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Bounds on component spectra of multispectral images

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ABSTRACT

A technique has been developed to estimate bounds on the spectra of major constituents of multispectral images. The bounds are two distinct sets of spectra, one in which the spectra are maximally independent from one another and another set in which the spectra are minimally independent. Both sets and their corresponding estimated abundance maps satisfy feasibility constraints for both spectral elements and fractional abundances. The actual spectra will have an independence measure between the minimal and maximum sets. An approach to mapping the feasibility region for all intermediate independence measures is described. In general, for a given level of independence there is an infinity of rotation axes about which small rotations of the spectra leads to another feasible set. In our approach, the selected rotation axis is the one which takes the maximally independent basis into the minimally independent basis. The effects of noise and low levels of additional components (impurities) are expected to have a larger effect on altering the spectra than the modifications due to small arbitrary rotations of feasible spectra. The technique is illustrated by application to a computer generated multispectral data array.

Keywords: multispectral, hyperspectral, subpixel analysis, pixel unmixing

1. INTRODUCTION

Imaging spectrometers can collect data in a large number of narrow bands and provide a low spectral resolution spectrum for each pixel. Pixel to pixel spectral variations can be attributed to varying concentrations of constituents and, in remote sensing applications, environmental variations. Identification of the material constituents provides for both interpretation and compression of the data. Identifying constituents by directly comparing data to laboratory spectra is hindered by pixel foot print size and by environment variations in illumination, atmospheric scattering and transport effects. Typically more than one constituent contributes to each pixel. An important first step in the analysis is the removal or reduction of atmospheric and environmental effects to produce apparent reflectance spectra.¹ Here, it is assumed that such a procedure has already been applied. This paper focuses on the subsequent problem of determining constituents directly from the apparent reflectance data. The estimation of spectral components from the hyperspectral data has traditionally been based on finding convex hulls of data base spectra.^{2,3} Several different techniques have been applied to laboratory spectra of mixtures. One such technique is self modeling where the entire feasibility region of spectra and abundances is mapped.⁴ However, this technique is limited to two components. Self mapping was extended to multiple components by Sasaki, Kawata and Minami.⁵ Their technique is to sequentially find the feasible minimum and maximum spectral response for each wavenumber bin of each spectra, while all other spectral elements and abundances remain feasible. This optimization needs to be performed sequentially, once per wavenumber bin per spectral constituent and can be a lengthy processes. If the feasibility regions are sufficiently narrow, then these regions provide a solution for the constituent spectra and abundances. If the feasibility regions are broad, then they provide bounds, but not actual component estimates. Two additional methods which do not determine the feasibility region, but provide a single estimate of spectral components and abundances include target transform factor analysis⁶ and an entropy minimization procedure.⁷ In the target transform approach, spectral peaks which are thought to belong to only one, or primarily to one component, are selected as targets. These targets are repeatedly projected onto principal components of the data array and by removing the negative components after each projection, each target converges to a feasible spectrum. This iteration procedure is repeated with all candidate independent target peaks until a feasible spectrum for each constituent is found. This method assumes that such peaks exist and are identifiable in the data. A systematic approach to selecting targets from a data set is presented in the cited work.⁶ The entropy minimization approach finds the set of feasible spectra which has the narrowest spectral peaks.

This technique uses the informational entropy function of an array which contains the absolute values of the second derivative spectra as its object function. The resulting spectra have narrow peaks and satisfies the constraint conditions. The characteristics

of these spectra closely resemble those found using the approach detailed here for one of the bounding sets, the maximally independent set.

The approach described here finds bounds on the spectra of the constituents of multispectral images. The bounds are two distinct sets of spectra, one in which the spectra are maximally independent from one another and one in which the spectra are minimally independent from one another. Both sets and their corresponding estimated abundance maps satisfy feasibility constraints for both spectral elements and fractional abundances. The actual spectra will have an independence measure between the minimal and maximum sets. An approach to mapping the feasibility region for all intermediate independent measures is described. In general, there is an infinity of pure rotations of the spectra which corresponds to a given level of independence. In our approach, only a few of the infinity of pure rotations are generated but feasible sets of spectra at all levels of independence are generated. The effects of noise and low levels of additional components or impurities are expected to have a larger effect on altering the spectra than the modifications due to small arbitrary rotations of spectra. The bounds, and hence the size of the feasibility region, can be narrowed by using additional information or constraints on spatial characteristics or constituents if such information is available. The methodology is outlined and illustrated by application to a computer generated example.

