NTF vs. PCA Features for Searching in a Spectral Image Database

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Abstract

A technique for searching in a spectral image database is proposed in this study. It is based on a similarity measure between spectral image features. New and convenient spectral image features are introduced and compared here. Non-negative tensor factorization (NTF) and principal component analysis (PCA) are applied in a spectral image domain to characterize colors of a spectral image. A new way of NTF with a multiresolution approach is used to accelerate the time complexity in the extraction of the features.

The proposed method is implemented and tested with a spectral image database. The images from the database are ordered according to the similarity between them and the tested image. Three similarity measures were applied in the two spectral image feature spaces. The results of the experiments are visually represented. The best combination of the spectral image feature and similarity measure in our opinion is proposed during a discussion part. Also further work will be proposed.

Keywords: NTF, PCA, Spectral imaging, database search.

Introduction

The interest in spectral image databases has been increasing over the last few years. The increase of importance of spectral image applications is one of the main reasons; these include e.g. digitization of a cultural heritage object [1]. Spectral images are images where color is represented accurately by a wavelength spectrum in each pixel [2]. The color spectrum may be represented as a *n*-dimensional vector, where *n* may be tens or even hundreds. This representation of the color image information requires more advanced methods than just management of the component images separately as is commonly done with RGB-images. Many effective techniques have been developed for RGB databases [3], [4], [5] but not all of them can be provided for spectral image databases.

A number of searching methods in the spectral image database have been proposed during last years [6][7]. Some of them are based on a similarity measurement between color characteristics of the image. We call these spectral color features. Those features have to characterize the color of the spectral image and the feature set should be small enough for rapid management. The similarity measure can be based on the distance (e.g. Euclidian or Kullback-Leibler distance) or the quality (e.g. PSNR, GFC) [8].

As the feature sets we compare two spectral expansion techniques. The first is Principal Component Analysis (PCA) [9]. It is a convenient technique for spectral data analysis. It finds an orthogonal basis for the spectral color space, where the original color spectra are from. The results of PCA are a spectral basis vectors and matrix of multipliers. Due to the orthogonality, the basis vectors consist also of negative elements.

Non-negative Tensor Factorization (NTF) is a new technique. It represents an original 3D non-negative matrix as tensor multiplication of non-negative bases. The non-negative basis for data description is useful for two reasons. First, the approach is natural since many measuring devices output only non-negative values. Secondly, non-negative filters can be physically implemented. Thus, many possibilities exist for the non-negative bases application. They include feature extraction in image databases, band selection in spectral imaging, and even image compression. The computational complexity of NTF is more complicated than that of PCA.

The structure of this report is as follows. First PCA and the multiresolution NTF algorithms are introduced. After that, we give the background for the database search and show the results from the experiments. The discussion and the conclusions are in the last chapter.

Principal Component Analysis

Principal Component Analysis consists in sequential search of factors (Principal Components). It is based on the statistical representation of a random variable $x=(x_1,\ldots,x_M)^T$. The mean of that population is denoted by $\mu_x = E\{x\}$ and the covariance matrix of the same data set is

$$C_x = E\{(x-\mu_x)(x-\mu_x)^T\} \tag{1}$$

where components of C_x, denoted by c_{ij}, represent the covariance between the random variable components x_i and x_j.

From spectral vectors $x_1,\ldots,x_M$, taken from a spectral image the spectra mean and the spectra covariance matrix can be calculated as the estimates of the mean and the covariance matrix. The eigenvectors e_i and the corresponding eigenvalues λ_i are the results of the solution of the equation

$$C_x e_i = \lambda_i e_i \tag{2}$$

where $i=1,\ldots,n$. Solving eigenvalues and corresponding eigenvectors is a non-trivial task, but many methods exist. By ordering the eigenvectors in the order of descending eigenvalues (largest first), ordered orthogonal basis with the first eigenvector having the direction of largest variance of the data can be found.

