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Robust Data Analysis Methods for Spectroscopy

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Abstract. This paper describes various methods for the analysis of spectroscopic data, particularly as they relate to wavelength calibration of echelle-format spectra. Methods that are robust to outlier values are highlighted.

1. Introduction

Classical statistical techniques usually lack the ability to reject outliers which appear in real data, resulting from measurement errors, mixed distributions, noise, etc. Different methods offer inherent robust properties in the presence of contamination. The application of robust methods to the domain of spectral data analysis is reviewed in this paper. A short introduction to robust regression by Least-Median of Squares is presented in Section 2. This algorithm is applied to the determination of echelle dispersion relations. Section 3 is an excerpt from a recently published article (Ballester 1994) related to the Hough transform and its application to echelle order detection and automated arc line identification. Wavelet transform can be useful in complementing robust techniques for multiresolution analysis, and Section 4 presents an application of the Mexican hat transform to the detection of spectral features.

2. Robust Regression

2.1. LS versus LMS

The sensitivity of least-squares (LS) regression to outliers is a traditional problem in data analysis, and as an alternative Rousseeuw (1987) introduced the Least Median of Squares (LMS) which consists of minimizing the term:

$$\text{med}\left\{(y_i - \alpha x_i - \beta)^2\right\}, i = 1, 2, .., N \tag{1}$$

This minimization cannot be obtained analytically and therefore requires repeated evaluations for different subsamples of size p drawn from the n observations. A complete trial would require $m = C_n^p$ evaluations which would rapidly become impracticable for large n and p values. Rousseeuw & Leroy (1987) determined the minimum number m of subsamples required to obtain a given probability α of drawing at least one subsample containing only good observations from a sample containing a fraction ϵ of outliers. By requiring α to be sufficiently close to 1 (e.g 0.95 or 0.99), m can be determined for given values of p and ϵ: $\alpha = 1 - (1 - (1 - \epsilon)^p)^m$

The smallest fraction ϵ of contamination that can cause the estimator to deviate arbitrarily from the estimate performed on the uncontaminated sample is called the breakdown point of the estimator. In the case of the LS estimator, only one outlier is sufficient to make the fitted parameters deviate arbitrarily from the expected value, therefore the breakdown point of LS is 0%. The LMS-based Reweighted Least Square (RLS) corresponds geometrically to finding the narrowest strip covering half of the observations. The breakdown point of the RLS is 50%. Most the other robust estimators do not attain a breakdown point of 30% (Rousseeuw & Leroy 1987). In the following sections of this paper, the applications have been realized using the `PROGRESS` algorithm available from the Statlib statistical library (e-mail: *statlib@lib.stat.cmu.edu*).

2.2. Iterative Dispersion Relation Determination

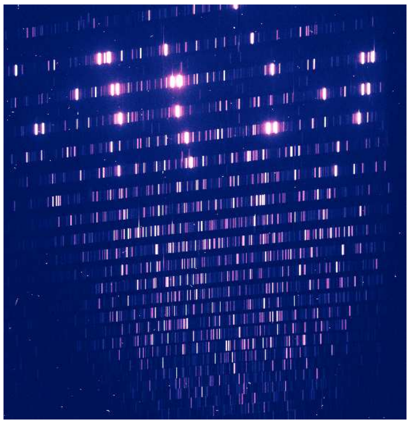
Wavelength calibration using an arc lamp exposure is a basic step in spectral calibration, usually requiring a careful analysis of errors and selection of lines, especially in echelle spectroscopy where arc spectra containing several hundreds of lines are commonly found. Several problems occur when using standard polynomial regression:

- LS regression assumes no error on the independent variables, whereas errors can occur both on the wavelength, due to line blending, misidentifications and quantization, and on the position, due to pixelation and centering errors.
- The lack of robustness to contamination will cause any outlier or misidentified line to affect the complete solution and introduce unnecessary errors into the residuals.
- In order to minimize the number of initial identifications, low-order relations are usually involved at the beginning of the calibration process (e.g., the echelle relation), introducing model errors.

Robust regression is an adapted method to take care of these problems. By combining Hough transform based automated arc line identification and robust regression, it is possible to perform an automated calibration, providing as information the central wavelength and the average dispersion in a single order. This first estimate is refined by Hough transform cross-matching and extended to the complete spectrum using the echelle relation ($m\lambda = f(x)$). However the accuracy of this relation is limited by several factors: in particular, optical misalignments occurring between echelle grating, cross-disperser, and detector. In the first iteration the unknown rotation angle is introduced into the error model of the echelle relation. Lines are then identified by a robust regression based iterative loop.

