A Revised Parameterization of the Dispersion Constants for High Dispersion IUE Spectra

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I. Introduction.

An overriding theme of physics is that discovering the correct representation of variables in a set of algebraic relations is the most important step in solving them. This is no less true in the representation of the wavelengths on a two-dimensional echelle format than it is for dynamical problems. In preparation for the creation of a high dispersion line-by-line file for the final archive processing of *IUE* images, this article sets forth the justification for the most economical parametric representation of wavelengths on the *IUE* camera format. Although this representation will be tailored to the particular circumstances of the *IUE* cameras the parameter representations can be incorporated analytically into any two-dimensional format. Some of the very peculiarities of the *IUE* cameras that make the flux calibrations so difficult for this instrument are also those that permit a simplification of the representation of dispersion constants.

The requirements for an optimal representation of the wavelengths are that:

1. there be a 1:1 correspondence between terms and physical causes,
2. the number of parameters be kept to a minimum,
3. the terms comprise an orthogonal set, so that errors in the terms are mutually independent,
4. the addition of unanticipated terms can be accommodated in a natural way,
5. the representation easily permit analyses in new ranges of parameter space or dimensions. For the *IUE* this might include dependences in time, camera temperature, intensity of exposure, etc.

II. Current Representation.

The solution of wavelengths in line and sample space in current *IUESIPS* requires the computation of a set of least squares constants A_i's and B_i's common to the entire image and is defined by the following linear equations:

$$\begin{aligned} \text{Sample Number} &= A_1 Z_1 + A_2 Z_2 + A_3 Z_3 + \ldots + A_7 Z_7 \\ \text{Line Number} &= B_1 Z_1 + B_2 Z_2 + B_3 Z_3 + \ldots + B_7 Z_7 \end{aligned} \tag{1}$$

In this representation the Z's are defined as follows:

$$Z_1 = 1, \qquad Z_2 = m\lambda, \qquad Z_3 = (m\lambda)^2, \qquad (2)$$

$$Z_4 = m, \qquad Z_5 = \lambda, \qquad Z_6 = m^2\lambda, \qquad Z_7 = m\,\lambda^2$$

The justification for this representation has not been documented in the *IUE* literature, although several terms do make obvious sense as will be shown below. The relations in (2) date back to the early history of the Project and to a suggestion by Dr. Sara Heap that the high order and cross terms might map out opto- electronic distortions. However, notice that the equations (1) and (2) preserve all aspects of the assumed s, l rectilinear coordinate system. They do not exhibit any r^n geometric dependences suggested by optical aberrations, even though the focus can be readily shown to be affected toward the edges of the camera field.

In the following we will analyze the parameterization of the two-dimensional spectral field in the *IUE* cameras and lay out a new plan for the representation of wavelength positions on the echelle format with only four parameters, a translational constant and a scale factor for each of the x, y axes. What makes this simple representation possible is the "virtual" property of pixels in the cameras, that is they are not fixed entities on the detector, and also the use of gratings to disperse light in both x and y directions.

III. Representation of a Single Echelle Order along the x Axis

To calculate the spectral dispersion of a single echelle order the normal procedure is to work in one dimension and to evaluate the angular dispersion of the grating, $d\beta/d\lambda = (m/d)\sec\beta$, where β is the echelle grating diffraction angle, and where β and λ change in the direction of dispersion. One generally evaluates the dispersion at an arbitrary position along the spectrum by computing the value of β there. However, one may equally represent spectral dispersion by a Taylor expansion of its value around a suitable fiducial "x" position. In the following it will be convenient to rotate the camera field so that the "x" and sample axes are aligned. Then the value of s is given by the equation:

$$s = s_o + f_{cam} \times \sum (1/n!) \times (m/d)^{n+1} \times d^n(\sec\beta)/d\beta^n \times (\delta\lambda)^{n+1} \qquad (3)$$

In this equation the reference position can be conveniently defined to be the echelle blaze maximum, corresponding to the blaze angle β_o, and all higher order derivatives are evaluated at that point.

Let's consider the first term of the series in equation (3), and in particular the expansion around the wavelength interval $\delta\lambda$. It is convenient to expand the term

$m\delta\lambda$ as follows:

$$m\,\delta\lambda \quad = \quad m\,(\lambda\ -\ \lambda_o\,) \quad = \quad m\,\lambda\ -\ m\,\lambda_o$$

Notice that the second term, $m\lambda_o$, is nothing more than the blaze wavelength for the echelle grating. Since it is a constant, it can be folded in with the initial translational constant that specifyies the position s_o of the blaze wavelength λ_o. Thus the first term in the summation in equation (3) merely introduces the parameter $m\,\lambda$.

