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Calibrating Echelle Spectra using Instrument Models

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Abstract. We have developed a generic model of echelle spectrographs, based on first optical principles, fully treating 3-dimensions. The geometrical part of it is capable of predicting detector positions for wavelength calibration spectra within 0.2 pix (1 sigma), solely using engineering parameters such as focal lengths, grating constants and configuration angles. First results are also available from the modeling code for grating efficiencies (blaze functions) for any given polarization, surface accuracy and random or periodic groove errors. Combined these tools allow one to carry calibrations of well observed modes into less well or even uncalibrated modes of operation.

1. Introduction

Current and future instruments provide astronomers with large amounts of high signal-to-noise, multi-dimensional observational data. In order to exploit optimally these data, the entire chain of the observation process from instrument configuration control through calibration, analysis and archival has to be tailored towards very high standards. In contemporary data calibration and analysis, very little has been done so far to relate the optical layout and its engineering parameters with the performance on scientific targets and calibration sources. Even less use has been made of the physical principles underlying the characteristics of a given instrument in predicting its performance to such a degree of accuracy, that it will allow to support and even substitute classical (i.e., empirical) calibration and analysis (cf. Rosa 1995).

One of the most demanding cases of data calibration and analysis are 2D echelle spectra. Traditionally, they require complex data reduction procedures to cope simultaneously with both the geometrical distortion of the raw data introduced by order curvature and line tilt, and the spread of the signal across the tilted lines and between successive orders respectively (cf. Hensberge & Verschueren 1988). We have studied (Ballester & Rosa 1997) the principles governing the accurate form of the echelle relation for off-plane echelle spectrographs, and have applied software models based on these equations to several echelle spectrographs at a ground based observatory (ESO's CASPEC, UVES) and to HST's STIS.

In the present paper we summarize the salient points of the above analysis, then discuss the potentials for application in model based calibration and analysis, and finally address the steps required to implement these techniques.

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2. Modeling Optical Principles in Echelle Spectrographs

The elements of a model for echelle spectrographs are mirrors, lenses, gratings, prisms, grisms. For the moment we will focus solely on the geometric aspects, i.e., the relations producing the spectral formats at the detectors. Luminosity aspects brought about by the interference terms, e.g., the echelle blaze function, line spread functions, as well as geometrical vignetting, reflectivity and transmissivity of materials, are remarked upon in Section 5.

Following the discussion in Ballester & Rosa (1997), the optical elements are placed into the 3D geometry of the instrumental layout, and then optical rays are followed through the system (here from slit to detector) using rotational matrices to change back and forth between the 3D instrumental geometry and the optical surfaces. This procedure allows one to write very compact code while retaining full visibility of the optical equations at each surface, a necessary requirement for studying the merits of first principle models in observation simulation. For example, all STIS modes can be completely described by the following operations at each reflective surface: 3 matrix rotations at entry, 1 matrix multiplication at the surface, and 3 matrix rotations on exit from the surface (collimator, X-disperser or mirror, Echelle or mirror, camera). A final rotation and projection deals with the detector.

In a complete optical train, the above strictly applies only for on-axis rays and does not take into account field distortions, camera aberrations and the like. In instruments like UVES (as described below) these effects can amount to discrepancies of several pixels at the detector. Distortions are specific to the optical elements and layout, and are usually predictable and stable in time. As was shown by Ballester & Rosa (1997), a model for a given instrument and mode will typically match 99% using the physical description as developed above. For most applications it will not pay off to develop further the description by introducing fully general off-axis optical equations. Instead, these percent-level effects can be accounted for by inserting at the proper location (eg. during projection onto the detector) low order polynomial functions whose coefficients can for example be produced with the help of a ray tracing program.

3. Comparison of Simulated and Observed Spectral Formats

The model represents adequately all effects for off-plane spectrographs, including line curvature with an accuracy close to one pixel. Because it is mostly based on linear algebra, it is straightforward to produce high performance code. Such code can be used to generate accurate simulations of lamp exposures through various slits (wavelength calibration observations). We have used such simulations to "re-find" the engineering parameters of CASPEC (ESO), which has been in operation for over a decade. We ran automatic feature line centering algorithms on the data frames to obtain x, y-location tables of about 560 Th-Ar lines. Optimization of the configuration parameter sets used the simulated x, y-positions on the basis of the catalogued wavelengths. The residuals between the measured and predicted positions are typically 0.4 pixel (3 sigma), where 1 pixel represents 0.5 true resolution elements. This result is excellent, since we can attribute most of the scatter to the difficulties generalized (Gaussian fitting, edge detection etc.) line centering techniques have in locating the centers of the tilted and curved emission line segments in the observed 2D echellograms.

As detailed in Ballester & Rosa (1997), we could show that the incident angle on the echelle grating remained very stable between 1984 and 1991 ($71\overset{\circ}{.}2 \pm 0\overset{\circ}{.}7$). A dataset from epoch April 1994 produces a configuration solutions with a value of $71\overset{\circ}{.}6 \pm 0\overset{\circ}{.}7$ for this angle. Although the shift of $0\overset{\circ}{.}4$ seems to be insignificant in the nominal error margin, it coincides with an overhaul and reassembly of the instrument in 1992, and may indicate that our conservative quotations of nominal errors are actually surpassed by the predictive power of the instrument simulation software.