2. METHOD

2.1 Determining the bounding sets of spectra

The multispectral or hyperspectral data array, H , is assumed to be composed of the sum of component arrays. It is also assumed that the contribution of each constituent is additive. Each component array can be represented by the product of the component spectra, S_k , and of the spatial abundances of the component, A_k . H is given by

$$H = \sum_k S_k A_k + noise . \quad (1)$$

For a linear sensor array, A_k is a simple vector of fractional contributions of component k for each element of the sensor array. For 2-D focal planes, A_k is taken to be a lexicographical vector. This device lets the representation of 3-D spectral spatial data as a 2-D spectral spatial matrix.

In the absence of noise the number of constituents determines the rank of the hyperspectral data matrix. Typically the number of constituents is not known, and must be determined, or guessed, by estimating the rank of the data matrix. Standard matrix rank determination algorithms derived from singular value decomposition (SVD) can be applied to the data matrix, H , to determine the number of components, n , present. In subsequent numerical analysis the matrix H can be replaced by the lower rank approximation, H_n , formed by the first n terms of the SVD expansion of the data matrix. H_n is expressed as

$$H_n = U h V^T = \sum_{k=1}^n S_k A_k , \quad (2)$$

where U and V are the matrices of left and right singular vectors, respectively, and h is the diagonal matrix of singular values. Using Equation 2 in place of Equation 1 removes some of the noise from the data. The singular vectors U and V are not acceptable solutions as spectra and abundances since they have negative components. The algorithm described below simultaneously finds feasible solutions for both the spectral components and their spatial abundances. The reason that this technique can determine the bounds is that the pixel to pixel variations in the multispectral image, are the combination of variations among the component spectra and the variations among the component spatial abundances. To bound the spectral and spatial variations, one must determine the maximum or minimum variation among the spectra (abundances) which is consistent with the constraints of positive component spectra, S_k , and the component spatial abundances, A_k . The variations among the spectra (abundances) can be measured by the extent that they overlap. The determinant of the singular value matrix of the data array is equal to the product of the determinants of the singular value matrices of the spectra, s , and the abundance, a . This expression is written as

$$|h| = |s||a| . \quad (3)$$

If the spectra and abundances are normalized to have fixed lengths, then the determinants remain finite and when one is a maximum, the other is a minimum. The overlap or metric matrix of the spectra or abundances can be formed and its determinant provides a measure of the variations among the spectra or abundances. In fact, $*S^T S*$ and $*A A^T*$ equal $*s^2*$ and $*a^2*$,

respectively. Maximizing or minimizing the determinant subject to the positivity constraints determines the maximally or minimally independent components, respectively.

Equation 3 provides the relation between the spectral component selection and the spatial abundance component selection. When the spectral components have maximum variation, or independence, the spatial abundance variation is at a minimum and when the spatial abundances have maximum variation the spectral component variation is at a minimum.

2.2 Geometric interpretation

A geometric interpretation of this approach can be made using convex cones. The components with minimum variations, or independence, are the generators or end members of the smallest convex cone of spectra that contains the hyperspectral data, H_n . The spectrum of every pixel can be represented by a non-negative linear combination of the spectral components with minimum variations. The abundance maps associated with these spectral components are the most varied. The components with maximum variations are the generators or corners of the largest convex cone of spectra that both contains the hyperspectral data, H_n , and whose predicted abundances satisfy positivity constraints. The spectrum of every pixel can be represented by a non-negative linear combination of the spectral components with maximum variations. The abundance maps associated with these spectral components are the least varied. All remaining feasible spectral components/abundances have measures of independence which lie between the most varied and least varied. The spectral components with minimum variations should be very similar to those obtained by finding the convex hull of the data set spectra. Like the convex hull spectra, the generators of the smallest convex cone will be "pure" component spectra only if pure single component pixels exist in the data array for all components. On the other hand, ignoring noise effects, the pure component spectra should be contained within the convex cone generated by the components with maximum independence.

2.3 Algorithm implementation

The following steps summarize application of the algorithm.