Similarly, the second term in the series involves the product $m^2 \times (\lambda - \lambda_o)^2$. The two lower order terms in its expansion, $m\lambda_o$ and $(m\lambda)m\lambda_o$, can be included into the first two parameters of the representation for wavelength; the only new one is the parameter $(m\,\lambda)^2$. Thus, so far the parameters representing wavelengths in a single order are:

$$1, \qquad m\,\lambda, \qquad (m\,\lambda)^2. \tag{4}$$

Of course, this parametric expansion could continue indefinitely. In the *IUE* spectrograph the echelle orders have $m \sim 100$. Thus, along a typical order in the camera field the nonlinearities in dispersion amount to about $\pm1\%$ and $\pm0.01\%$ from the first and second terms, respectively. The first of these is significant, but we will judge the second to be negligible and therefore neglect terms of higher order than $m^2\lambda^2$ in this discussion. In the actual implementation described in Section VI, higher order terms can be easily included without introducing complications into the parametric representation.

IV. Two-Dimensional Visualization.

Our key to a good visualization is a picture provided by Dr. Ted Gull, shown in *Figure 1.* This figure shows an optical echellogram of a Hg-vapor lamp aided by a relatively powerful cross-dispersing grating. The lines drawn in the figure identify the following coordinate system:

1. an x axis defined along a reference echelle order; any order may be chosen for convenience,
2. a y axis perpendicular to the x axis,
3. a locus of constant λ, indicated by a shallow dashed line,
4. a "λ vector" perpendicular to #3, also indicated by a dashed line.

The spectrum in *Figure 1* is so overexposed that both the continuum and the strong Hg emission lines are readily visible. The x axis is identified with the direction of dispersion of a reference echelle order. Hence, the parameter $m\,\lambda$ can be thought of a vector aligned with the x axis. The cross dispersing grating is aligned perpendicularly to the echelle so that it disperses light perpendularly, that is along the y axis. As one moves up the y axis one encounters new echelle orders, and the wavelengths differ from the preceding ones by the ratio of echelle orders, m_{lower}/m_{upper}. Hence, we see that 1/m may be taken as a vector, and therefore a continuous variable, aligned with the y axis.

Now notice the three emission lines along the dotted shallow line. These are actually the same line in adjacent echelle orders, so the line adjoining them is the locus of constant wavelength. Look carefully at the features of this slanted "spectrum". These features are caused by ruling errors of the echelle grating; one can even see patterns from the brightest ones replicated in mirror image on opposite sides of a bright line. Physically, this "spectrum" is the monochromatic scattering function resulting from both gratings. If they were perfectly ruled and the gratings were infinite in extent, there would be no "continuum." Next, one can identify the vector perpendicular to this locus with the λ parameter. The sharp spikes trailing above and below the sharp lines show the monochromatic scattering image from the cross dispersing grating alone.

The two dimensional format is not quite uniform over the entire image. Because both gratings disperse light, the λ vector is the vectorial sum of the dispersions of the two gratings, $m\lambda$ and λ. An angle ψ between them can be equated to the arctangent of the ratio of various grating parameters. The most significant of these parameters is the spectral order, *i.e.,* $\tan(\psi) \sim m_{Xdisp}/m, = 1/m$ for the *IUE*. Notice that as one moves vertically along the y axis, the echelle order m varies, and this causes the angle ψ to change as well. This fact has two consequences. First, it means that adjacent echelle orders are not quite parallel. This departure from parallelism can be called "order splaying." Second, if one were to proceed along an echelle order some distance one would find eventually that the local value of ψ had changed relative to its value at the blaze, (*i.e.,* at $y = 0$), and thus the order is slightly curved. For most grating cross-dispersers, this curvature is negligible along the useful range of the echelle blaze function. However, for spectrographs using prismatic cross dispersers the angle of "diffraction" is a function of wavelength, and the curvature is much more noticeable (*e.g.,* Schroeder 1987). It should be added that the effective "β_o" of the cross disperser in the *IUE* cameras is only about one degree. Therefore, the change in $\sec\beta_{Xdisp}$ along the y axis, and therefore the nonlinearity in cross dispersion, is altogether negligible.

