Recent developments in the optimal extraction of UVES spectra

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1 Introduction

The UVES data reduction pipeline[1] uses optimal extraction to achieve higher signal-to-noise (S/N) of faint objects, corresponding to an increase in effective exposure time up to 70% compared with a simple aperture extraction (see Horne[2] and the further developments by Marsh[3] and Mukai[4] for an introduction). Initial releases of the UVES pipeline had limitations in the extraction quality at certain S/N ranges. We describe the implementation in version 3 of the pipeline, working in the CPL[5] context, which shows significant improvements with respect to earlier versions. The new implementation is used operationally since the beginning of P79.

2 Algorithm

In order to measure the spatial profile a preliminary estimate and subtraction of the sky is carried out by taking the median of all pixels (after masking out the object using a rough object localization). The algorithm then follows Horne's scheme but with the following differences:

- The spatial profile is measured either using an analytical (Gaussian or Moffat) profile (as described in [4]), or by resampling the empirical profile to a grid with a resolution of 0.2 pixels in the spatial direction, and fitting a low order polynomial to the spatial profile at each resampled position.[5] See also figure 3.

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[5] While resampling the data is often avoided because it introduces resampling noise[3], this resampling noise is smoothed when fitting a low-degree polynomial to

- In order to fully exploit the peculiarities of the echelle format the free parameters of the respective models (analytical profile centroid and width, or virtually resampled profile at each spatial position) are modelled as 2D polynomials in wavelength *and* order number. In this way, regions (which may span entire orders) where the profile cannot be accurately determined due to very low signal are interpolated from neighbouring regions having presumably higher S/N.
- Horne's formula for the optimally extracted flux (which is equivalent to profile fitting at every wavelength[2]) assumes that the sky background has been already subtracted, and furthermore that the interpolated sky level is effectively noise-free. Because of the short slits typically used in echelle spectrography (to ensure order separation), the assumption of a noise-free sky determination may not be valid; we therefore generalized the method to give combined optimal sky and object flux estimates by minimization of

  $$\chi^2 = \sum_i \frac{(f_i - (S_i + Fp_i))^2}{\sigma_i^2} \tag{1}$$

  where f_i and σ_i^2 are the flux and variance at the i'th pixel, p_i is the normalized spatial profile, and F and S_i are the object flux and sky levels to be determined. Assuming a simple model where the sky background is constant, $S_i = S$, a two-parameter minimization of eq. (1) yields

  $$F = \frac{(\sum_i 1/\sigma_i^2) \sum_i p_i f_i/\sigma_i^2 - (\sum_i p_i/\sigma_i^2) \sum_i f_i/\sigma_i^2}{D} \tag{2}$$

  $$S = \frac{(\sum_i p_i^2/\sigma_i^2) \sum_i f_i/\sigma_i^2 - (\sum_i p_i/\sigma_i^2) \sum_i p_i f_i/\sigma_i^2}{D} \tag{3}$$

  with variances

  $$V(F) = \frac{\sum_i 1/\sigma_i^2}{D}; \qquad V(S) = \frac{\sum_i p_i^2/\sigma_i^2}{D}, \tag{4}$$

  where $D = (\sum_i 1/\sigma_i^2) \sum_i p_i^2/\sigma_i^2 - (\sum_i p_i/\sigma_i^2)^2$, and where the error bars of p_i and σ_i^2 are not propagated because the final variances are dominated by the contribution from f_i (following Horne). The object and sky spectra are extracted by applying eqs. (2) and (3) to the non-sky subtracted image. In comparison with a separate sky subtraction, this method improves the final object S/N by a few percent (see figure 1) in the low to intermediate S/N range. While this is not a dramatic improvement, we consider it worth the effort because the additional computational cost is practically zero.

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the spatial profile. However, when the model profile is later used to extract the data, it is important that the model is rebinned to the sampling of the data rather than the other way around. Mukai dubbed this "virtual resampling".

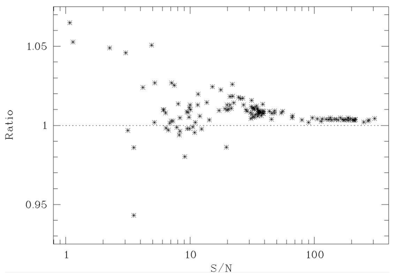

Fig. 1. Ratio of the S/N obtained with the optimal sky subtraction and the S/N obtained with a separate, initial sky subtraction. Each point in the figure corresponds to the extraction of one echelle order in various data sets with different count levels.

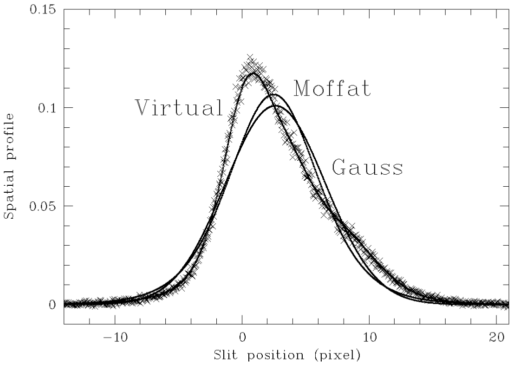

Fig. 2. Empirical spatial profile (crosses) and three models (lines). At intermediate or high S/N the analytical methods usually cannot fit the object spatial profile accurately. (The UVES instrumental PSF is known to be slightly asymmetric, but the high degree of asymmetry shown here for illustration purposes is due to the source being double.)