- I. Use SVD of data array to determine number of components.
- II. Maximize the independence of the spectra by maximizing the determinant of the spectral metric matrix, $* S^T S *$, while the lengths of the vectors S_k are held fixed. The lengths of spectral component vectors and abundance vectors are chosen symmetrically. This can be written as

$$S_k^T S_k = h_k \quad (4)$$

and

$$A_k A_k^T = h_k, \quad (5)$$

with hard constraints requiring all components and abundances to be positive and soft constraints requiring that the sums of all abundances of each pixel add to unity in the least square sense, that is the abundances satisfy

$$-I_m \quad A^T \quad I_n \quad - = 0 \quad (6)$$

where I_m is a unit vector of length equal to the number of pixels and I_n is a unit vector of length equal to the number of components. The solution yields the most linearly independent spectra and the least linearly independent abundances.

- III. Maximize the independence of the abundances by maximizing the determinant of the metric matrix of the abundances, $* A A^T *$, while the lengths of the vectors are held fixed as in step II above. The same set of hard and soft constraints which were used in step II are again applied. The solution yields the most linearly independent abundances and the least linearly independent spectra.

2.4 Mapping the feasibility region

Once the extreme, bounding solutions are obtained, solutions for spectra and abundances with varying levels of independence are sought. A means of finding such solutions is obtained by considering the transformation from one extreme basis to the other. A linear transformation, T , transforms the maximally independent basis into the minimally independent basis. T is defined as

$$S_{min} = S_{max} T, \quad (7)$$

and

$$A_{min} = T^T A_{max}. \quad (8)$$

Partial transformations are sought which define a path within the feasible region from the maximum to the minimum sets of spectra. Consider the singular value decomposition of T given by

$$T = W t Y^T, \quad (9)$$

where W and Y , the left and right singular vector matrices of T , are orthogonal and correspond to rotations of the basis functions amongst themselves. While the matrix t of singular values corresponds to a dilation or stretching. The singular vector matrices of T , W and Y , are related to the polar expansion of the transformation matrix T given by

$$T = D O = O B, \quad (10)$$

where D and B are symmetric matrices with eigenvalues identical to the singular values of T , and O is an orthogonal rotation matrix. The dilation matrices D and B are given by

$$D = (T T^T)^{1/2} \quad (11)$$

and

$$B = (T^T T)^{1/2}, \quad (12)$$

respectively. O is the rotation about W followed by the reverse rotation about Y and can be expressed as

$$O = W Y^T. \quad (13)$$

The transformation T , is the combination of rotations about W and Y in combination with either dilation of the maximum basis S_{max} by D before rotation, dilation of an intermediate basis by t , or dilation after rotations by B . The determinant of the metric matrix of S_{min} is related to the determinant of the metric matrix of S_{max} by

$$|S_{min}^T S_{min}| = |t|^2 |S_{max}^T S_{max}|. \quad (14)$$

Partial transforms, smaller dilations and smaller rotations will define sets of feasible spectra that lie in the feasible region and which have independence intermediate between the maximum and minimum measures. Because the determinant of the metric matrix only depends on the extent of dilation, a continuous evolution of the minimally independent basis from the maximum to the minimum is defined by the fraction of the dilation performed by D^α , t^α , or B^α where α , is the fractional power of the dilations with $0 \neq \alpha \neq 1$.

The independence of the intermediate basis spectra/abundances are controlled by the amount of dilation determined by the value of α . In the absence of noise, the actual component spectra correspond to a rotation of the feasible spectra at some level of independence, i.e. the levels of independence are the same. This relationship can be written as

$$|S_{actual}^T S_{actual}| = |(t^\alpha)^2| |S_{max}^T S_{max}| \quad (15)$$

and

$$|A_{actual} A_{actual}^T| = |(t^\alpha)^\beta| |A_{min} A_{min}^T|. \quad (16)$$

Considering only the dilation and using a fractional power of T as the partial transform will not necessarily lead to feasible intermediate solutions. The fractional power of T corresponds to full rotations about W and Y, but partial dilations. In order to map portions of the feasibility region, fractional or partial rotations are defined by O^β where $0 \neq \beta \neq 1$ and $(O^\beta)^{1/\beta} = O$. The feasible partial transforms are then given by

$$T^{\alpha,\beta} = D^\alpha O^\beta, \quad (17)$$

$$T^{\alpha,\gamma} = O^\gamma B^\alpha, \quad (18)$$

and

$$T^{\alpha,\delta,\xi} = (W)^\delta t^\alpha (Y^T)^\xi. \quad (19)$$

The feasible basis spectra and resulting feasible abundances are given by

$$S^{\alpha,\beta} = S_{max} T^{\alpha,\beta}, \quad (20)$$

and

$$A^{\alpha,\beta} = (T^{\alpha,\beta})^l A_{max}. \quad (21)$$

The range of β , γ , δ , and ξ which map out feasible solutions provide a portion of the feasible spectra/abundances for a given level of independence.

