DECONVOLUTION OF SIMULATED HST SPECTRA. II
EXTENSION TO VARIABLE PSF AND NEW TECHNIQUES

Ronald L. Gilliland
Space Telescope Science Institute, 3700 San Martin Drive
Baltimore, MD  21218

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This continues the series of reports addressing the impact of poor OTA focus on the HST spectrographs. In particular we investigate the potential role of reconstruction techniques in maximizing the scientific return of spectral observations. Unlike the cameras, the spectrographs can acquire data in which the primary impact is simple loss of light, without any degradation of resolution, through use of narrow slits. Thus we must face the question: Should the observations be obtained through a narrow slit at intrinsically poor S/N, but good resolution, or through a broad slit with deconvolution applied to restore resolution, but at the price of degrading the initially better S/N? The above question is posed for consideration of spectral resolution on an isolated source; as with the cameras work in spatially crowded fields is compromised – here the narrow slits are of little help.

In this report we explore the use of more powerful restoration techniques: constrained nonlinear methods, and maximum entropy. (Previous report addressed Fourier deconvolution with optimal Wiener filtering.) These approaches offer significant gains in the accuracy of restored, simulated spectra, and can be extended trivially to deal with point spread functions that vary over the domain of a single observation (as will occur for FOS).

A future report will begin to address more realistic spectral simulations, inclusion of residual flat-fielding errors and the inherent undersampling of the first generation HST spectrographs. Both of these issues complicate the consideration of tradeoffs between use of narrow versus broad slits.

Analysis of simulations continues to suggest that observations should be acquired through the small spectrograph apertures, with concurrent loss of light, if the limiting spectral resolution is desired. We do not find that deconvolution works well enough to argue for a switch to large apertures, followed by deconvolution, for routine observations.
I. INTRODUCTION

The previous report in this series showed that one would in general be better off (if limiting instrumental resolution is to be retained) to observe through a small slit, keeping spectral resolution at the start, rather than using a wider slit and deconvolution. Why continue the investigation of deconvolution techniques for the spectrographs? There are several reasons:

1. Use of more powerful techniques could in principle reverse the initial conclusion, making observation through wider slits more attractive.

2. The one-dimensional work on spectral reconstruction can serve as a path-finder for the much more computationally burdensome 2-d imaging problem.

3. The choice of slits for the GHRS is limited to only two, a very narrow one at 0.25", and a broad 2.0" aperture. Should the adopted focus provide less light through the small slit than assumed in these simulations (a distinct possibility), the wide slit might then be a generally preferred option.

4. The FOS has a variable line spread function inherent to the spectrograph; even if the OTA focus were not a problem, development of techniques to remove this variable internal smearing would be desired.

5. For a limited subset of observations (where low resolution is required) the use of deconvolution of wide-slit data is already seen as preferable to the narrow-slit observations.

In this report we introduce the use of two relatively new techniques, compare accuracy of resulting restorations with the more familiar Fourier technique, and demonstrate their successful treatment of a variable smearing function. We will also provide mention of a few techniques that were tried, but that did not produce results competitive with other approaches.

The approaches discussed in this report follow largely from the book: Deconvolution With Applications in Spectroscopy by P. A. Jansson, 1984. The (possibly) original contributions herein are: 1) adoption of a better smoothing function required for the constrained nonlinear method, 2) demonstration of utility for a variable PSF, and 3) a proposal for optimal termination of iterative solutions to reconstruction problems.

II. CONSIDERATION OF ADDITIONAL TECHNIQUES

We present first a short discussion of two techniques that work well for the spectral reconstruction case, and that can be trivially extended to handle a variable PSF. For completeness, mention will also be made of all techniques that were implemented, but that failed to produce impressive results, either due to inherent limitations of the technique, poor match to current problem, or even possibly inadequate coding.

a. Jansson's nonlinear constrained method

The best of many techniques tried to date for the reconstruction of spectral data is also the simplest to outline. Jansson’s approach is an iterative reconstruction that makes use of information
in the current spectrum estimate to control certain aspects of the iteration, and is hence non-linear. The method allows full use of simple prior information, such as a positivity constraint. Injection of a seemingly innocuous constraint such as positivity can make deconvolutions for certain problems dramatically more accurate. The constraint can also include an upper bound, as would be appropriate for a spectrum composed of a continuum with superposed absorption features. Taken together the inclusion of these two constraints, an upper and lower bound to the allowed solution, allow a significantly improved deconvolution. The bounds to the solution are enforced by a simple relaxation function. The iteration proceeds via small corrections to the estimate for the true spectrum. The Jansson technique works by forcing corrections near the bounds to be small, and by changing the sign of corrections that would extend beyond the bounds. Presentation of the algorithm and a graph of a relaxation function should make this clear. The problem at hand is to solve the integral equation:

