialize matrices W_{init} and Z_{init} as follows:

$$W_{init} = |U_r|, \qquad Z_{init} = |S_r V^T|.$$

The rank r defines the maximum number of basis functions. In experiments we use the number r_b of basis functions, $r_b \leq r$.

The initialization made for the standard NMF can be used to generate only one individual. Therefore, we modify this approach to initialize the whole population. We employ the SVD initialization followed by NMF with the update rule called local non-negative matrix factorization (LNMF) [12]:

$$Z \leftarrow \sqrt{Z. * (W^T * (X./(WZ)))},$$
$$W \leftarrow W. * ((X * Z^T)./(WZZ^T)).$$

We take each even solution of the first 100 iterations of the SVD-NMF algorithm to obtain the population size 50. To determine the population size we follow suggestion that the optimal population size for problems coded as bitstrings is approximately the length of the string [13]. Though we use real valued strings we follow this rule. Hence, the population size, i.e. 50, is approximately defined by the number of wavelengths, i.e. 61.

3.2   Selection, crossover and mutation

The operation *select-mates* makes the tournament selection of parents. The operation *crossover* is based on uniform crossover with probability $pc = 0.9$.

The operation *mutate* is different for W and Z. For individuals of W, the gene value w_{ij} is randomly selected and changed using a random value $a \sim \mathcal{N}(0, 1)$ as follows: $w_{ij} = w_{ij} + 0.0005a$. Similarly for z_{ij}, $z_{ij} = z_{ij} + 0.2a$. When the value w_{ij} or z_{ij} become less than zero it is set to zero. The selected value for probability of mutation is $pm = 1/61$.

The designed algorithms have the deterministic initialization but selection is still random. Therefore the results have small variations at each algorithm run which can be neglected.

3.3   Smoothing

The crossover and mutation may produce abrupt changes of values in the neighbor genes of the chromosomes that lead to spiky basis functions. To solve this problem we introduce the smoothing operation *smooth* for columns of W and for rows of Z with a simple averaging window comprising three elements. Testing shows that a good probability of smoothing is about 10 times less than the probability of crossover, i.e. $ps = 0.1$.

3.4   Evaluation and fitness functions

The three proposed algorithms have different operation *evaluate*. For the algorithms GA-NMF-S and GA-NMF-C the fitness functions are the same as the objective functions: Eqs. 1 and 2, respectively.

In multiobjective optimization (GA-NMF-M) a Pareto ranking approach is utilized [14]. The objective value of each solution is not assigned in this case. The population is ranked according to a dominance rule in the objective space. The operation *evaluate* is replaced by three operations: *evaluateS*, *evaluateC* and *rank*:

$E_s(t) := evaluateS\ (P(t));$
$E_c(t) := evaluateC\ (P(t));$
$rank\,(E_s(t), E_c(t));$

The operations *evaluateS* and *evaluateC* calculate the objective functions $E_s(t)$ (Eq. 1) and $E_c(t)$ (Eq. 2), respectively. Finally, the solutions are evaluated using the operation *rank* which calculates fitness value based on solution rank in population. We adopt the fitness assignment ranking based on a lower rank corresponding to the best solution [14,15].

4.   Experiments

The experiments were conducted with MCC spectral colors in two spaces: spectral and color. The number of wavelength of spectra was taken at 5nm intervals in the VIS range (400-700nm). The number of basis functions tested was three. Two light sources (D65 and Halogen) were utilized in tests. Three spectral datasets were used in experiments (Tab. 1). For the paint dataset we increased the number of

wavelengths originally taken at 10nm from 31 to 61 using linear interpolation.

Table 1 Spectral datasets. The first dimension of size is the number of wavelengths and the second one is a number of samples.

| Dataset	Size
Macbeth ColorChecker	61×24
Munsell color dataset [16]	61×1269
Paint dataset [17]	61×91

4.1   Spectral space

The non-negative matrix factorization was implemented in spectral space. The Algorithm 1 with fitness function according to Eq. 1 and initialization described in Section 3 was used.

The parameters for GA were as follows. The individual length for columns of W was 61. The individual length for rows of Z corresponded to the number of samples (Tab.1). The number of iterations was 200,000, except for the Munsell set it was 1,000,000 iterations. The population size was 50 for all tests.