The entire feasibility region for a given level of independence is not mapped by all possible (feasible) values of β , γ , δ or ξ . To map the entire feasible region more general rotations are required about arbitrary axes. If the unmapped feasibility region is fairly narrow, then these general rotations will be small and the actual spectra should be identifiable from one of the sets generated with the same level of independence.

3. APPLICATIONS

The model has been applied to synthetic multispectral imagery where the spectral components and their abundances are known. The imagery was constructed using reference reflectance data.⁸ Such data provides a testbed for the determination of the tightness of the bounds and the effects of noise and the effects of selecting an incorrect number of components. If all of the constituents are present at 100% in some pixels, then the minimally independent spectra should predict the actual spectra. However, if none of the pixels contain pure component spectra, the pure spectra lie outside the convex cone formed by the spectra. In the absence of noise, the pure spectra lie within the convex cone formed by the maximum variance spectral components.

To illustrate the approach, four reference spectra were selected: dry and wet clay, limestone and silt. Figure 1 shows the four reference reflectance spectra. The synthetic mixed pixels were constructed as follows. The wet and dry clays and the limestone were taken as real components of a mixture. Random amounts of these three components were taken with the constraint that no pixel contained more than 80% of any one component, and no pixel contained less than 10% of any one component. Randomly generated noise was produced with small additions of the silt with a maximum of 10% of any pixel being "noise". The noise in real data is often a low level component. An SVD of the synthetic data matrix was taken and a rank three approximation to the data matrix using the expansion in the three largest left and right singular vectors was used throughout the analysis. The algorithm was applied to the synthetic data, with results illustrated in Figures 2 and 3. The bounds found ($\alpha=0$) maximum spectral independence with minimum abundance variation, and ($\alpha=1$) minimum spectral independence with maximum abundance variation in Figures 2(a) and 2(b), respectively. Two intermediate spectral independence results coming from transformation Equation 17 with $\alpha = \beta = .6$ and $.7$ are illustrated in Figures 3(a) and 3(b), respectively. In this example choosing $\alpha = \beta$ for all α , $0 \neq \alpha \neq 1$ leads to feasible spectra and abundances. The path through the feasible region for $\alpha = \beta$ for the three components is illustrated in Figures

4. The derived spectra for the intermediate independence values are in reasonable agreement with the actual spectra. Deviations of extracted spectra from the input is caused primarily by the noise floor which contains low levels of the silt component. The spectral components with maximum measure of independence have spectral peaks that are not present in the actual component spectra. Maximizing the independence among the spectral is a mathematical rather than physical criteria and this behavior is to be expected. In this example the minimum measure of independence spectra is a blend of the actual spectra, as expected whenever there are no pixels containing pure isolated component. The feasibility region and its bounds can be tightened by adding additional constraints to the model if any are known. Such constraints can come from using context or a reference library to identify one or more components, or by using spatial constraints such as restricting spatial autocorrelations among the pixels to place constraints on the spatial abundance components.