\[ \phi(x) = \int \psi(x-y)P(y)dy \]

where \( \phi(x) \) is the observed spectrum, \( P(y) \) is the known point spread function blurring the true spectrum \( \psi(x) \) that we desire a robust estimate of. In this notation the Jansson, constrained approach involves the following steps. Iterate the equation:

\[ \psi^k(x) = \psi^{k-1}(x) + r^k[\psi^{k-1}(x)][\phi(x) - \int \psi^{k-1}(x)P(y)dy] \]

where the relaxation function \( r^k \) is given for example by:

\[ r^k[\psi^{k-1}(x)] = r_{max}^k \left( 1 - \psi^{k-1}(x) - (A + B)/2 \right) / (B - A) \]

where \( r_{max}^k \) is a constant controlling iterative step size, \( B \) is the allowed upper bound (e.g., continuum level), and \( A \) is the lower bound (zero enforces positivity). For a spectrum that has been normalized to extend from limits of 0.0 to 1.0, the relaxation function with \( r_{max}=1.0 \) is shown in Figure 1.

Reconstruction processes remain an art form, as opposed to a well defined science. There is much freedom in detailed choice of the relaxation function to be used. Furthermore it is well known that presmoothing of the data should be used as input to the iteration shown above. There is much discussion in the book by Jansson about finding the best choice of data smoothing. We believe that application of the classically defined optimal Wiener filter (simple Fourier smoothing) actually is the best possible choice.

Figure 2 shows the primary test spectrum used for these experiments. The input spectrum consists of a continuum level at 10,000 with many randomly positioned, sharp gaussian absorption features. The lower panels show the results of convolving through the SSA and LSA of the GHRIS with addition of sqrt(N) gaussian distributed noise. The lost throughput of SSA and lost resolution of LSA are easy to see.

In the previous memo on this subject the result of optimal filter deconvolution was shown. In Figure 3 we compare the deconvolutions of SSA and LSA spectra for Fourier (Wiener filter) deconvolution and Jansson's technique. The upper two panels show difference spectrum of deconvolution relative to perfect input spectrum for Fourier case, the lower two panels show same
for the Jansson technique. Clearly the Jansson technique shows better results. (A numerical comparison of resulting quality of restoration will be given after discussion of other techniques.)

It is worth pointing out some limitations of the Jansson approach. The nonlinear iteration does not force flux conservation, in the current tests a non-conservation occurs at the level of 0.3%; since the total flux in the input is known one could make a correction of this magnitude simply by scaling the resulting total back to correct level. A possibly more serious objection is that the errors shown in Figure 3 are apparently more correlated with spectral features in the Jansson technique, than in the intrinsically noisier optimal filter deconvolution. We have further investigated this by plotting the differences (as in Figure 3) against the input spectrum in Figure 4. Indeed, there is a suggestion of greater systematic errors for the strongest lines. Two things can be said of such systematic errors: 1) systematic errors remaining in data reductions are bad, but 2) if the errors are systematic the effect can be calibrated out. Thus, if deconvolution with the Jansson technique were to be seriously pursued, then it might be worthwhile to apply a calibrated correction as function of line depth (and probably smearing function width). Given that the r.m.s. error resulting from the Jansson technique is already smaller than from Fourier deconvolution, any removal of the slightly greater systematic errors would be even more favorable to the Jansson technique. Of course applying corrections of this nature would require excellent understanding of both the technique, and a model for the observation.

A further useful approach to examining differences between reconstructions is to look at power spectra of the differences. Figure 5 shows the power spectra corresponding to differences as plotted in Figure 3. Frequency is in cycles/pixel from zero to the Nyquist limit. High frequencies are suppressed by the optimal Wiener filter for the Fourier deconvolutions. The high frequencies in the Jansson technique restorations do in fact contain useful information that contribute to the lower realized errors of the deconvolution. The power spectra of differences allow a useful conclusion concerning relative utility of SSA and LSA observations. At the lowest spectral frequencies the LSA observations produce smaller errors. At the higher frequencies (where spectral line information will usually reside) the SSA does better. Clearly these comparisons carry implications for proper selection of aperture depending on the details of what one is trying to extract from the spectra.

