OPTIMAL SMOOTHING OF ASTEROID REFLECTANCE SPECTRA: THE SEARCH FOR FAINT ABSORPTION BANDS. D. Shestopalov[1], L. Golubeva[1], and L. McFadden[2]. [1]Shemakha Astrophysical Observatory, Shemakha, Azerbaijan 373243 (shestopalov_d@mail.ru). [2]Department of Astronomy, University of Maryland, College Park, MD 20742-2421 (mcfadden@astro.umd.edu)

Background: Faint absorption bands (FABs) arise in the visual range of mineral and rock spectra due to petrologically important transition elements (Fe^{2+}, Fe^{3+}, Ti^{2+}, Ti^{3+}, Cr^{3+}, Ni^{2+}, etc) situated in a crystal lattice of minerals. The intensity of these bands is small for the following reasons. First, abundance of these elements is low in the rock-forming minerals and, second, the electron transfers in envelopes of cations, situated in electrostatic field of ligands, are spin forbidden. At the same time FABs bear important information about crystallographic, chemical and physical properties of minerals and, consequently, about their origin and evolution [1,2].

Lately spectrophotometric surveys, including thousands of asteroids from different optical types and dynamical groups, have been obtained [3-5]. Large telescopes and modern CCD-spectrometers produced spectra with good signal-to-noise ratios even for faint asteroids. After dividing the observed asteroid spectrum by the observed solar analog spectrum the resulting spectrum displays high-frequency oscillations of the reflectance coefficients and looks like a fine-tooth comb. This effect is conditioned, in particular, by photometric errors of the measurement of low light levels from an asteroid and a star. Just these oscillations contain information about FABs.

We suppose that the measured asteroid reflectance spectrum is the sum of three components: low-changing regular trend, low-amplitude modulation (useful signal) of the trend and a random noise (see Fig.1a as an example). The trend is easily approximated by the classic least square estimation. The task, consequently, is to separate the useful signal from the noise.

Method of the optimal smoothing of the asteroid spectra: For the smoothing of the initial asteroid spectrum we use the running box, which may contain 5, 7, 9, …, n (odd number) of y-points and moves along x-coordinate of a spectrum, changing position by one point. Because of small number of y-points, situating within boundaries of the box, the shape of probability distribution of random value of y_i is unknown. To define correctly the center position of the probability distribution, we calculate five different estimations of the distribution center (Y_1,…,Y_5) for the variation series $y_1<y_2<\ldots<y_n$ inside the box during its movement along abscissa axis. Here Y_1 is usual arithmetic average; Y_2 is *center of hinges*, defined as half-sum of 25% - and 75%- quantile; Y_3 is *median* or 50%-quantile of the variation series; Y_4 is *mean range*, defined as half-sum of the maximum and minimum value of the variation series; and Y_5 is the *cut average*, calculated after cutting the equal portion (25%) of points off the ends of the variation series. Median (MY5) from these five different estimations gives the final estimation of the distribution center of the random value y_i. That kind of algorithm, based on the ideas voiced in works [6,7], is free from assumptions about the distribution function of the random value y_i, and is well protected against the misses which may be among y_i.

Numerical experiments with artificial spectra have been carried out in order to investigate the properties of the smoothing algorithm. The artificial spectrum was constructed as a sum of a linear trend, absorption bands with Gaussian contour, and random noise, having uniform probability distribution of amplitude (Fig.1b). We go into the question: is there the optimal size box (n_{opt}) to take off (or at least to suppress) the noise but to preserve the useful signal (FABs) in a spectrum? To answer this question we studied the statistics of signal and noise in the artificial spectra at various n. If n increases the smoothed spectrum approaches regular trend without any local maxima or minima in the spectrum. The signal to noise ratio (S/N) for the smoothed spectra decreases with growth of n. On the other hand the accuracy of calculating the smoothed spectra increases together with n. Therefore the number of discernable gradations (g) of the signal also increases if n increases. In a result the product gS/N has maximum at some n. This effect is preserved, of course, when we process the real asteroid spectra (see Fig.2). The value of n_{opt} obtained in such a way determines the optimal size of the box for the smoothing of the noisy reflectance spectra. Fig.1 shows the result of the optimal smoothing of 3268 De Sanctis spectrum (from [3]) and the artificial spectrum.

Artifacts: The second approach that we have in mind is the following. Let a spectrum be optimally smoothed and some faint oscillations along a trend are seen. What is it - the real bands or artifacts? For the noiseless artificial spectrum we exactly know characteristics of the absorption bands - their position (λ_e) and equivalent width (W). Note λ_e is the position of center of gravity of an area under band counter after removing a linear continuum, which passes through band wings. Having added a random noise with different amplitude in "clean" spectrum we calculated differences ΔW and $\Delta\lambda$ between exact values and values obtained (W_c and λ_c) after the optimal smoothing of the noisy spectra. We calculated the ratio (η) of summary area of the noises around a band contour to W_c for the smoothed spectra so that influence of the noises might be taken into account. The plots of ΔW vs η and $\Delta\lambda$ vs η are shown in Fig.3. We see the scattering of ΔW and $\Delta\lambda$ around zero is small if $\eta \lesssim 1$, and strongly increases if $\eta > 1$. Therefore we come to the following conclusion. The given absorption band in the optimal smoothed spectrum is regarded as real if $\eta \lesssim 1$. Otherwise the existence of an absorption band in the smoothed spectrum raises doubt.