4. Application: Wavelength Calibration and Order Extraction

The model technique described above represents adequately all effects for off-plane spectrographs including line curvature with an accuracy better then an actual resolution element. Because it is mostly based on linear algebra, it is straight forward to produce high performance code. Such code can for example be used to generate accurate initial solutions of the dispersion relation using the grating positions as provided by encoders. This allows to implement fully automatic, boot-strapping wavelength calibration procedures, considerably easing the chore of generating calibration reference data.

One of the most demanding cases for the implementation of un-supervised pipeline data reduction is the target extraction and wavelength calibration of high resolution, large field 2D echellograms. Typically (e.g., the `calstis` software package for STIS), a complex structure of code segments is supported by a large number of tables to define expected "average" solutions and to provide the capability to adjust to shifts, tilts and rotations of the actual spectral format. Underlying is the assumption that two spectral formats with only small deviations in one or more of the angles defining their generating optical paths can be affinely transposed into one another. Unfortunately, the various features of an off-plane echelle spectral format (e.g., order separation, order curvature, line tilt and line curvature) cannot easily be predicted simultaneously to the same accuracy by simplistic transformations and scaling laws.

In the classical schemes it is therefore necessary to provide a dense coverage of the actually observed range of spectral formats (e.g., shifts induced by non-repeatability of grating mechanisms or off-center location of target on extended slits) with reference data from empirical calibrations. Also required is a mechanism to align the nearest solution with the actually observed case and then to translate predicted dispersion solutions and order locations using linear offsets. Typically one uses correlation techniques to find these shifts—the result on an actual scientific dataset being insecure in the case of low S/N, or even undetermined in the case of, e.g., pure emission line spectra. Also, the requirement of finding and following the ridge of a spectral order for optimal extraction schemes is most demanding exactly where the scientific (target) signal is low compared to the background (eg. in the valleys of deep and broad P-Cygni absorption profiles).

It is obvious that predictive algorithms based on first optical principles can provide more exact solutions for any observed situation. Empirical calibration exposures in this scheme are used to optimized configuration parameter sets. The classical "alignment" task then reverts into, e.g., estimating the actual value of a grating tilt angle, and predicting a new full dispersion solution, instead of estimating a zero point shift only for a prefabricated "approximate" solution.

5. Implementation Requirements and Current Activity

This concludes the exploratory stage, in which we developed from first principles the formalism of optical equations for spectral formats in echelle spectrograms, suitable for high performance code. Lately we have successfully configured models for a broader range of instruments, and the list now includes FOS, STIS (HST), CASPEC, UVES (ESO), and all 8 "modes" of IUE (SW, LW; Primary and Redundant cameras; low and high resolution).

Current activity is concentrated on linking the spectral format code with multi-parameter non-linear optimization software, such as simulated annealing. This will yield software ready to be applied routinely for calibration purposes, e.g., to automatically produce optimized configuration sets for the plentitude of STIS modes, and to apply our first principle predictive technique in a routine manner to the spectral extraction from STIS frames.

Up to now we have concentrated on instrument model code that deals exclusively with the geometrical aspects (spectral formats). In a next step we will include the luminosity aspects. As is well known, the basic textbook grating and echelle blaze function equations do not generally produce sufficiently accurate predictions of the efficiency curves from real spectrographs (excluding simple corrections such as vignetting or reflectivities of materials). The failure has its physical basis in the necessity to find a solution to a set of N Maxwellian equations, where N is equal to the total number of grooves illuminated by the beam. The simple equations work best for first order, low resolution gratings in near Littrow configuration, where groove shaping errors, and the permeability and conductivity of the coating and the substrate play a lesser role.

Therefore predictive code for the luminosity aspects will probably have to be based on a capability to simulate real gratings from the superposition of a large multitude of idealized textbook gratelets, and the goal is to find a compromise between accuracy and speed. Once this second aspect of spectrograph simulation can be predicted with the same success as in our geometrical code, a fully model-based predictive calibration will be a question of package implementation rather than principle.

Our work is closely linked with the calibration and data flow activities of instrument supported at two major observatories, namely HST and ESO's VLT, with a view towards next generation instrumentation. These two current instruments are well supported by "classical" calibration and data reduction techniques and therefore provide an ideal testbed for our predictive calibration and forward data analysis scenario (cf. Rosa 1995). We anticipate that user-friendly packages on the geometrical aspects of STIS and UVES will become available for the respective communities in mid-1998.

References

Ballester, P., & Rosa, M. R., 1997, A&AS, in press

Hensberge, H., & Verschueren, W., 1990, A&A, 240, 216

Rosa, M.R., 1995, in *Calibrating and Understanding HST and ESO Instruments*, ed. P. Benvenuti (Garching: ESO), ESO Conf. Proc. No. 53, p. 43