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Analysing spectral signatures with multiscale methods

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Abstract

A new spectral analysis method based on wavelet decomposition and on a multiscale vision model is presented here. This method was developed to process reflectance spectra from planetary surfaces and to extract the relevant information from highly correlated data, where it only represents a small fraction of the overall variance. The outcomes of the analysis are a description of the bands detected, and a quantitative and reliable confidence parameter. The bands can be described either by the most appropriate wavelet scale only (for rapid analyses) or after reconstruction from all scales involved (for more precise measurements). An interesting side effect is the ability to separate even narrow features from random noise, as well as to identify low-frequency variations i.e., wide and shallow bands.

1. Introduction

Modern space borne instruments produce very large data sets that require automated processing and analysing methods. Imaging spectroscopy data can be particularly difficult to handle because they consist in very correlated data sets where the relevant information only bears a small fraction of the overall variance. For this reason, analyses using multivariate methods often require a preprocessing step to extract the useful signal. A first step in such a processing is to rapidly detect absorption bands and characterise them in terms of band centre, width, and depth. A new method based on wavelet decomposition and a multiscale vision model is presented here, which is partly derived from image analysis techniques (e.g. [1]).

Wavelet decomposition is particularly well suited for analysis of NIR spectral data, because it intrinsically performs a correction of the local continuum. The Wavelet Transform of a spectrum therefore presents a negative minimum wherever an absorption band is detected at a given scale.

The present detection method, through noise filtering and multiscale analysis has the following properties:
• it requires no assumption on the data: the only free parameter is the detection threshold in terms of noise standard deviations
• it detects absorption bands of various width and strength, even when entangled and dissymmetric
• it provides first order band characteristics with a confidence parameter

2. Wavelet transform

Wavelet coefficients are computed for each wavelength and for scales in geometric progression, using continuous wavelets (adapted from the IDL code by [2]). We use DOG2 wavelets (Mexican hat), that are best adapted to peak detection: the central lobe mimics the band profile, while the negative secondary lobes perform a subtraction of the local continuum. Only the negative coefficients are retained here, because they correspond to absorption features in the spectra.

The noise is handled as in [1]: the scale distribution of a unit white noise is multiplied by the data noise at all wavelengths involved. Wavelets coefficients smaller in absolute value than 3-5 times the noise are discarded. At a given scale, bands are typically detected in structures of consecutive channels grouped around a distinct minimum.

3. Multiscale analysis

Because of the high redundancy of the wavelet algorithm used, bands are detected at 3-4 consecutive scales. Structures at different scales corresponding to the same band are identified and connected using a multiscale model (e. g. [3]), which is optimized for planetary reflectance spectra.

Two types of objects are identified simultaneously (Fig. 1): bands (sets of structures connected at different scales) and envelops (leftover in the connection process). For each band a dominant structure is identified, which provides the best short

description of the absorption. Envelops usually result from interferences between neighbouring bands, but in complex cases they may actually describe a wider absorption overlapping narrow bands.

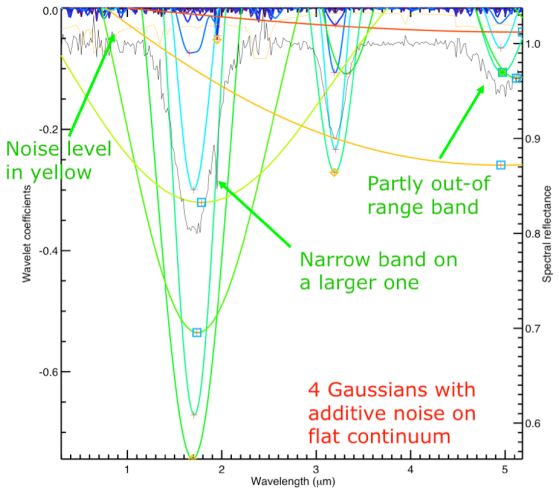

Figure 1: Assessment on a simulated spectrum. Detected bands are marked by yellow diamonds.

4. Band characterisation

A dominant scale is identified for each band during the connection process. In general, this is the scale that provides the strongest response. The corresponding structure provides the best short description of the band. To reduce computation time and to allow for quick analyses of large data sets, the bands may be characterized by their dominant scale only: centre, width, strength and signal to noise ratio.

Detections near the edge of the spectral range are uncertain, and artefact may occur in the case of tilted or non-linear continuum. Warnings are issued whenever the band is incomplete (shoulder missing on one side) or undecidable (minimum reflectance at the edge, one wing missing).

5. Applications & prospects

Intense testing has been performed with simulated data (Fig. 1), laboratory spectra of meteorites and minerals (Fig. 2), and observational spectra of asteroids and TNOs. This technique has already been used for analysis of NIR spectra of Ceres (from the VLT [4]), Mercury (from the NTT [5]), and Lutetia (from the Rosetta spacecraft [6]). On Mercury, it has been used to identify a detection threshold and an upper limit to the abundance of FeO in silicates.

Future developments will focus on analysing spectral image-cubes, i.e. identifying variations of signatures in a series of spectra.

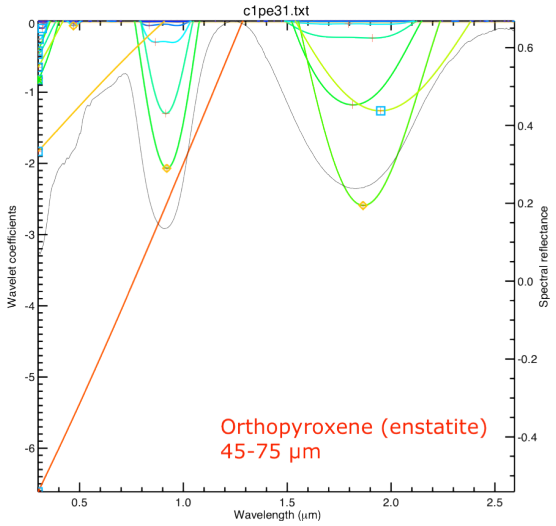

Figure 2: Assessment on a laboratory spectrum. Blue boxes and green stars mark incomplete bands (pyroxene spectrum from RELAB).

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