To summarize, *Figure 1* provides a visualization of the geometrical orientation of the parameters $m\lambda$, $1/m$, and λ as vectors x, y, and y', respectively. It is convenient to associate the blaze angle β_o with $x = 0$, and a reference echelle order with $y = 0$. Because only one order is exactly aligned with the x axis, some provision must be made for splaying of the orders. Finally, the nonlinear term in relation (4) can be thought of simply as a term in x^2.

V. Two Dimensional Parameterization.

The echelle orders in a grating cross-dispersing system can be represented by a series of hyperbolas, given by the equation $x\ y\ =\ constant$. Parametrically, this is a term in λ, which was already identified as parameter Z_5 in relation (2). Recall that the slope of this line is given by the angle ψ, which angle changes across the camera field. The "splaying function" can be approximated as a straight line segment of the full hyperbola as long is m is large and $m\chi_{disp}$ is small. Note that the λ vector generates splaying only when used with the nearly parallel vector 1/m. Of course, the errors in these two terms will be strongly correlated. Note also that operationally, m remains discrete only in the term $m\lambda$, where it is used in a look-up table to assign each wavelength to a unique echelle order.

This parametric analysis can be generalized to handle spectrograph formats with special features. For example, those with prismatic cross-dispersers will have curved echelle orders and perhaps even "S-shaped" distortions that can be parameterized by $y = x^2$ $(m^3\lambda^2)$ and $y = x^3$ $(m^4\lambda^3)$ dependences, respectively, Additionally, it is possible in principle to handle optical aberrations at the edges of the field by rewriting 1/m and $m\lambda$ in polar coordinates.

From the foregoing, we can drop terms Z_6 and Z_7 because they are inappropriate representations of the optical formatting in the spectrograph. In those cases for which it is possible to rectilinearize the orders, the splaying (Z_5) term can be eliminated and the s and l (sample and line) equations decoupled from one another. We will now also advocate the linearization of the high dispersion wavelengths, and therefore the elimination of x^2 (Z_3) or higher terms. In that case, each equation becomes represented in the simplest possible way, by a constant and scale factor:

$$\begin{aligned} s &= A_1 + A_2\, m\lambda \\ l &= B_1 + B_4\, 1/m \end{aligned} \qquad (5)$$

This is the logical conclusion of our efforts and our recommended parametric representation for the final archiving of *IUE* spectra. Once again, it should be stressed that one cannot remove terms Z_3 and Z_5 in the representation of all echelle formats because in many cases their detectors consist of real fixed pixels.

VI. Rectilinearing the Orders, Linearizing the Wavelengths

In the next *Newsletter* Shaw will discuss a strategy to correct for image distortions of *IUE* images. The plan calls for correcting the measured reseau positions to their known values by interpolation with two dimensional cubic splines. The implict idea behind such an approach is to exploit the "virtual' property of *IUE* pixels to modify the centroid of each pixel slightly with respect to its neighbors. There is virtually no penalty for fractional adjustments in the floating-point pixel positions provided that the adjustments are done *prior* to the final resampling, i.e., their conversion to integer values. We propose to correct for order splaying and wavelength nonlinearities along an echelle order by explicit geometric mapping, that is, by adding two more vector terms to the de-distortion field. There are a few rationales for this vector approach. The first is convenience: constant spacing for the relevant physical variable, wavelength, permits its linearization. The convenience offered by de-splaying is a simple (and conceivably shorter) extraction slit. A second rationale is the reduction of dispersion constant in equation (1), particularly when they can be calculated precisely from known grating constants. A third advantage is the benefit realized in the stability and errors of the solution by removing nonorthogonal and cross-coupling terms such as x^2 and xy.

Operationally, the vector-mapping procedure consists of the following steps:

Step #1 : Rotate the camera format.

Rotate the camera format about its center until the x axis is aligned with a convenient order.

Step #2 : De-splay the orders.

This is accomplished by rotating each order around its $x = 0$ point. A straight line representation is adequate for *IUE* spectra though linearity need not be imposed. The angle ψ is computed at the center of each echelle order and a reference order angle ψ_o is subtracted from it. It is sufficient to estimate the y positions of these orders at $x = 0$ from the dispersion constants from previous wavelength calibrations. The vector shifts from this de-tilting are applied to virtual pixel locations along each echelle order.

Step #3 : Linearize wavelengths.