Multiresolution Non-Negative Tensor Factorization

The basic approach of NTF is to find a solution for the problem

$$\min_{u^m, v^m, w^m \geq 0} \left\| G - \sum_{m=1}^{k} u^m \otimes v^m \otimes w^m \right\| \quad (3)$$

where $\otimes$ is a tensor multiplication, u^m is basis for the first spatial domain of the image height, v^m is basis for the second spatial domain of the image width domain and w^m are basis for the spectral domain. G is the 3D non-negative matrix representing the original spectral image. All elements of u^m, v^m and w^m are non-negative and k is the factorization rank. The factorization process is schematically presented in Figure 1.

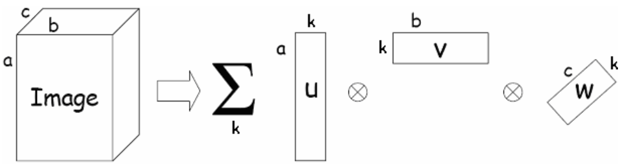

Figure 1. *Non-negative tensor factorization for 3D data.*

A multiplicative update rule for the NTF minimization problem (3) is given in [10]. The approach minimizes the reconstruction error in the Frobenious norm sense. The iteration step to update all i values is defined as follows:

$$u_i^j \leftarrow \frac{u_i^j \sum_{s,t} G_{i,s,t} v_s^j w_t^j}{\sum_{m=1}^{k} u_i^m < v^m, v^j >< w^m, w^j >} \quad (4)$$

$$v_i^j \leftarrow \frac{v_i^j \sum_{r,t} G_{r,i,t} u_r^j w_t^j}{\sum_{m=1}^{k} v_i^m < u^m, u^j >< w^m, w^j >} \quad (5)$$

$$w_i^j \leftarrow \frac{w_i^j \sum_{r,s} G_{r,s,i} u_r^j v_s^j}{\sum_{m=1}^{k} w_i^m < u^m, u^j >< v^m, v^j >} \quad (6)$$

where $<.,.>$ refers to the inner product and $r = [1,\ldots,a]$, $s = [1,\ldots,b]$, $t = [1,\ldots,c]$. Note that the update rule preserves non-negativity provided that the initial values for the vectors u, v, w are non-negative. In iteration (T) of the update process, the values of u^j are updated Jacobi style with respect to the entries u_i^j for $i = 1\ldots t$ and are updated Gauss-Seidel style with respect to the entries of other vectors $\{u^m\}_{m \neq j}$ and vectors $\{v^m, w^m\}_{m=1}^{k}$.

The algorithm convergence is long due to process is iterative and initialization is random. The multiresolution approach is based on an approximation of the original data [11]. Wavelet transform performs the appropriate approximation of the data. The original data is transformed to the approximative component and to the detail components [12]. In the inverse wavelet transform these components are used to reconstruct the data, see Figure 2. The wavelet transform carries the perfect reconstruction property. The principle of multiresolution is illustrated. The lower level approximation is received as values a_{j+1} etc. from the original values a_j. In practice the transform is performed using convolution with low-pass filter h and high-pass filter g. In definition of the filters different requirements can be set [12].

The wavelet transform is one-dimensional in nature. In the two-dimensional case, the one-dimensional transform is applied to the rows and columns of the image. In the three-dimensional case, the one-dimensional transform is applied to the spatial and spectral domains separately. In Figure 2, c), the principle of the three-dimensional, separable transform is shown.