We make a comparison of GA-NMF-S with a standard NMF algorithms which can be divided into several classes: Multiplicative update algorithms, gradient descent algorithms, and alternating least squares (ALS) algorithms. For these algorithms the statements about convergence (global or local) have not been proven though the ALS algorithm will converge to a local minimum in certain special cases [3]. The multiplicative update algorithms are the first well-known NMF algorithms which often converge in practice. They have become the baseline versus the new developed algorithms. Therefore, the multiplicative update algorithms were selected for comparison with GA. The statement about convergence of GA has been neither proved. However, it is known that GA may have tendency to converge to the local minimum. The GA algorithms are widely used to obtain high-quality solutions for hard complex optimization problems.

For comparison we give the result for MCC using the standard NMF algorithm, 200,000 iterations (Fig. 1b) [4]. The result for GA-NMF-S is shown in Fig. 3a. The results are similar. In addition, the MSE values for each spectral color are given (Tab. 2). The GA-NMF results are slightly better than those of the standard NMF. We implemented algorithms in Matlab and used a 2.5GHz laptop computer with Windows. The computational time for standard NMF obtained 101s versus the GA-NMF-S computational time 220s. At this point the most important factor for us is to achieve an accuracy similar to the standard NMF. At the next step we will modify the GA-NMF algorithm to obtain the new functionality to work in color space which the standard NMF has not. The standard NMF is based on an update rule working in the physical spectral space and is not capable to work in color space. It will be shown that the optimal basis functions related to color space approximate significantly
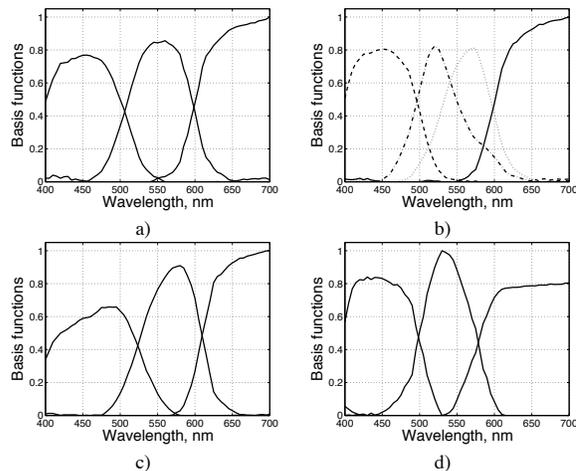
Fig. 3 Algorithm GA-NMF-S. a) Three normalized basis functions for MCC. b) Four normalized basis functions for MCC. c) Three normalized basis functions for paint dataset. d) The three normalized basis functions for Munsell dataset.

Table 2 Spectral approximation. MSE for standard NMF and GA-NMF-S. The table cell order corresponds to the order of color patches of MCC.

| Standard NMF, average: 0.0031					
0.0005	0.0035	0.0013	0.0010	0.0037	0.0049
0.0045	0.0011	0.0031	0.0017	0.0032	0.0052
0.0014	0.0018	0.0045	0.0049	0.0040	0.0035
0.0125	0.0055	0.0022	0.0008	0.0002	0.0000
GA-NMF-S, average: 0.0014					
0.0004	0.0006	0.0004	0.0007	0.0028	0.0037
0.0035	0.0004	0.0005	0.0021	0.0008	0.0033
0.0009	0.0013	0.0024	0.0003	0.0031	0.0034
0.0012	0.0004	0.0003	0.0001	0.0000	0.0000
GA-NMF-M, average: 0.0017					
0.0004	0.0006	0.0005	0.0011	0.0034	0.0042
0.0048	0.0005	0.0007	0.0025	0.0006	0.0051
0.0012	0.0014	0.0030	0.0007	0.0040	0.0046
0.0013	0.0005	0.0004	0.0003	0.0001	0.0001

better colors.

Though our main purpose is to study three-band systems we test the potential of our method also for a four-band system. We note that SVD initialization define the rank of matrix factorization [12]. According to this approach the rank cannot be higher than four, i.e. four basis functions, for MCC. The result is shown in Fig. 3b.

In addition, we tested other datasets. The results are shown in Figs. 3c,d. The results for the paint dataset differ from the previous one. This can be explained by different colors presented in a set particularly for artistic purposes. The results for Munsell dataset is much closer to the test results with Macbeth colors.