The nonlinear terms (in practice only $n = 2$) can be computed as a function of β, and therefore s or x positions from equation (2). In practice, the values can be computed explicitly for the $y = 0$ order and then scaled to other orders by the ratio of their m's, which takes into account the "compression" of the blaze function toward shorter wavelengths. The computation of the nonlinearity proceeds by incrementing outward along the sample direction from $x = 0$ and computing the new angle β and the term $\sec\beta\tan\beta$ at each pixel. Note that this is equivalent to evaluating a Taylor series at a fixed point $x = 0$ with several higher order terms (eqn. 3). This computation determines the shift of each pixel relative to the preceding one as well as the aggregate shift for this pixel before the operation began. Notice that this algorithm also permits a small correction for the curved camera focal plane. Computing the linearization requires knowledge of both β_o and mean dispersion values for each camera, but these are already known.

VII. Final Recommendations.

Dr. Tom Ayres has pointed out that the current coefficients in the solution for dispersion constants given by eqn. (1) range over 10 orders of magnitude, and that these vast inequalities can promote instabilities in the solution. Therefore, we would underscore his recommendation to the April, 1989 meeting of the *F.A.D.* Committee workshop that all parameters be normalized to a value appropriate to the middle of the cameras.

With only a spatial and scale constant representing each dimension in eqn. (5), one can afford to solve for constants over small spatial scales rather than over the entire camera image. This opens the possibility of analyzing the behavior of each of the four A_i, B_i coefficients as a function the smallest spatial unit, an individual echelle order. Such analysis provides an insurance policy that all spatial mappings "upstream" are correct. If they are not, they will show up as trends, wiggles, or even as discontinuities (in the case of camera fault lines separating "tectonic plates") that could require fine-tuning of the vector shifts. In addition, all time and temperature calibrations to date have resulted only in a camera-averaged translational shift, but perhaps higher order dependences are imposed across the camera field. The solution of the dispersion relations order-by-order would permit such evaluations rather easily.

Figure 2 shows histograms provided by Mr. Randall Thompson based upon a new line library of Pt wavelengths suggested by Ayres. In order to provide solutions for 4 variables, each echelle order should contain five lines; to be safe, let's say six lines. These histograms show that for both cameras (the LWR and LWP are identical) the line density is just high enough to permit a wavelength solution for an individual order. At the top and bottom of the camera fields, it may become necessary to group together two or three orders. It should be admitted also that this library assumes that the wavelength calibrations would be made over a large range of exposure times, which unhappily has not always been possible. Still, it is clear that it should be possible to reduce substantially the spatial averaging required for the positions of high dispersion wavelengths in the *IUE* cameras.

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References

Schroeder, D. 1987 *Astronomical Optics*, (San Diego: Academic Press, p. 287.