A full determination of utility of a given deconvolution technique depends in detail upon the information a scientist wishes to extract from an observation. Consideration of how well the technique performs for: a) determining equivalent widths of weak lines, b) core depth of strong lines, c) continuum shape, might well lead to quite different conclusions.

b. Maximum entropy reconstruction

We have adopted the maximum entropy package of Gull and Skilling, 1984 (MEMSYS Users' Manual) as modified by Keith Horne. Keith had previously modified the maximum entropy codes to allow imposing bounds at a continuum level, as was useful in the Jansson approach. It is beyond the scope of this report (or the author's knowledge) to provide a discussion of the maximum entropy technique. For this report it is sufficient to note that a well tested maximum entropy code was adopted (with much help from Keith Horne) and tested with the standard spectrum. Figure 6 shows the results for the best solution with maximum entropy, the upper panel is perfect input spectrum, middle panel is reconstruction, and the lower panel
is the difference spectrum. The maximum entropy solution is significantly better than Fourier
(optimal) filtering, but not quite as good as the Jansson iteration in terms of a simple r.m.s.
measure. It is quite possible that a maximum entropy solution would be preferred for some
classes of science.

The Gull and Skilling implementation of maximum entropy deconvolution does not include
constraints of smoothness directly in the objective functions being solved. The current best
solution with maximum entropy smoothes the spectrum estimate between iterations by a 3-
point boxcar low-pass filter (using code added by Keith Horne). While this works quite well, I
imagine a similar constraint imbedded more directly in the basic solution would produce superior
results. Maximum entropy solutions could probably be developed that would outperform the
Jansson technique in accuracy within a more robust theoretical framework, although at a much
higher computational burden. (For the 2-d problem the extra machinery of maximum entropy
solution might not impose such a severe relative overhead, since the simple convolutions done
in support of any iterative technique would require considerably more resources.)

c. Other methods implemented

We have tried two other techniques, neither of which performs as well as the simple optimal
constrained approach (positivity constrain only) that has met with considerable interest from
the astronomical community. A second approach is attributable to Bracewell, 1958 (Proc. Inst.
Radio Eng. v. 46, 106) and Helstrom, 1967 (J. Opt. Soc. Am. v 57, 297) and provides a variant
of the Wiener optimal filtering that minimizes errors between observations and solution. Table
I contains a comparison of the five approaches discussed above.

<table>
<thead>
<tr>
<th>Technique</th>
<th>rms(LSA)</th>
<th>rms(SSA)</th>
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<tbody>
<tr>
<td>Jansson</td>
<td>237.</td>
<td>183.</td>
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<tr>
<td>Maximum Ent.</td>
<td>245.</td>
<td>—</td>
</tr>
<tr>
<td>Fourier</td>
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<td>215.</td>
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<td>Lucy</td>
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<td>246.</td>
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<tr>
<td>Bracewell</td>
<td>788.</td>
<td>518.</td>
</tr>
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III. EXTENSION TO VARIABLE PSF

The FOS is expected to have problems with variable point spread functions from two effects:
1) near the ends of their free spectral range the gratings will introduce line spread function
asymmetries of opposite sense at the extremes of wavelength, 2) over the large spectral range
covered by single low-resolution spectra, the OTA spatial PSF input may vary. (GHRS spectra
in the lowest resolution mode might suffer from similar effects at a reduced level. The problem of
variable PSFs and deconvolution is fundamental to proper treatment of WF/PC observations.)

A variable smearing function is introduced simply by making \( P(y) \) from Eq. 1 dependent upon
\( z \) also. If the convolutions are done algebraically (in fact this is faster than use of FFTs, given
the narrow width of the PSF), then it is easy to see how the variable PSF can be introduced
both to produce a simulated spectrum (evaluating Eq. 1 with everything on right hand side
known). It is equally easy to make the solution of Eq. 2 follow with use of a variable PSF. In our case the constant PSF is a vector with 5 elements for the SSA and 33 elements for the LSA of GHRS (simulations are done with GHRS apertures, although problem is more important for eventual application to FOS), the variable PSFs are simply matrices of 5x2000, and 33x2000 that are easily stored in computer memory. (Note that direct extension to the 2-d WF/PC case would require huge arrays; here one would tabulate the PSFs on a maybe 10x10 grid and interpolate as needed.) The variable PSF is also easy to implement within the maximum entropy package.

Figure 7 shows the variable PSF that we have adopted for this test. The left to right asymmetry is shown as top and bottom panels; the asymmetry magnitude scales as the square of distance away from spectrum center, so that it primarily impacts only the outer regions of the spectrum. The simulation is an exaggeration of what is expected for FOS spectra. The variable PSF, over 2000 spectral points, thus varies smoothly between the cases shown in Figure 7.

We have deconvolved the convolution of the variable PSF with the standard test input of this note, with three different approaches: 1) Fourier optimal filtering using the PSF from center of spectrum, 2) variable PSF and Jansson's technique, 3) variable PSF and maximum entropy. This was done only for the LSA. Resulting r.m.s. measures of success were: Fourier: 443., Jansson: 250., Maximum Entropy: 266. Figure 8 shows the results for Fourier and Jansson reconstructions as the second and fourth panels. The Fourier solution does not take into account the variable PSF, with resulting large errors where deviations of the PSF symmetry were significant. The Jansson deconvolution handles the variable, asymmetric PSF as well as a constant PSF.