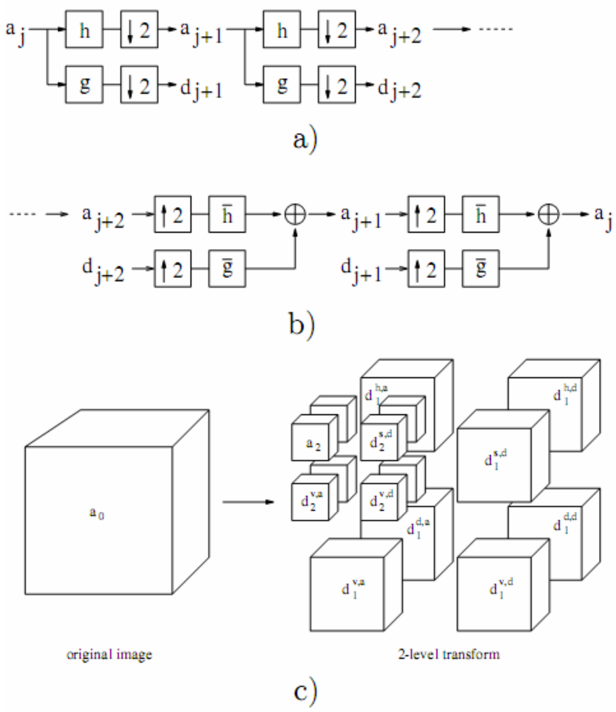

Figure 2. *Wavelet transform. a) Forward transform. b) Inverse transform, c) Separable three-dimensional wavelet transform applied twice.*

One of the most simple and well-known wavelet transform which also was used in this study is Integer Wavelet Transform (IWT). The basic form of the IWT subtracts the even samples from the odd samples to get the difference d_1 and the new approximation a_1 as

$$d_{1,l} = a_{0,2l+1} - a_{0,2l}, \quad a_{1,l} = a_{0,2l} + \lfloor d_{1,l}/2 \rfloor \quad (7)$$

where the original data is stored in a_0. The second subscript refers to the index in the sample vector. The exact reconstruction comes from calculating the values in reverse order as

$$a_{0,2l} = a_{1,l} - \lfloor d_{1,l}/2 \rfloor, \quad a_{0,2l+1} = a_{0,2l} + d_{1,l} \quad (8)$$

In general, the IWT consists of prediction and of update based on the lifting where the number of vanishing moments is increased.

Finally, multiresolution approach for NTF computation consists of the following steps:

1. Compute the lowest resolution transform using (7) for the original data set.
2. Compute u, v, and w (Eqs. 4, 5, 6) for this lowest level in multiresolution.
3. Interpolate u, v, and w for the next higher level in multiresolution.
4. Use (8) to compute the next higher level in multiresolution.
5. Compute u, v, and w for the current multiresolution level.

6. If u, v, and w are computed for the highest level in multiresolution, then stop. Otherwise, goto Step 3.

Search Method

The search method consists of two steps. First is the feature extraction process by NTF and PCA. Second is the measuring of the similarly between extracted features. This process is shown in Figure 3.

In the NTF each spectral image was applied as a 3D non-negative matrix. Basis *u*, *v*, and *w* were obtained using multiresolution NTF algorithm introduced before. The non-negative basis for the spectral domain (normalized *w*) defines the spectral image feature. In the PCA each spectrum vector from a spectral image was stored to 2D matrix row wise order. Then according PCA theory covariance matrix in a spectral content was calculated for each spectral image matrix. An orthogonal basis that consists in ordered eigenvectors of the covariant matrix defines the spectral image feature.

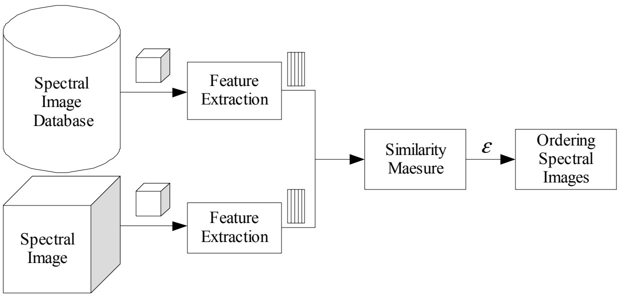

Figure 3. *Spectral image database search process.*

If the number of the eigenvectors in PCA is equal of factorization rank in NTF, then finally we obtained two sets of $c \times k$ matrixes corresponding to each spectral image from the database. The corresponding size of the eigenvectors and *w* matrixes are significantly smaller than the database of the original images. This allows to find a similarity between database units faster. For each new image to be added into a database or to be compared with database images, the corresponding eigenvectors and *w* must be found using PCA and NTF algorithms introduced above.

