On principal components of variations of cloud and surface brightness spectra in the $2-5.5~\mu m$ wavelength range inferred from aircraft measurements of outgoing radiation

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Received May 23, 2000

We discuss the emission spectra of natural underlying surfaces measured from an airborne platform. The spectra were measured with the resolution about $0.07~\mu m$ in the wavelength range from 2 to $5.5~\mu m$. The principal components of the covariance matrices of logarithms of spectral brightness are calculated for two types of the surface: clouds and the ground. It is shown that the subspaces of principal variations in the spectra of the surfaces of both types are close to each other. The spectral behavior of principal components is briefly interpreted, as is its relation to the physical factors that influence the radiative field.

The emission spectra of natural underlying surfaces in the 2 to 5 μm spectral range depend on many physical factors, and both the solar and thermal components of these emission contribute significantly to radiative properties in this transitional region of the spectrum. The multicomponent character of the spectra necessitates the use of experimental methods of determination of the principal components of the spectrum variations.

In this paper we analyze the spectra of natural surfaces, inferred from airborne measurements made between 0.15 and 10 km altitudes using a SP–102 airborne spectrometer 1 in the wavelength range 2 to 5.5 μm with the spectral resolution about 0.07 μm . The spectra were recorded during level flights over homogeneous (if possible) natural objects.

The diversity and random character of multiple factors influencing the spectra of outgoing radiation in the wavelength range 2 to 5 μm necessitates the use of statistical description of the variations in the spectrum.

This paper presents the results of analysis of principal components of covariance matrices of spectral brightness; for a convenience, the spectra are treated in the logarithmic representation. In the wavelength range from 2 to 5.5 μm studied here, the dynamical range of brightness at the spectral resolution of 0.1 μm spans several orders of magnitude. When the logarithmic representation is used for analysis of the structure of variations of the entire spectrum, at a set of wavelengths, the levels of variations, differing by an order of magnitude, can be readily adjusted, and so the variations of the shape of the entire spectrum can be clearly visualized.

The specific feature of spectral data analysis is that all spectral components of a realization have same dimensionality, and so one can use the eigenvectors and eigenvalues of covariance matrices to analyze the structure of the covariance. In analysis of multidimensional data, in which different components of a realization have different dimensionality, the eigenvectors of only the correlation matrices have a sense, while those of the covariance matrix do not (see, e.g., Ref. 2).

For analysis of internal structure of covariance, the experimental spectra were classified into two representative ensembles, namely, clouds and the ground. For these, the eigenvalues and eigenvectors of sample covariance matrices of logarithms of spectral brightness were then calculated.

The eigenvectors of a covariance matrix define a certain direction in space of logarithmic brightness spectra. (By definition, the eigenvector \mathbf{u} of the covariance matrix S satisfies the equation $Su = u\lambda$, where λ is the eigenvalue corresponding to the vector u). In the case considered here, they define directions in 34-dimensional space. Their main distinctive property is the lack of correlations between projections of the spectra (from here on, the spectra are treated on log scale) on the directions corresponding to different eigenvectors of the covariance matrix.³ Every eigenvector is orthogonal to a subspace defined by all the other vectors. Thus defined, the eigenvalues corresponding to eigenvectors of a covariance matrix represent the variances of the projections of spectra onto the eigenvectors.³ For a convenience, these vectors are normalized and, as such, have unit lengths.

Table 1 presents eigenvalues of sample covariance matrices for background ensembles of clouds and ground surfaces. The eigenvalues and the corresponding eigenvectors are given in the order of decreasing eigenvalues.

The eigenvalues were calculated iteratively by $Hotelling\ method^4\ using\ specially\ written\ computer\ program^5\ because the existing computer codes for calculating the eigenvectors do not provide required accuracy of computations.$