2.3. Results

Figure 1 shows the calibration of a Th-Ar exposure taken with the EMMI spectrograph at La Silla observatory. The wavelength range covered is 380–940 nm



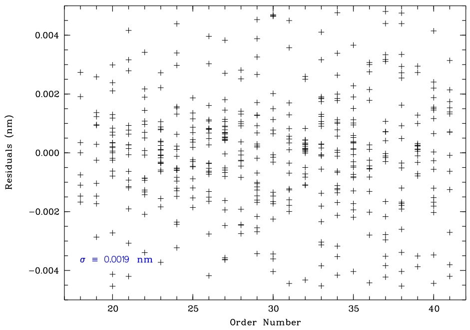


Figure 1. Th-Ar exposure obtained with the EMMI spectrograph at La Silla observatory and figure of residuals.

over 24 orders. The combination of arc line identification by Hough transform and robust regression allows to perform the calibration with the only information of central wavelength (679 nm ± 50 pixels), average dispersion (0.03 nm pixel^{-1} ± 30%) and absolute order number (24) for the relative order 18. The method requires no instrument dependent knowledge and allows for a relatively large inaccuracy of the initial solution. The figure of residuals shows a final accuracy of about 1/15 pixel rms. The Th-Ar line catalog was provided by H. Hensberge and corrected for line blending (De Cuyper & Hensberge 1995).

3. Hough Transform

A description of the Hough transform and its astrophysical applications can be found in Ballester (1994) and Ragazonni & Barbieri (1994). For the application of the HT to the detection of echelle orders, we use a representation of the HT assuming no preliminary segmentation of the image, since the sought-for features are brighter than the background. Accumulating a function of the intensity makes it possible to detect the orders by order of brightness.

The identification of arc lines consists of associating a list of line positions in pixel space with a list of reference wavelengths. The principle of the method is to perform all possible associations in a pixel-wavelength space. A three-dimensional HT allows us to detect, within a given range of central wavelength and average dispersion, the non-linear dispersion relation maximizing the number of associations. In the general case, the maximum is searched for in a cube of the Hough space, providing the parameters $(\lambda_c, \alpha, \beta)$ of the dispersion relation: $\lambda = \lambda_c + \alpha x(1 + \beta x)$. Usually the simplification $\beta = 0$ makes it possible to use a two-dimensional HT.

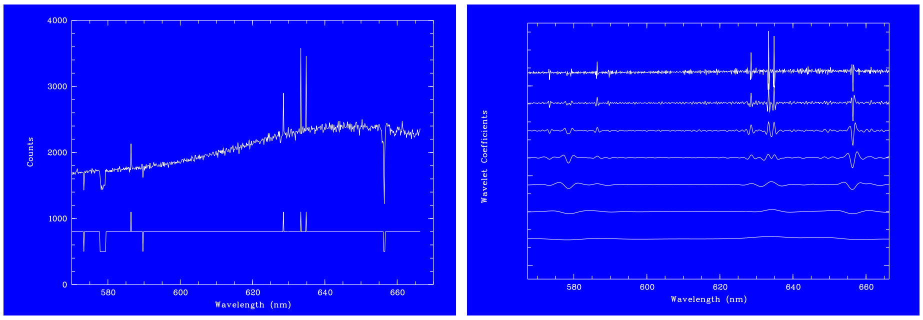


Figure 2. Spectrum of a standard star and associated binary mask (after scaling and translation), and dyadic Mexican hat transform of the above spectrum decomposed on 7 scales. The coefficients of the sharp positive features are concentrated at small scales. Coefficients of the absorption lines are maximized at different scales, depending on their spatial extension.

4. Wavelet Transform

The wavelet transform has been widely described (e.g., Starck, Murtagh, & Bijaoui 1995) and consists of the convolution product of a function with an analyzing wavelet. By choosing a wavelet which is the second derivative of a smoothing function, the wavelet coefficients become proportional to the second derivative of the smoothed signal. The Mexican hat transform involves the wavelet: $\psi(x) = (1 - x^2) \exp(-x^2/2)$ which is the second derivative of a Gaussian. Since the continuum of a spectrum varies smoothly, its second derivative will show increased values at the position of sharper spectral features. Figure 2 shows the Mexican hat transform of a spectrum presenting emission features, as well as absorption lines, of different widths. The wavelet coefficients become maximum (in absolute value) at different scales depending on the spatial extension of the features. The Mexican hat transform can be used to generate a multiresolution mask of the spectral features. The transformation applied to the wavelet coefficients at the different scales includes segmentation, generation of windows, and multiresolution recombination using a coarse-to-fine approach. After segmentation at each scale, the coefficients are compared between successive scales. The process starts from the largest scale and a feature will be retained at the next scale if its associated wavelet coefficients are larger. After recombination the mask is binarized and provides a schematic representation of the spectrum, providing the positions of the continuum and of the features.

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