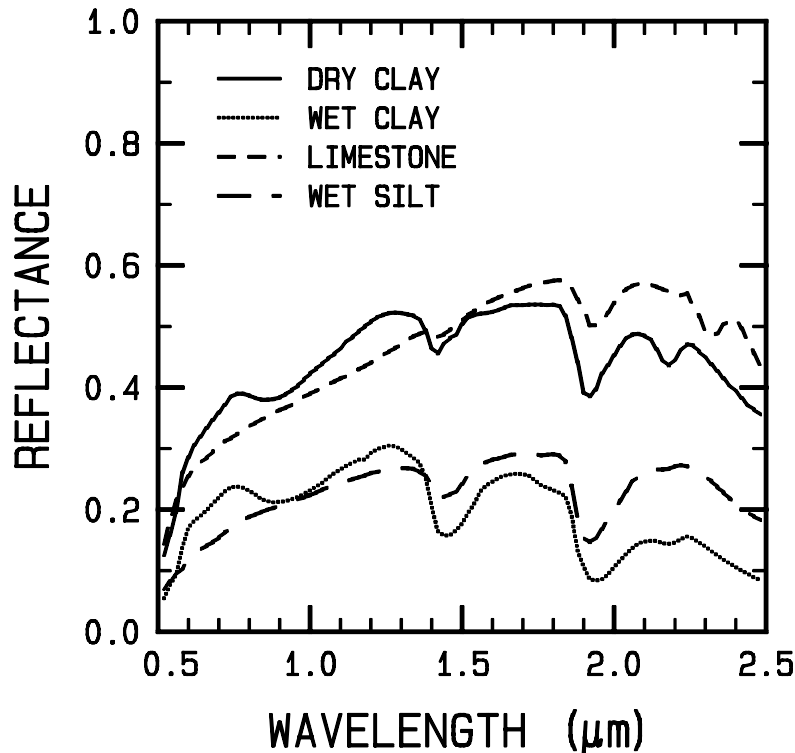


Figure 1. Reference spectra for synthetic multispectral images

4. SUMMARY

The approach discussed in this paper determines bounds on the spectra of the constituents of multispectral images. The bounds are two distinct sets of spectra, one in which the spectra are maximally independent from one another and one in which the spectra are minimally independent from one another. Both sets and their corresponding estimated abundance maps satisfy feasibility constraints for both spectral elements and fractional abundances. The actual spectra will have an independence measure between the minimal and maximum bounding sets. An approach to mapping the feasibility region for all intermediate independent measures was described. The bounds, and hence the size of the feasibility region, can be narrowed by using additional information or constraints on spatial characteristics or constituents if such information is available.

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— DRY CLAY — WET CLAY — Limestone GUESS 1 - - GUESS 2 - - GUESS 3

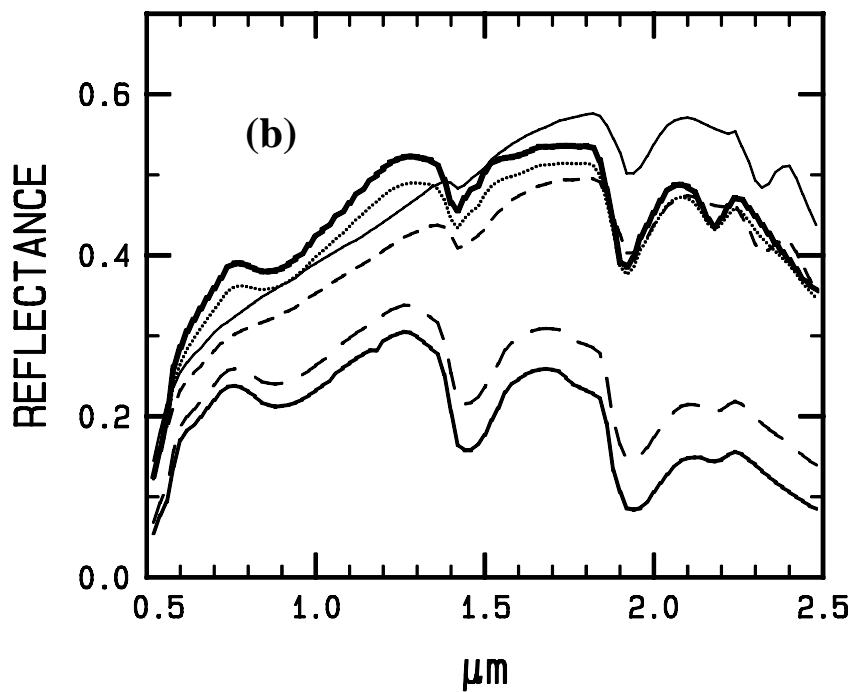
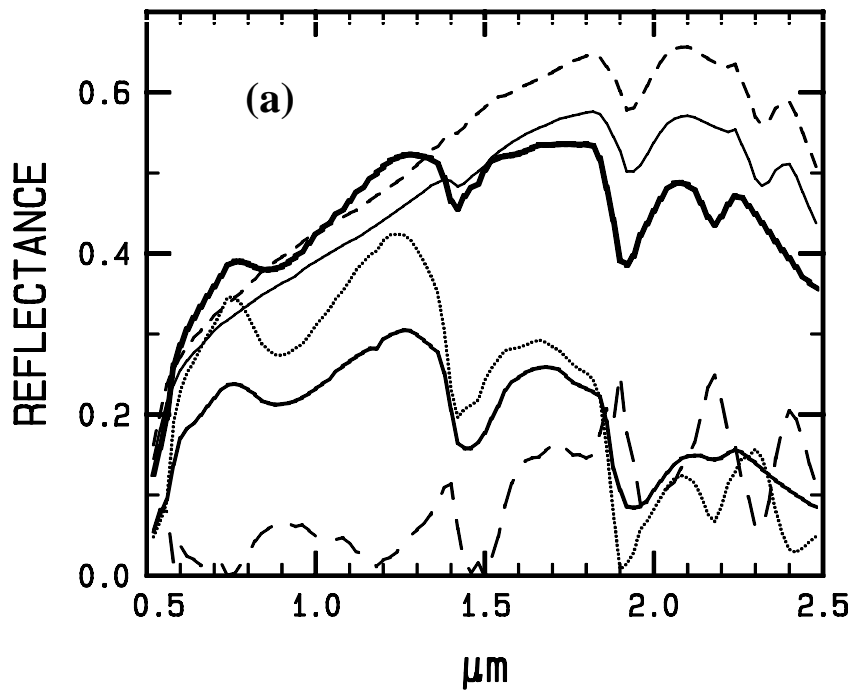