3 Robust automatic data reduction

Considering the default resolution of 0.2 pixels, a 30 pixel slit length and a two-dimensional 2nd degree polynomial, the virtual method needs to determine 1350 polynomial coefficients from the science image. In contrast, the analytical methods use only 18 coefficients for the two 2nd degree polynomial fits to the centroid and width of the spatial profile. For this reason, the analytical methods are more robust at very low S/N (see figure 4). However, at higher S/N the often significant mismatch between the analytical profile and the empirical profile (see figure 2) is known to bias the extracted flux[3] and make the rejection of cosmic rays unreliable.

In order to have a fully automatic data reduction with always good quality science results the appropriate profile measuring method is selected at runtime, depending on an initial estimate of the object S/N. If it is less than 10, an analytical method is used, otherwise the virtual method is selected. The Gauss and Moffat methods usually give very similar results, and the Gauss method is chosen as default because it makes the data reduction slightly faster.

Also, the degrees of all two-dimensional, low-order polynomials involved are determined at runtime by starting from (0, 0) and increasing the degrees in steps of one or two as long as the residuals decrease significantly. All polynomial fits are weighted, and outliers are rejected iteratively using a robust kappa-sigma clipping. Although this method of determination of the optimal polynomial degrees involves some ad hoc heuristics, it has proven to consistently give better results than setting the degrees manually.

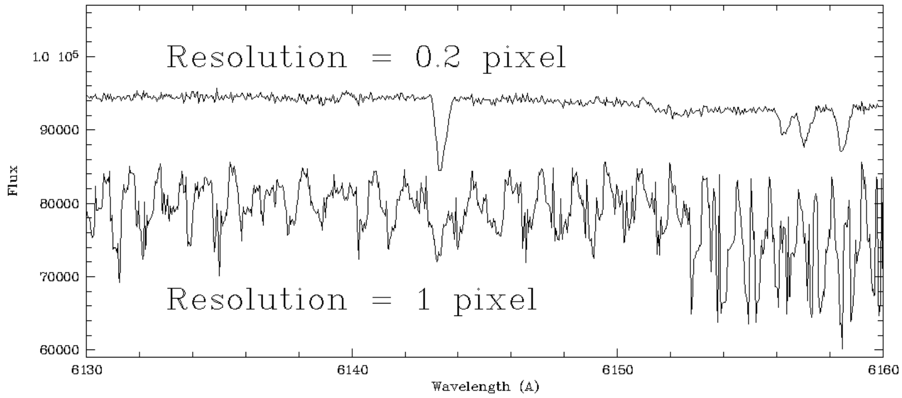

Fig. 3. Zoom of spectrum with S/N ≈ 290. Using a model profile of too low resolution may cause a quasi-periodic pattern in the extracted spectrum.

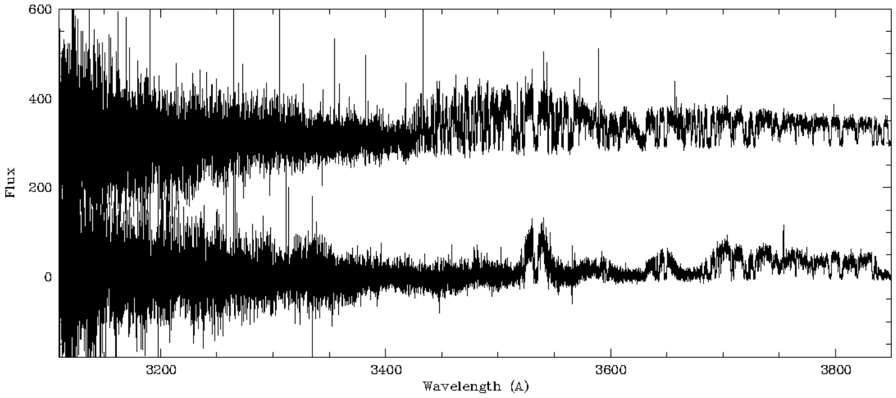

Fig. 4. Comparison of an extracted spectrum obtained with the new algorithm, analytical method (upper spectrum, shifted +300 units for clarity) with the same spectrum as produced using the previous algorithm (lower spectrum). The latter presents regions of missing signal because the object tracing fails in some orders. The global model allows to locate and extract the object in every order in a robust manner.

References

1. P. Ballester et al., ESO Messenger 101, p. 31-36 (2000)
2. K. Horne, PASP, 98:609-617 (1986)
3. T.R. Marsh, PASP, 101:1032-1037 (1989)
4. K. Mukai, PASP, 102:183-189 (1990)
5. www.eso.org/cpl