The similarity between the spectral images features were calculated in this study using Euclidian distance, goodness of fit coefficient (GFC) and peak signal-to-noise ratio (PSNR) as follows:

$$\varepsilon_{Euclidian} = \underset{j}{mean}\left(\sqrt{\sum_{i=1}^{c}\left(w_1(ij) - w_2(ij)\right)^2}\right) \tag{9}$$

$$\varepsilon_{GFC} = \underset{j}{mean}\left(\frac{\sum_{i=1}^{c} w_1(ij)w_2(ij)}{\left(\sum_{i=1}^{c} w_1(ij)^2\right)^{1/2}\left(\sum_{i=1}^{c} w_2(ij)^2\right)^{1/2}}\right) \tag{10}$$

$$\varepsilon_{PSNR} = \underset{j}{mean}\left(10\log_{10}\frac{\hat{w}_j^{\,2}}{\underset{i}{mean}\left(\left(w_1(ij) - w_2(ij)\right)^2\right)}\right) \tag{11}$$

where w_1 and w_2 corresponding features matrixes (eigenvectors for PCA or *w* for NTF) and $\hat{w}_j$ is the theoretical maximum of w_1 and w_2 in columns.

However due to the random initialization, NTF produces different matrixes for the same spectral image. Though basis vectors represented by those matrixes will be same but the order can vary. Therefore the similarity measure must be order independent. To find the similarity between two bases we calculated the similarity between all possible combinations of the vectors in the bases. The best value (minimum for Euclidian distance, maximum for GFC and PSNR) was defined as an answer.

Experiments

In this study 107 spectral images were used. The images come from different sources and they were measured in Joensuu University (Finland) [13], Lappeenranta University of Technology (Finland), Chiba University (Japan), Saitama University (Japan), University of Bristol (United Kindom) [14] and Marine Biological Laboratory (Maryland, USA). All spectra were limited and normalized in a range from 400nm to 700nm with 5nm interval. The size of spectral images varies from 3Mb to 56Mb. The RGB representation of all images is in Figure 5. The calculations were done in Matlab. The initializations of the NTF bases *u*, *v*, and *w* were done by assigning small numbers from the random number generator. The number of level in the IWT in multiresolution NTF was 4. The corresponding number of the iterations beginning from the lowest resolution was 200000, 60000, 30000, 500 and 100 for the level of the original spectral image. The factorization rank in NTF and the number of the eigenvectors in PCA was 5. So finally we had two features sets, each consisting of 107 matrices. The size of each one was 61×5. An example of the spectral bases for three images is in Figure 4.

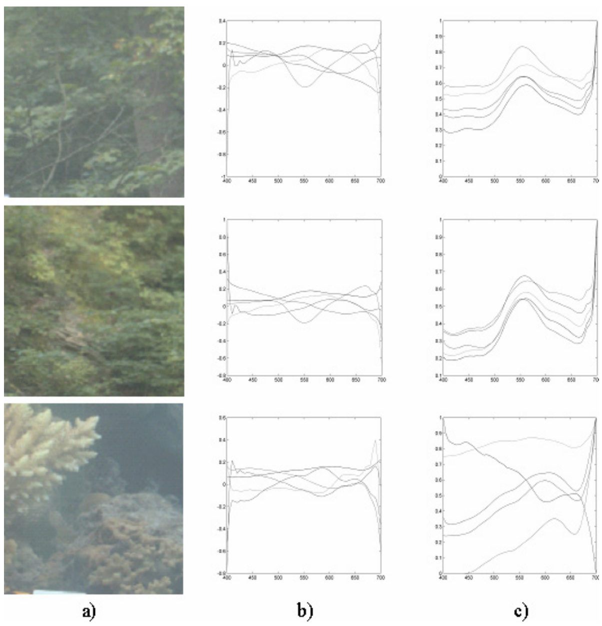

Figure 4. *Example of the corresponding features; a) original image; b) PCA basis; c) NTF basis.*

The similarity measure was calculated by using Euclidean distance, GFC and PSNR. To compare measures, those values were calculated between six sample images with different sources and all other images from the database. Since the measures in Equations 9, 10, 11, the similarity between same images is highest. The algorithm finds the same image from the database as the closest one. To visualize the results the images are shown in Figure 6, Figure 7, Figure 8, Figure 9, Figure10, Figure 11 in a order of similarity. First image in the left is the sample image. Due to the restricted amount of a space, only 6 images of the search results are shown.