Figure 2(a,b). Slices of feasible component surfaces for (a) maximum spectral component independence, $\alpha=0.0$, and (b) minimum spectral component independence, $\alpha=1.0$.

COMPONENTS
 — DRY CLAY — WET CLAY — Limestone GUESS 1 --- GUESS 2 — GUESS 3

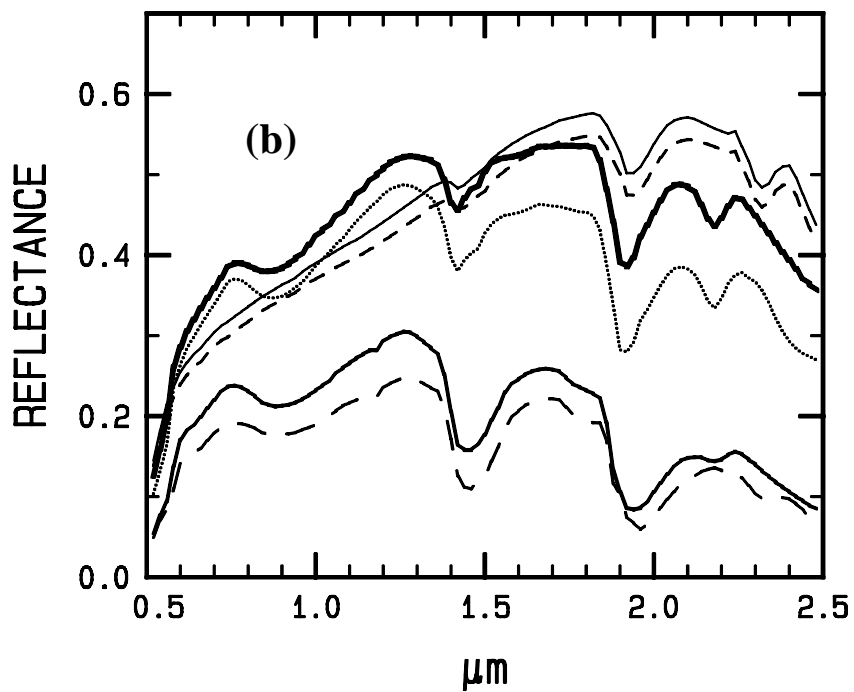
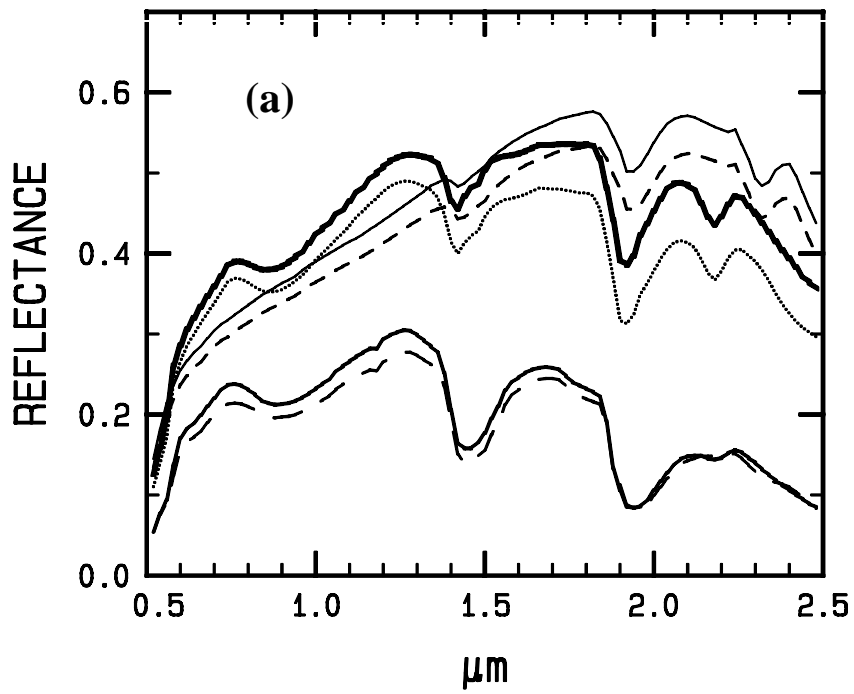