In accordance with this rule all the local minima in the smoothed spectrum of 3268 De Sanctis should be recognized as questionable (Fig.1a). The sole absorption band near 500 nm is purported to be real in the smoothed spectrum in Fig.1b, other bands "are drowned" in noises.

Influence of the width of the running box on absorption band characteristics: With the help of the artificial spectra we studied the variation of W_c and λ_c in regard to exact values λ_e and W at different maximum amplitude (A_{max}) of random noise and width (n) of the running box. We did not find any essential shifts of W_c and λ_c in the smoothed spectra relative to exact values in the range of $5 \leq n \leq 23$ points and $|A_{max}| \leq 0.05$ (see Fig.4 as an example). For an asteroid spectra n_{opt} is always less than 23 points, therefore we think that the operation of smoothing of the noisy spectra by the method described above does not give systematic shifts for estimating the band characteristics at least for the absorption bands that meet the condition $\eta \lesssim 1$.

Conclusions: Method of the optimal smoothing of the noisy spectra, which is described here, is quite admissible for searching FABs in the asteroid spectra obtained within the framework of large spectrophotometric surveys. In some cases the estimation of the absorption band characteristics (equivalent width and band center) is possible. Note, however, that we can not investigate a precise absorption band profile by this method. For this aim spectral observations of the asteroids with more high accuracy and spectral resolution are essential.

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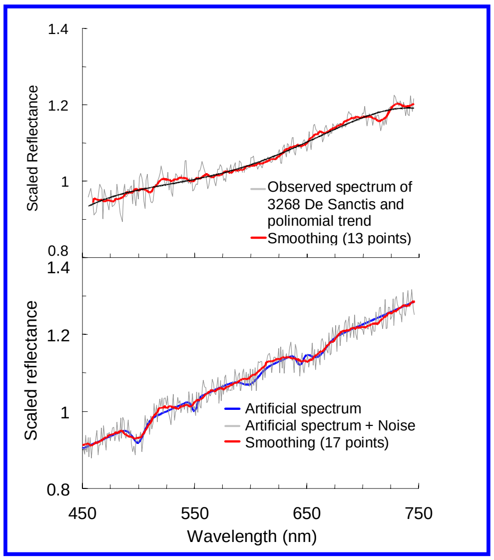

Fig. 1 ←

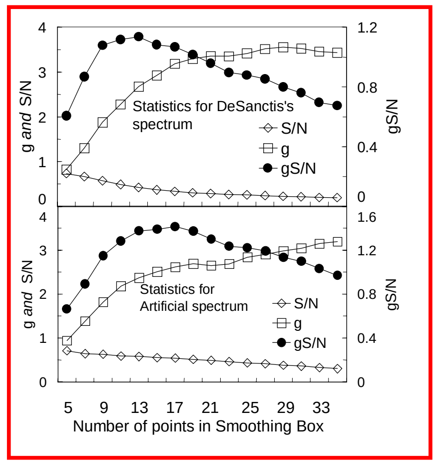

Fig. 2 →

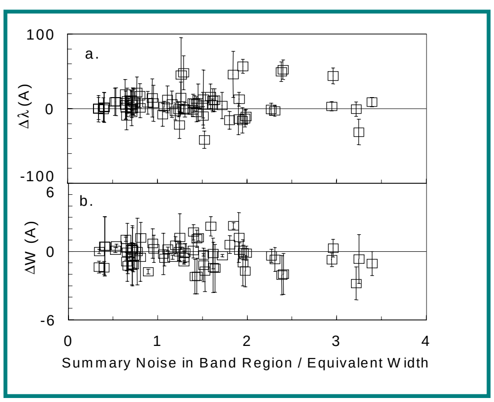

Fig. 3 ←

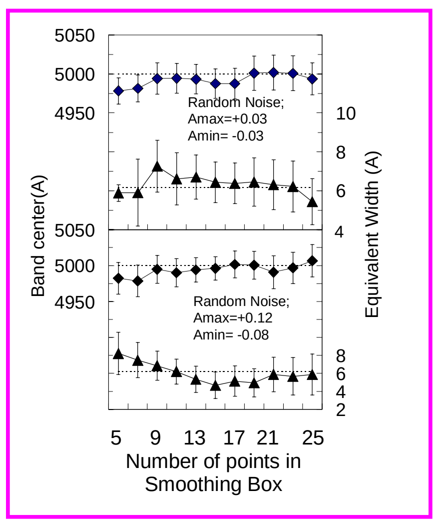

Fig. 4 →