Discussion

The search method in the spectral image database was implemented and tested with three different similarity measures. NTF and PCA bases were calculated and defined as the spectral color features. A new technique of similarity measurement between spectral bases was proposed, and spectral images were ordered according to those similarities.

It was shown that features proposed in this study are useful for spectral image database search. They are presented in a compact form and represent color of the spectral image with high quality. Also the experiments show that proposed similarity measurements are suitable to be used between spectral bases.

According to the obtained results we can conclude that PSNR measure shows better results than GFC and Euclidian distance (e.g. Finla in Figure 8.). Also, it can be assumed that NTF features represent a better result then PCA ones (e.g. Icon in Figure 9. and Faces in Figure 11.). The disadvantage of NTF case is that the method is iterative. Although the method was improved by a multiresolution approach, it still takes more time then PCA.

The next goal of this research is to include the content based features to the proposed method. Also the time complexity of the feature extraction must be improved.

Figure 5. *The RGB representation of the tested images.*

Figure 6. *Ordered output for spectral images in the case of NTF and PCA features uses. The similarity measures used, row by row from top to bottom are: PSNR, GFC and Euclidian distance.*

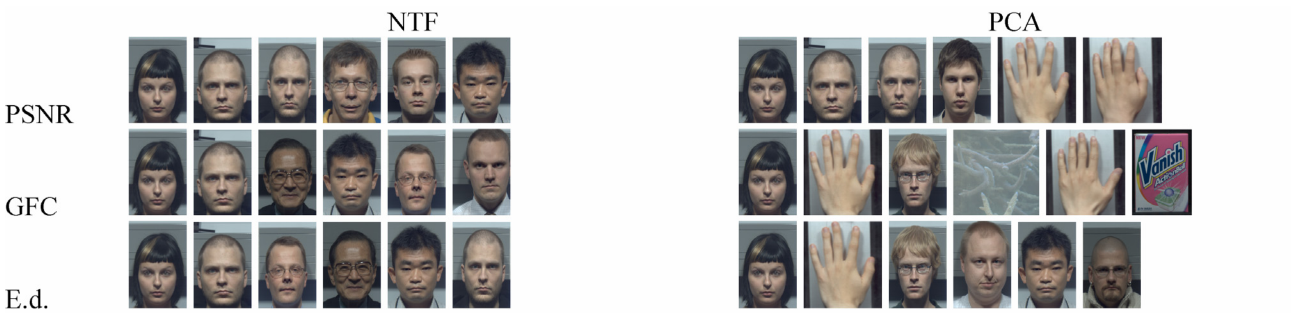

Figure 7. *Ordered output for spectral images in the case of NTF and PCA features uses. The similarity measures used, row by row from top to bottom are: PSNR, GFC and Euclidian distance.*