Figure 3(a,b). Slices of feasible component surfaces for intermediate values of spectral component independence (a) $\alpha=0.7$ and (b) $\alpha=0.6$.

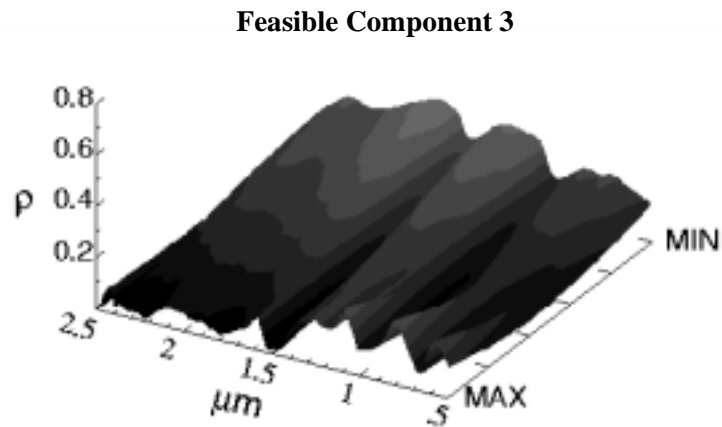
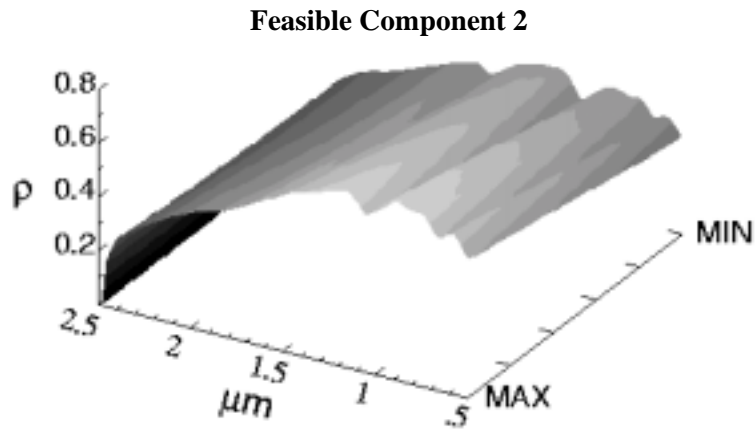
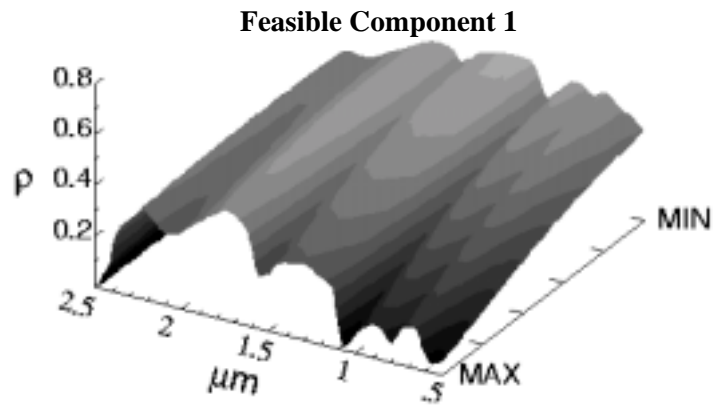


Figure 4. Feasible components for independence ranging from maximum to minimum. Black corresponds to low reflectance (ρ) and white corresponds to high reflectance.

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