

Gaussian Extraction of Low Resolution Spectra from IUE Images of Point Sources: The *GEX* Programs

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I. Introduction: The Basic Method

The IUESIPS method of extracting spectra from IUE images sums signal from the central 9 lines of an image and subtracts background that is the sum of two 5-line wide swaths on either side of, and separated by 5 lines from, the central 9 lines. (These numbers are for 55-line-by-line format; double them for 110-line-by-line files.) It has long been recognized that this does not produce the best signal-to-noise, particularly for a faint signal above a high background. It has the advantage that the center line need not be well-defined and the spectrum need not be well focussed; however, since most of the signal is concentrated in the central 5 lines, the IUESIPS method adds unnecessary noise. Also, determining background in the standard manner introduces systematic error because the background is observed to change smoothly over the camera face; that is, the summed background in the IUESIPS extraction may be quite different from the background appropriate to the center of the signal 10-15 lines away. The statistical fluctuations in the background intensity using only 10 lines may also be large. Furthermore, the IUESIPS extraction procedure does not discriminate between cosmic ray hits and photons, so that spurious emission features arise.

For these reasons, other extraction techniques have been developed, and one of these is the Gaussian extraction method described here. The basic approach was developed by Karen and Richard Hackney (Hackney, Hackney, and Kondo 1984, IUE 4th Year Conf. Proc.), who in turn were following a suggestion by Koorneef and DeBoer (IUE Newsletter No. 5). The Gaussian Extraction, or *GEX*, programs, were written in IDL by the present authors with help from Randy Thompson of the Goddard Regional Data Analysis Facility (RDAF) staff, and are implemented on the Goddard RDAF Vax.

GEX consists of two passes on the line-by-line file,¹ one coarse and one fine. The first pass, *GEX1*, fits a linear background plus a Gaussian to a series of cross-cuts (signal perpendicular to the dispersion direction). All fit parameters are stored in a table. In an intermediate step, the Gaussian widths are fitted to a quadratic, allowing for a smoothly changing focus along the spectrum. The second pass, *GEX2*, uses the same Gaussian-plus-linear-background model, but calculates only the height of the Gaussian for each cross-cut, taking the appropriate linear background coefficients and Gaussian centers from the table (interpolated where necessary) and imposing Gaussian widths determined from the quadratic fit. The width and height of the Gaussian determine its area and thus the flux at that particular cross-cut.

II. Details of the *GEX* Programs

Now a few details about each pass. After the line-by-line (LBL) file is read, the fluxes are scaled from 0 to 1 to better suit the fitting algorithms. The "signal" and "background" regions are then defined. For a 55-LBL (110-LBL) file, the current version of

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¹ A better procedure would be to operate on the unsampled file.

GEX uses lines 1–23 (1–46) and 33–55 (65–110) as background and 24–32 (47–64) as signal. The Gaussian center is set to line 28 (55) as an initial guess for the fits to the cross-cuts; during the fits the center is allowed to vary as a free parameter.

For each pass, the user selects the desired number of samples (*i.e.* the desired extent in wavelength) per cross-cut. For an exposure of reasonably good signal-to-noise, a typical first pass would look at 10-sample “chunks”, or about 17Å in wavelength for the SWP and 27Å for the LWR or LWP cameras. A typical second pass would be sample by sample. For the weakest signal, one barely visible on the photo-write, a first pass of 50-sample chunks and a second with 6-sample chunks generally works well.

In *GEX1*, the background region of a chunk is fitted to a linear function using the standard RDAF *LINFIT* program (similar to the Bevington routine of the same name). The standard deviation of the points around the fit is returned as σ . Then any points deviating by more than 2σ are ignored and the remaining points re-fitted to a line. The slope, intercept, and standard deviation are then saved. In practice, ignoring 2σ deviations removes clear outliers while leaving enough points to determine the background accurately. We did not find it useful to repeat the rejection and re-fitting steps.

A word about the background region selected: in general, the background varies smoothly over the camera face, and a linear fit is quite good — tests show a quadratic fit is no better. However, at the long-wavelength end of the SWP camera, one can clearly see the circular edge of the detector in lines 1–15. Thus we plan to change the *GEX* code to exclude lines 1–15, at least for the relevant part of the SWP image. No other such systematic problems have been seen in extensive tests of many different images.

After the linear background has been determined, the appropriate values are subtracted from the signal vector for that chunk. If the average remaining signal in the central region is less than $\sigma/2$, where σ is still the standard deviation from the linear background fit, then no Gaussian fitting is done, zeroes are written to the intermediate file, and the fit parameters for this chunk will be ignored in the second pass.