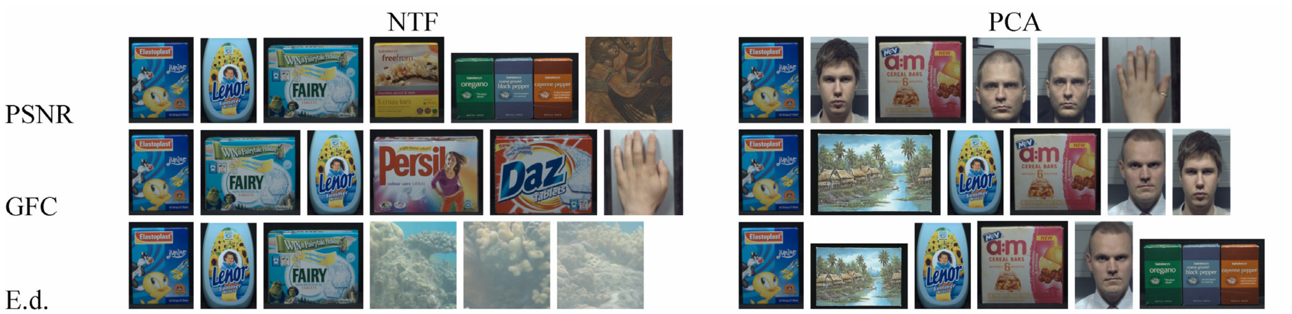

Figure 8. *Ordered output for spectral images in the case of NTF and PCA features uses. The similarity measures used, row by row from top to bottom are: PSNR, GFC and Euclidian distance.*

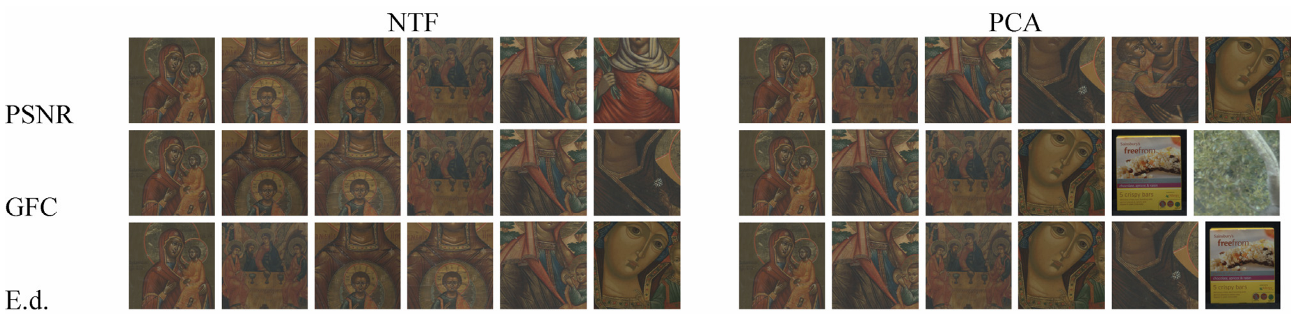

Figure 9. *Ordered output for spectral images in the case of NTF and PCA features uses. The similarity measures used, row by row from top to bottom are: PSNR, GFC and Euclidian distance.*

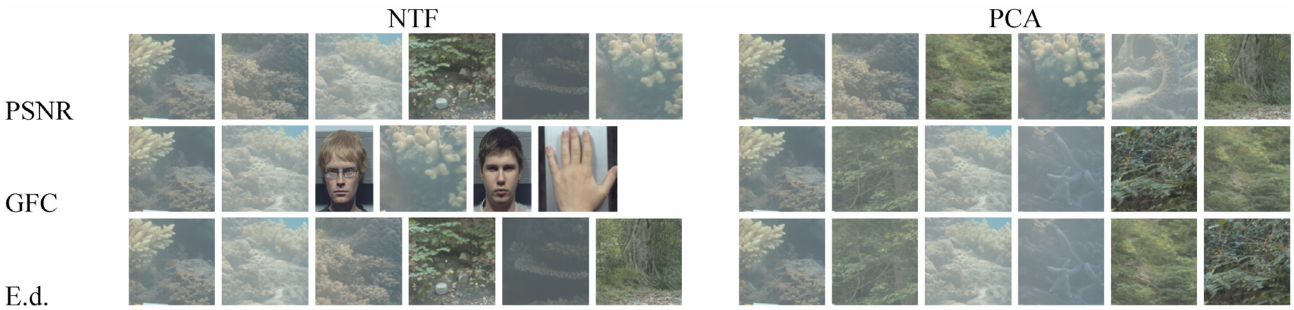

Figure 10. *Ordered output for spectral images in the case of NTF and PCA features uses. The similarity measures used, row by row from top to bottom are: PSNR, GFC and Euclidian distance.*

Figure 11. *Ordered output for spectral images in the case of NTF and PCA features uses. The similarity measures used, row by row from top to bottom are: PSNR, GFC and Euclidian distance.*

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