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	Eigenvalues		Accumulated sum				
Vector			of t	first	as a fraction		
number				values	of trace		
	Clouds	Ground	Clouds	Ground	Clouds	Ground	
1	13.055	7.8371	13.055	7.837	0.558	0.428	
2	4.9741	4.8514	18.029	12.688	0.770	0.692	
3	1.4441	2.1522	19.473	14.841	0.832	0.810	
4	0.9779	0.8629	20.451	15.704	0.874	0.857	
5	0.7104	0.7455	21.161	16.449	0.904	0.898	
6	0.5899	0.6151	21.751	17.064	0.929	0.931	
7	0.4641	0.3351	22.215	17.399	0.949	0.949	
8	0.2705	0.2041	22.486	17.603	0.960	0.961	
9	0.2172	0.1644	22.703	17.768	0.969	0.370	
10	0.1728	0.1473	22.876	17.911	0.977	0.977	
11	0.0916	0.097	22.968	18.008	0.981	0.983	
12	0.0825	0.072	23.050	18.080	0.985	0.987	
13	0.0793	0.063	23.129	18.143	0.988	0.990	
14	0.0728	0.047	23.202	18.190	0.991	0.993	
15	0.0538	0.030	23.256	18.220	0.993	0.994	
16	0.0345	0.0277	23.290	18.248	0.995	0.996	
17	0.0243	0.0177	23.315	18.266	0.996	0 997	
18	0.0201	0.0124	23.335	18.278	0.997	0.997	
19	0.0157	0.0087	23.350	18.287	0.997	0.998	
20	0.0130	0.0077	23.363	18.294	0.998	0.998	
21	0.0078	0.0057	23.371	18.300	0.938	0.999	
22	0.0073	0.0052	23.379	18.305	0.999	0.999	
23	0.0064	0.0043	23.384	18.310	0.999	0.999	
24	0.0050	0.0036	23.390	18.313	0.999	0.999	
25	0.0044	0.0029	23.394	18.316	0.999	0.999	
26	0.0036	0.0024	23.398	18.318	0.999	1.000	
27	0.0029	0.0019	23.401	18.320	1.000	1.000	
28	0.0038	0.0017	23.404	18.322	1.000	1.000	
29	0.0021	0.0011	23.406	18.323	1.000	1.000	
30	0.0017	0.0010	23.407	18.324	1.000	1.000	
31	0.0014	0.0008	23.409	18.325	1.000	1.000	
32	0.0011	0.0006	23.410	18.326	1.000	1.000	
33	0.0009	0.0005	23.411	18.326	1.000	1.000	
34	0.0007	0.0002	23.412	18.326	1.000	1.000	

The computations are difficult in that the sample covariance matrices are close to degenerate ones while, at the same time, they are not such with the unity probability.⁶ For instance, for clouds the smallest eigenvalue is 0.0007449, i.e., about six hundred thousandths of the maximum eigenvalue. The need for a special codes to calculate eigenvalues was also motivated by large dimensionality of realizations and, hence, covariance matrices.

It can be seen that, on the whole, the eigenvalues rapidly decrease as the eigenvalue number increases (see Table 1). The eigenvalues have the meaning of variances of projections onto the eigenvectors, and these projections for different vectors do not correlate; therefore, the sum of eigenvalues, or the trace of a covariance matrix, serves as a certain accumulated measure of spectrum variability. From the accumulated sums presented in Table 1 it can be clearly seen that the total spectrum variations mostly consist of variations in the directions of only a minor part of all the 34 vectors. Even variations of projections onto the direction of only first vector are 55 and 43% of the trace for clouds and ground, respectively. Projections of

only first three vectors account for over 80% of the total variance. Five first eigenvalues account for 90% of the trace of the matrix, for first eight vectors this amounts to already 96%, and variations in directions of first 14 vectors account for over 99% of the trace.

The last vectors have associated with very small variances of projections of realization from the sample (see Table 1). The fact that projections onto last vectors are stable suggests that they are orthogonal both to directions of variations of the signal, and to directions of variations of the noise (indicating that the noise components are spectrally correlated).

Seemingly, the directions of principal signal variations correspond to first vectors since the mean level of variance of the noise (of the order of 0.02) is small compared with first eigenvalues, and since the fraction of noise projection onto first eigenvalues, even for strongly correlated noise, is much less than the variance of variations of useful signal.

The direction cosines of first eight vectors are plotted in Fig. 1 for the cloud ensemble and in Fig. 2 for the ground one. (For the sake of brevity, the words direction cosines will be omitted in the below discussion, and just plots of vectors, or vectors, will be used instead of plots of direction cosines of vectors. By direction cosines of a vector in its geometrical interpretation we mean simply the values of its components, since all the vectors are appropriately normalized).

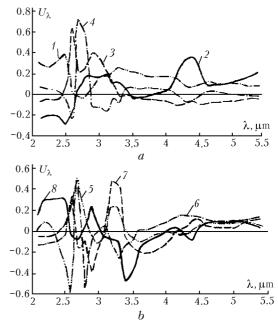


Fig. 1. Eigenvectors of sample covariance matrix of logarithms of spectral brightness of clouds. Numbers at the curves indicate the vector numbers.