If sufficient signal is present, the background-subtracted signal is fitted with a Gaussian (using the standard RDAF routine *WFIT*), with height, center, and width all free parameters. The version currently in the RDAF experimental library uses the background-fit σ as the uncertainty on each point, so that all are weighted equally. This is clearly not optimal since the central few lines contain most of the signal. A better method would specify uncertainties using a plausible error model such as $\sigma = V_0 + F/Q$, where V_0 is a constant term reflecting the magnitude of the fixed pattern noise (analogous to the readout noise for a CCD), F is the expected flux in DN at the point (initially the observed value of the data, and then the height of the fitted Gaussian plus background for subsequent re-fits), and Q is the conversion factor between the number of incident source photons and the observed data number.² The DC term V_0 can be found from null images, and Q is known from pre-flight calibration of the cameras to be 2.7 for the SWP camera and 3.4 for the LWP and LWR cameras (Bohlin *et al.* 1980, *Astr. & Ap.*, **85**, 1). The line-by-line linearized flux units (FN) must first be converted into DN; conversion factors are given by Bohlin *et al.* (1980). This improvement to the error estimate should be implemented in the *GEX* routines shortly.

² We are grateful to Keith Horne for suggesting this improvement to the error estimate; see his contribution, this volume, or Horne 1986, *P.A.S.P.*, **98**, 609–617 for a discussion of estimating the variance of the data.

After finding the best-fit Gaussian, the cross-cut is checked for points more than $n\sigma$ away from the fit, where initially $n = 2$. Occasionally this would result in more than half the signal points being thrown away; if so, n is increased to 3 and points are checked again. This continues until at least half the signal points remain. (An improvement would be to keep all points within 2σ of, or else the half closest to, the first fit Gaussian, whichever includes more points. However, in practice the cycle to increase n is rarely invoked.) With the bad points discarded, new Gaussian parameters are determined. As with the background, only one re-fitting is done. If the suggested improvement to the error model is made, the re-fitting would be iterated until no new points are rejected.

At this point, background and Gaussian parameters have been determined for one chunk. The process is repeated for each successive chunk, and the values are stored in an intermediate table which is then used for the second pass and also to evaluate the success of the first pass. In particular, do the Gaussian widths vary more or less smoothly with wavelength, or is there a large amount of scatter? For a judiciously chosen coarseness in the first pass, the scatter in the widths from chunk to chunk will be small compared with the overall variation with wavelength; if this is not the case, then the first pass should be done more coarsely. In non-batch-mode processing it is useful to check the quadratic fit to the widths (and the amount of scatter), but experience generally indicates the proper intervals to use (see below).

Some nitty-gritty details of the intermediate step: zeroes in the table are ignored, since they indicate the first-pass chunk was too faint; Gaussian widths that are too large (≥ 3 or ≥ 6 for 55-LBL or 110-LBL files, respectively) are ignored; remaining widths are fitted to a quadratic function of λ ; and Gaussian centers are pegged to the range 27-29 or 53-58, but are not fit to any smooth function. An alternative, fancier version also allows for hand-editing to remove additional unacceptable values of Gaussian width or center (independently).

The second pass, while done on a finer scale than the first, is computationally much simpler, and therefore does not take a lot of time. The cross-cut is extracted and scaled from 0-1. The background slope, intercept, and standard deviation, and the Gaussian center are interpolated from values in the table; the Gaussian width is calculated from the best-fit quadratic. At present, all signal points are weighted equally. Since the Gaussian height is the only free parameter, one solves for it directly instead of using *WFIT*. The standard deviation of the fit, σ , is also calculated. Just as in the first pass, points deviating by more than $n\sigma$ where n starts at 2, are deleted and the Gaussian height and sigma are recalculated once. The [uncalibrated] flux associated with the mean wavelength of the current cross-cut is simply the area under the Gaussian, and the statistical uncertainty in the flux is related to the area and the sigma of the fit.

The following improvements to the second pass are the same as those discussed for the first pass: (1) to weight the signal points according to an error model, (2) to iterate the discarding-points-and-refitting process, and (3) to remove points one by one rather than according to multiples of σ . These changes may be implemented in the near future, as they require minimal changes to the code. Additional improvements might be to allow for asymmetric Gaussian profiles (see below), and to use a more accurate functional form for the variation of profile width with wavelength.³ These improvements would involve

³ Based on studies of high signal-to-noise, well-focused spectra, Cassatella *et al.* (1984, IUE Newsletter No, 24) and more recently Altner (1987, private communication) have found

some rewriting of the code but could be accommodated fairly simply.

The only subjective intervention required in the *GEX* scheme is the choice of first- and second-pass sampling grids. Depending on the quality of the spectrum, from good to poor, chunks should be between 10 and 50 samples for the first pass and between 1 and 6 samples for the second pass. Guessing correctly requires a little experience with the method. One typically starts with a 10-sample first pass and checks the resulting width and center plots (as a function of wavelength) to assess its success. If the signals in the 10-sample chunks are strong enough that the fits are not too noisy, *i.e.*, if the widths vary smoothly with wavelength without a large degree of scatter, if few (or none) of the widths are 0 or ≥ 3 (or ≥ 6), and if the centers are not "too erratic",⁴ then the 10-sample first pass is fine. Otherwise, a 20-sample first pass is tried. And so on.