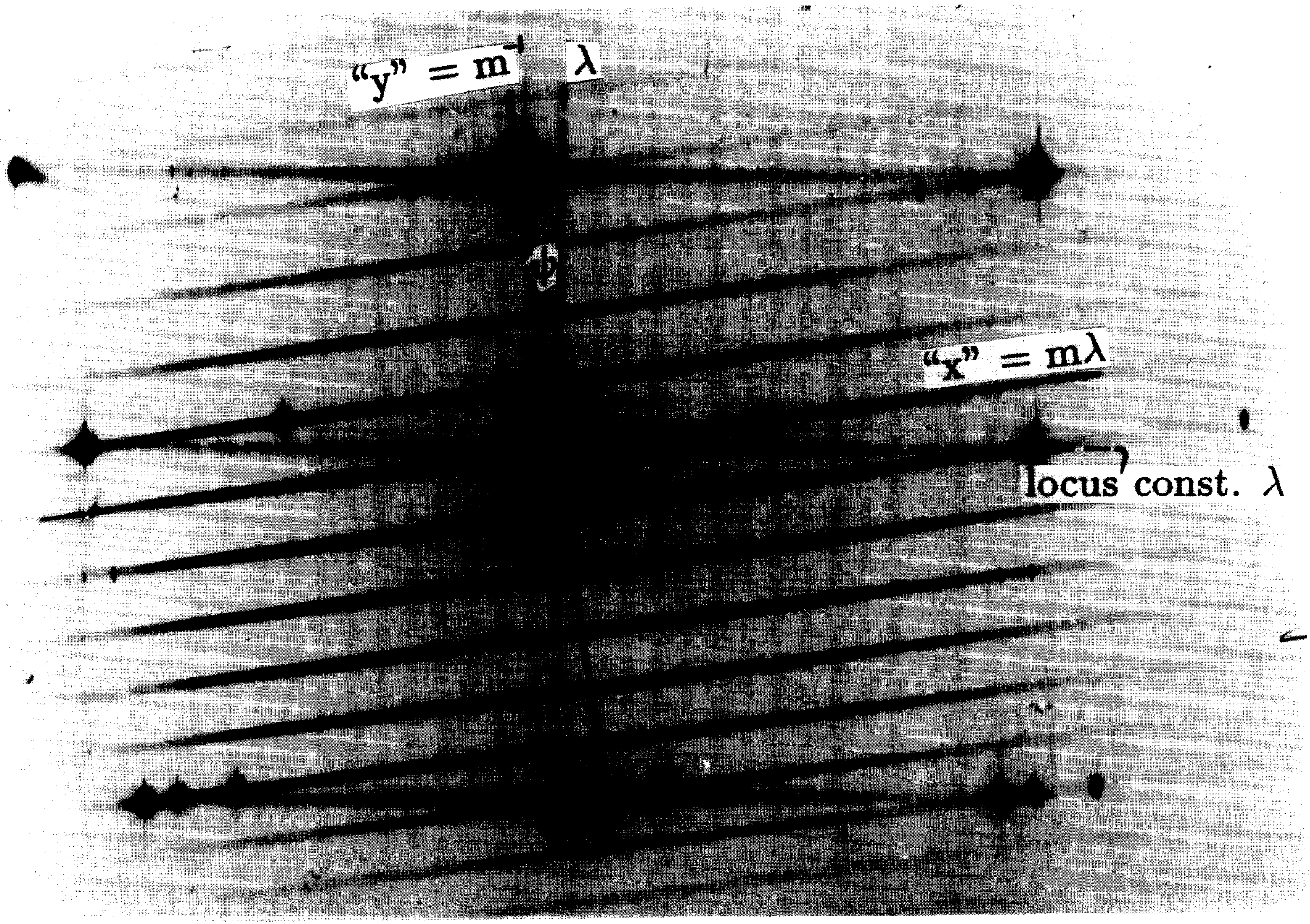

Figure 1 -- Echellogram of Hg-vapor spectrum with superimposed coordinate system.