From Figs. 1 and 2 it is seen that the first vectors are rather smooth, and that the both the rate of oscillations and the number of zero crossings increase with the growing vector number. Each of the vectors, as a rule, is not attributable to spectral manifestation of any single physical factor influencing the spectrum, but

rather it reflects a combined effect of a set of factors. This is because both the factors themselves and their influence on the spectrum correlate. Nevertheless, some vectors can certainly be attributed to some dominating factor. For both ensembles, the first vector (Figs. 1a and 2a) reflects the principal energy variations in the spectrum, primarily associated with variations of scattered solar radiation reaching the device. However, even this primary effect, associated with the first vector, is distorted somewhat because of a complex relationship between the conditions of observations and variation's variances of different levels for different wavelengths.⁷

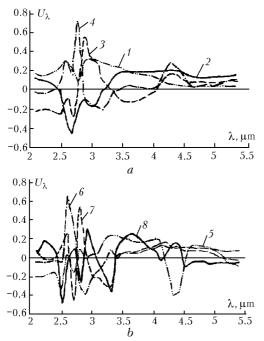


Fig. 2. Eigenvectors of sample covariance matrix of logarithms of spectral brightness of the ground. Numbers at the curves indicate the vector numbers.

The correctness of this interpretation of the first vector is confirmed by Table 2, which gives the correlation coefficients of projections onto the first vectors with the parameters characterizing the observation conditions. In Table 2, H is the flight height; P is the pressure at the flight height; T is the temperature of the atmosphere; h_V is the viewing angle; t is the solar elevation angle; t is solar azimuth angle; and t is the scattering angle. In particular, for clouds that, on the average, produce much higher solar radiation background than other backgrounds, the projection of the spectrum onto the first vector is strongly correlated (in the absolute value) with the scattering angle (see Table 2).

The second vector for clouds characterizes variations in thermal emission of the clouds. Since most of the measurements were made at a low height above the clouds, the recorded air temperature well correlates with the cloud top temperature; while a weaker correlation was found between flight height/pressure and temperature of the emitting part of the clouds. This

most clearly manifested itself in that the projections of the spectrum onto the second vector much closer correlate with temperature than with the altitude and pressure (see Table 2).

In the ground ensemble, the projection onto the second vector also strongly correlates with the air temperature and, moreover, its correlation with height and pressure is no weaker than with the temperature. The spectral behavior of direction cosines of the second vector for ground ensemble (see Fig. 2a) strongly differ from that of the cloud ensemble. This is because the spectral brightness in the ground ensemble depends on the flight height and air temperature at this height only in the regions of atmospheric gas absorption bands and slopes of these bands, primarily since only in these spectral intervals the sensor receives thermal radiation emitted by the atmosphere, and does not records surface emission. The difference in the shape of the second eigenvectors of both ensembles thus reflects the difference of the spectral coefficients of correlation between logarithms of brightness and temperature. On the contrary, the vectors with large numbers are not amenable to such a simple physical interpretation. Only for particular vectors the spectral behavior of their direction cosines can be explained quite straightforwardly.

For instance, the third vector in the ground ensemble (resembling somewhat the second vector of cloud ensemble) can be interpreted as the contrast between logarithms of brightness in the slope regions of the $2.6\text{--}2.8\,\mu\text{m}$ water vapor and carbon dioxide absorption band and logarithms of brightness in the thermal and shortwave regions.

The fifth vector of the ground ensemble is seemingly associated with the brightness contrast in the $4.3~\mu m\ CO_2$ absorption band and in the neighboring relatively transparent windows. For clouds, whose temperature correlates with the air temperature, this contrast is much lower and so it is only apparent in ninth and tenth vectors. Spectrally, they behave similar to the fifth vector of the ground ensemble. Cosines of the angles between fifth vector of the ground ensemble and ninth and tenth vectors of the cloud ensemble were 0.528 and 0.523, respectively.

To compare principal directions of spectrum variations in cloud and ground ensembles, we calculated the cosines of angles between eigenvectors of these ensembles. Table 3 gives scalar products of first eight eigenvectors of ground ensemble (see Fig. 2) and eight vectors of cloud ensemble (see Fig. 1).