III. Advantages and Disadvantages

The *GEX* extraction routines were developed more or less empirically — first optimized for very weak spectra, and then adapted to suit high quality spectra also. Most of the details enumerated in the previous section were evolved through extensive testing rather than as a result of some clear computational philosophy. Despite this lack of intellectual purity, the method works well. Here is a list of advantages:

- (1) The Gaussian profile is usually very good. In the highest signal-to-noise SWP spectra, one can see a slight asymmetry toward the higher-line-number side. A special version of *GEX* fits an asymmetric Gaussian according to the form prescribed by Cassatella *et al.* (1984, IUE Newsletter No. 24) but the "lost flux" is on the order of 1% of the total flux, and so for most purposes the asymmetry is unimportant.
- (2) The Gaussian extraction clearly improves the signal-to-noise of the extracted spectrum over the IUESIPS procedure. For a typical weak spectrum, the rms deviation about the mean in the Gaussian case, for 100Å bins, is 0.7 of the rms deviation for the IUESIPS case. This is comparable to the improvement obtained using the Optimal Extraction Method described by Horne, *op. cit.*.
- (3) The *GEX* programs accommodate the "wobble" in the spectrum. Eventually reprocessing with geometric corrections may remove this wobble, but for the present it exists in the LBL file. Horne's Optimal Extraction Method may not allow for variations of sufficiently high frequency along the wavelength direction.⁵
- (4) The programs exist! and run! at the RDAF. As do auxiliary programs such as a batch-job submission routine that prompts for wavelength ranges and sampling intervals for first and second passes; a routine to access the intermediate table to

that the widths of the instrumental profiles vary as functions of wavelength which are *close* to quadratics but are actually somewhat flatter.

⁴ There is a real "wobble" of the center of the signal with wavelength (see work by Randy Thompson). Thus one expects to see the center of the Gaussian wander about some mean position. However if the first-pass is too fine relative to the quality of the spectrum, the center will oscillate back and forth rapidly simply because there was not enough signal for the Gaussian to be well-determined.

⁵ This depends on the degree of the polynomial describing the instrumental profile as a function of wavelength. In principal, one could include enough terms to describe the wobble, but the computation may then become unwieldy.

display the *GEX1* results; a routine that extracts a spectral vector from the *GEX2* output and absolutely calibrates it; a routine that corrects the Gaussian-extraction-produced sigmas according to the value of the IUESIPS eps vector; and so on.

- (5) The *GEX* extraction handles emission lines well. Since the programs were developed for (and tested on) continuum sources, this is a pleasant bonus.
- (6) One of the purposes of the Gaussian extraction was to remove uninteresting signal from the source signal in the image. With *GEX*, most hits and reseaux are removed, and infrequent saturated points are properly handled.

On the debit side, there are some disadvantages, and some unknowns:

- (1) The approach is fairly unsophisticated relative to the afore-mentioned Optimal Extraction Method. Beyond the original two-pass idea, the details of *GEX1* and *GEX2* were determined empirically, and while the programs have been well-tested on a variety of spectra, they may not work well in every case.
- (2) Some spectra may require subjective judgements, although impartial criteria could be hard-wired into the program with a little effort.
- (3) In high signal-to-noise images, the Gaussian-extracted flux is systematically lower than the IUESIPS-extracted flux, typically by 1-3%. This may be due in part to flux missed in the asymmetric part of the Gaussian, in which case the IUESIPS method produces a better number. Or it may be because curvature in the background makes the IUESIPS estimate of the background systematically low.
- (4) *GEX* does not always remove reseaux completely, does not remove hits if they are in the center of the spectrum, and does not handle a badly oversaturated continuum spectrum.
- (5) Computation time? At present, the program contains a lot of bells and whistles — options to plot, lots of I/O, extra values written to the table for special purposes — as well as non-optimized code. If the IUE RDAF VAX is not heavily used (as in a typical evening), then ~4 spectra can be extracted in ~1 hour with the present code. Is this fast enough and could it be faster with a few modifications? How does it compare to the Optimal Extraction Method (which has not been tested with the same kind of machine under similar loads)? These questions can be answered with a few simple tests.
- (6) Currently *GEX* works on low resolution, untrailed spectra of point sources only.⁶ It may work on high resolution spectra, but only with substantially more programming (and computation time!).

IV. Summary and Conclusions

To anyone who has worked with low resolution IUE spectra of faint point sources, it is clear that the IUESIPS extraction is inadequate. Some sort of optimized extraction method is necessary. Whether it should be the *GEX* routine or the Optimal Extraction Method of Keith Horne or IUESIPS with a narrow-slit or something else depends on a number of factors, including the following.

⁶ In principal one could determine the instrumental profile from an observation of a point source and deconvolve it from the image of an extended source, but whether this scheme would actually work in the presence of noise and temporal variations of focus and so on, is unclear.

- (1) Faithfulness to the image, as judged by looking at the fits to the cross-cuts.
- (2) Apparent signal-to-noise, as judged by the rms deviation about the mean in a fixed-size wavelength bin.
- (3) Processing time; comparing methods with identical data on the same computer, even if programs are written in different languages.
- (4) Success in removing hits and reseaux and in compensating properly where the spectrum is saturated.

Each of these points should be evaluated for a variety of exposures (low, medium, and high signal-to-noise), for continuum objects and strong-line objects, and for standard calibration stars. It may be that the different methods should be used in different cases. Whatever the outcome, there is no reason that an optimized extraction method cannot do all of the "right" things.