4.2   Color space

GA-NMF gives a simple and straightforward way for matrix factorization optimized for color difference. This does not apply to the standard NMF. We utilized GA-NMF-C with a fitness function based on color difference (Eq. 2) and
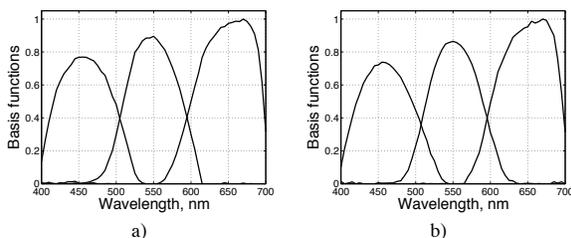
Fig. 4 Normalized basis functions calculated using GA-NMF-C for MCC and different light sources: a) D65. b) Halogen.
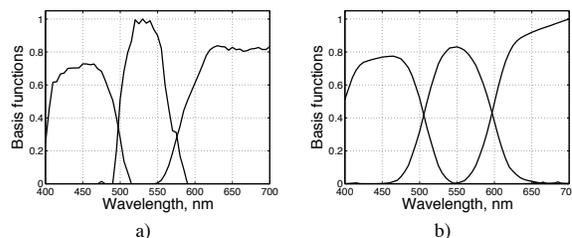

Fig. 5 Normalized basis functions. a) Algorithm GA-NMF-C for Munsell dataset. b) Algorithm GA-NMF-M for MCC.

initialization described in Section 3. The rest GA parameters are indentical to that of GA-NMF-S. The spectrum-to-color conversion was used for decoding [10]. For conversion we use the illuminants: D65 and Halogen, and CIE 1931 color matching functions. The results were obtained using 200,000 iterations. The results are presented in Fig. 4 and Tab. 3.

Table 3 Color approximation, light source D65. The color difference CIELAB ΔE. The table cell order corresponds to the order of color patches of the MCC.

GA-NMF-S, average: 6.47					
2.10	1.55	2.20	7.90	6.92	12.85
14.24	3.62	4.18	8.75	7.62	11.58
10.93	13.45	11.86	3.25	5.09	16.28
2.22	2.49	2.20	1.96	1.36	0.77
GA-NMF-C, average: 1.14					
2.62	0.10	0.14	1.46	1.32	0.64
0.67	1.15	1.72	0.80	1.14	1.42
0.96	0.54	0.80	0.52	1.21	2.85
0.43	1.44	1.31	0.68	0.96	2.37
GA-NMF-M, average: 2.99					
2.07	1.51	0.90	2.82	3.97	6.09
4.98	0.84	2.00	4.23	2.33	5.01
1.32	4.68	4.38	2.71	3.12	6.00
2.37	2.00	1.39	1.49	1.59	4.05

From the basis functions and color matching functions in Figs. 1a, 3a, and 4a, and Tab. 3, one can clearly see that the basis functions optimized in color space are much more accurate than in spectral space. For Macbeth colors ΔE_{avg} is reduced about six times (Tab. 3). The basis functions are quite bell shaped, and better define the wavelength subranges and modes of the curves. For the long-wavelength curve the result is still not good but this curve at least approximately defines the subrange of wavelengths. Surprisingly, the results does not change much if light is varied (Fig. 4a,b).

In addition, we tested the paint dataset and the Munsell dataset using the GA-NMF-C algorithm given 200,000 iterations and 1,000,000 iterations, respectively. The light source D65 was used. For the Munsell dataset the basis functions become more bell shaped (Fig. 5a) than those in Fig. 3d though the functions are less smooth. The similar result was obtained for the paint dataset. For GA-NMF-S (paint dataset) $\Delta E_{avg} = 15.05$ and for GA-NMF-C $\Delta E_{avg} = 7.56$. For GA-NMF-S (Munsell dataset) $\Delta E_{avg} = 12.53$ and

for GA-NMF-C $\Delta E_{avg} = 8.52$.

4.3 Multiobjective optimization

In the final conducted experiment we explored the advantage of GA in multiobjective optimization (GA-NMF-M). We search the optimal basis functions for both spectra and colors using criterion based on the Pareto front described in Section 3. The results are presented in Fig. 5b, Tabs. 2, and 3. The results represent the trade-off between two marginal cases: spectral and color optima. The algorithm is less accurate than corresponding single objective algorithms in color space. The multiobjective algorithm can be used in digital image archiving to help to use one set of basis functions instead of two sets: spectral and color.

5. Conclusions

We developed three new algorithms for NMF using GA. The first algorithm GA-NMF-S finds the optimal basis functions of spectral color set in the spectral space. The algorithm performs as well as the standard NMF algorithm. The second algorithm GA-NMF-C finds optimal basis functions for color space. To the best of our knowledge this is a new result. The basis functions in this case are closely bell shaped and shows more accurate the mode locations of the spectral curves. The algorithm accurately approximates colors. The third algorithm GA-NMF-M uses multiobjective optimization in spectral and color spaces.

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