The entries of Table 3 can be considered as the coordinates of the eigenvectors of ground ensemble in the coordinate system coinciding with the eigenvectors of cloud ensemble (and vice versa). From Table 3 it is seen that the first vectors of both ensembles are very close (their scalar product is 0.814). The second vector of the ground ensemble is close to the third vector of cloud ensemble, while third vector of the ground ensemble is close to the second vector of the cloud ensemble (cf. Figs. 1*a* and 2*a*).

Table 2. Coefficients of correlation between projections onto eigenvectors and parameters characterizing observation conditions

Table 3. Scalar products of eigenvectors of sample covariance matrices of logarithms of spectral brightness of clouds and ground surface

Type of	Vector number	Clouds							
background		1	2	3	4	5	6	7	8
Ground	1	0.814	0.450	-0.206	-0.029	0.025	-0.07	0.049	0.224
	2	0.095	0.272	0.724	0.322	0.359	0.267	0.123	-0.207
	3	0.511	-0.715	0.288	0.161	-0.277	0.015	0.002	0.001
	4	0.067	-0.266	-0.382	0.458	0.661	-0.056	0.313	-0.070
	5	0.114	0.087	0.067	-0.248	0.037	-0.206	-0.060	-0.464
	6	0.031	0.025	-0.384	0.249	-0.157	0.686	0.375	-0.196
	7	-0.125	0.270	0.048	0.690	-0.471	-0.262	-0.190	0.080
	8	0.111	0.170	0.006	-0.122	-0.072	0.249	-0.655	-0.194

Overall, we can note the closeness of subspaces defined by first three vectors of both ensembles. (For both ensembles, sum of the first three vectors accounts for over 80% of trace of the covariance matrix). Since each vector has unit length, in any orthogonal Cartesian coordinate system the sum of squares of its direction cosines is identically unity. The sum of the squares of first three direction cosines of the first vector of the ground ensemble is 0.908 in the coordinates of the eigenvectors of cloud ensemble, implying that this vector lies almost totally in the subspace defined by first three vectors of the cloud ensemble. For the second and third vectors of the ground ensemble, these sums were found to be equal to 0.607 and 0.855, which also suggests the closeness of subspace of first three vectors for both ensembles.

With regards to the subspace of the first eight vectors of the cloud ensemble, the first eight vectors of the ground ensemble lie almost totally in this subspace, except for the fifth vector which, as was already noted above, is close to the ninth and tenth vectors of the cloud ensemble.

The closeness of subspaces of principal spectrum variations of both backgrounds originates from the similarity of physical mechanisms and, hence, from resemblance of the responses in the spectra of main factors influencing the spectrum.

Analysis made indicates that the variability domain of the spectral brightness is spectrally bounded in multidimensional space, and that these domains are close for different backgrounds; which may be significant for the development of concise methods of spectrum description.

We conclude by noting once again that the choice of representation of spectrophotometric data is very important for analysis of the covariance structure. The use of logarithmic scale, in particular, had allowed us to study the structure of variations in the spectrum shape.

On the other hand, the variances of the absolute spectral brightness are proportional to the mean brightness values by virtue of the lognormal distribution of the spectral brightness (e.g., see Refs. 8–10). Therefore, analysis of brightness itself gives a trivial result that the principal variations are concentrated in

the spectral region where the mean brightness is high. In particular, the variance of projections of brightness spectrum, on a linear scale, onto the direction of the first vector for the cloud ensemble is 94.4% of the trace. At the same time, the cosines of the first vector are proportional to the mean spectrum. Thus, when the variations of the absolute spectral brightness are considered, the method of principal components virtually provides information only on the integrated characteristics of the brightness spectrum.

This situation, seemingly, is typical for analysis of quite a wide range of spectral data sources; which is supported by many studies dealing with analysis of eigenvectors of covariance matrices (see, e.g., Refs. 11–13). All of them indicate that almost all variance in the spectrum is associated only with variations in direction(s) of one (two) eigenvectors of the covariance matrix

In our case, the use of logarithmic scale of brightness measurements had allowed us to perform meaningful analysis of the structure of spectral covariance, in particular, via calculation of eigenvalues and eigenvectors of the covariance matrices.

The covariance structure has proven physically informative; so it is advisable to consider the possibility of using this structure for different practical

applications and, in particular, to construct imitation model for brightness spectra of natural underlying surfaces in the 2 to $5.5~\mu m$ wavelength region.

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