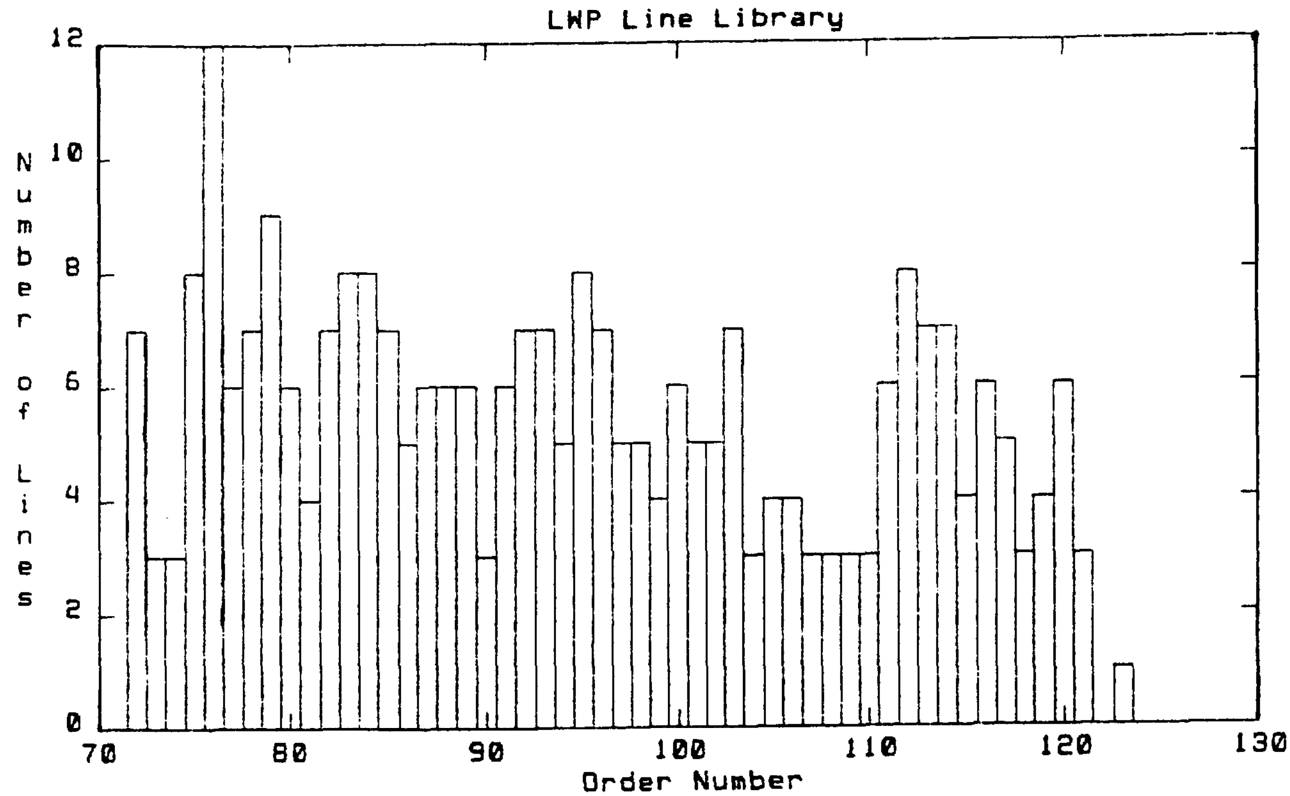

Figure 2A -- *Histogram of acceptable lines in proposed wavelength calibration library, LWP camera.*

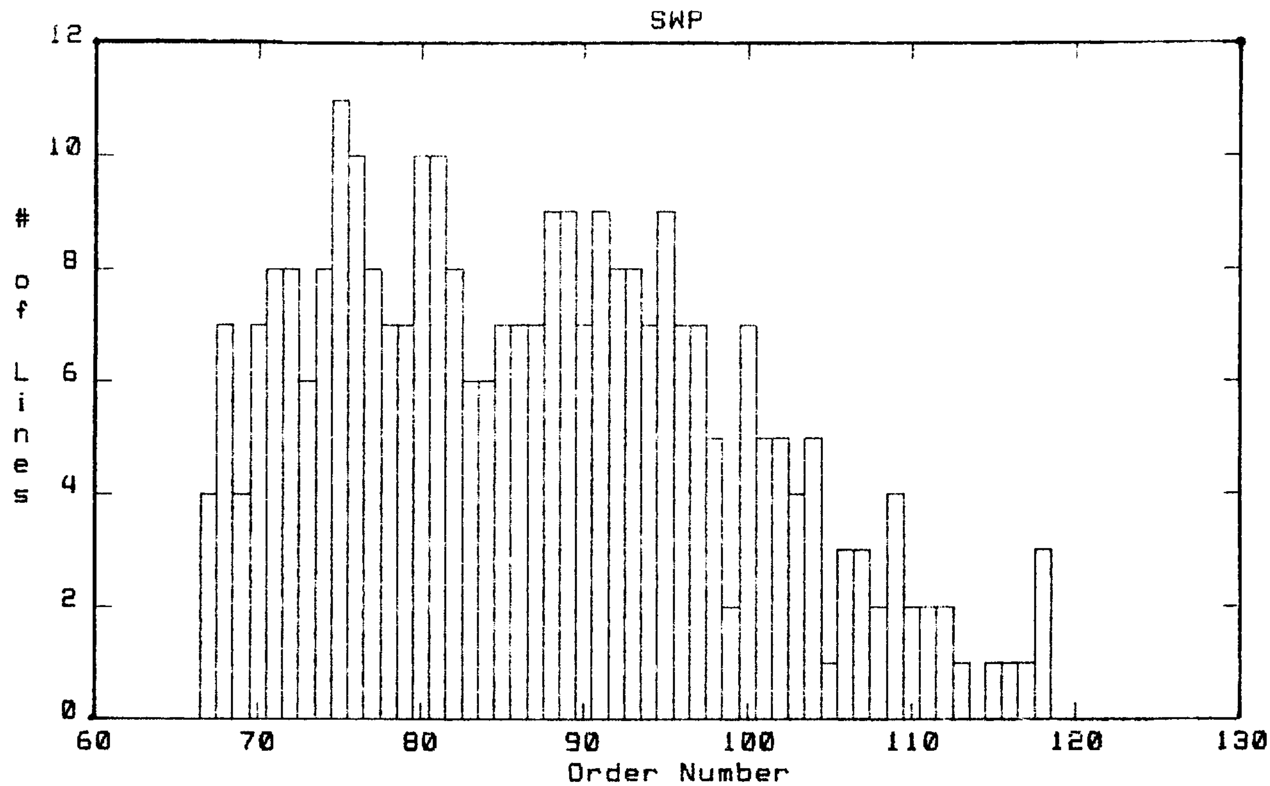

Figure 2b -- *Histogram of acceptable lines in proposed wavelength calibration library, SWP camera.*