Computationally the Jansson approach (with variable PSF) converges in about 20 steps (for this test case) requiring about 4 seconds per spectrum on a sparcstation. The maximum entropy solution requires more than an order of magnitude more time.

IV. COMMENTS ON USE OF NONLINEAR DECONVOLUTION TECHNIQUES

A primary problem encountered with any of the iterative spectral restoration approaches is knowing when to stop the iteration. Stopping at $\chi^2 = 1.0$ is a common approach, but this may not provide the best solution. In our test cases to date we know precisely the true solution, and the level of induced noise. We may estimate $\chi^2$ precisely (not possible in general), as well as more direct measures of how well the reconstruction matches the known input spectrum. For definiteness note that we define $\chi^2$ as:

$$\chi^2 = \sum \frac{(\phi_{obs} - \phi_{calc})^2}{\phi_{calc}}$$

The normalized value with expectation of unity value is obtained by dividing by the number of data points, $\phi_{calc}$ is the convolution of estimated object spectrum and smearing function at each step in the iterations. In these simulations, where we know truth, the r.m.s. between reconstruction, $\psi_{calc}$, and the known input spectrum, can be followed. The closest approach of $\chi^2$ to unity is not necessarily the same as minimum r.m.s.; or minimum of any other measure of quality of reconstruction. Given that for a real problem one does not know the prior truth to allow termination of the iterative process, but only an estimated $\chi^2$, how should a solution be reached?
The following process should work well:

1. Produce a spectral reconstruction terminating the iteration at $\chi^2 = 1.0$.
2. Adopt the reconstruction as a model for the true spectrum.
3. Decide on a measure (e.g., r.m.s. deviation) that a good reconstruction should minimize to define best solution.
4. Produce a model observation by convolving the model for true spectrum with smearing function, and add in appropriate noise.
5. Form iterative nonlinear solution for both the observed and model spectra, stopping at the minimum of quantity defined in step 3 for the model spectrum restoration.
6. If desired repeat steps 2 through 5 with an updated model spectrum.

The choice of optimal reconstruction measure adopted for step 3 above may well depend on the science one wishes to derive from a given observation. This approach is clearly not amenable to "pipeline" processing, but should provide a robust way of approaching the best possible reconstruction for well defined assumptions.

V. SUMMARY

The use of prior information, such as positivity constraints and continuum limits, can improve the fidelity of spectral reconstructions. The nonlinear deconvolution techniques produce results that contain many subtleties. The choice of whether to use deconvolution techniques at all, if so, which one, and how it should be used in detail, will depend on the information to be derived from the observation.

In general, current results suggest that use of the small apertures (without need for following application of deconvolution) on the spectrographs will generally be preferred. This conclusion could be modified in response to less than expected UV throughput in the small apertures.
FIGURE CAPTIONS

Figure 1. Example of a relaxation function used with Jansson's nonlinear constrained solution. Function forces iteration corrections to be small near boundary, and imposes a sign change if solution attempts to go beyond the imposed solution limits.

Figure 2. Top panel shows perfect input spectrum used for all simulations in this note. Input is a continuum at 10,000 with 200 superposed gaussian absorption lines of random position and amplitude. Lower panels show result of convolving (with an observed optical PSF derived from WF/PC data) the input spectrum though SSA and LSA apertures of GHRS, sqrt(N) gaussian noise has been added.

Figure 3. Difference spectra for deconvolutions of the SSA and LSA spectra of Figure 2, relative to the perfect input. Upper two panels are for SSA and LSA with optimal filter Fourier deconvolution. Lower panels are same for Jansson's technique reconstruction.

Figure 4. Same information as in Figure 3, but displayed as scatter plots of differences versus values of the input spectrum. Useful for pointing out systematics with line strength.

Figure 5. Power "spectra" of the difference spectra shown in Figure 3. Useful for visualizing what spectral frequencies are handled best by different aperture observations, or deconvolution technique.

Figure 6. Shows results of best maximum entropy reconstruction. Upper panel is input (truth), middle panel is the reconstruction, and lower panel are the differences.

Figure 7. Three values of continuously variable PSF used in testing capability of restoring data in which the smearing function changes through the data domain. PSF at top is applied on left side of spectrum, PSF at bottom to right side, with continuous variation through case at middle as shown.

Figure 8. Difference spectra for deconvolution of the variable PSF as illustrated in Figure 7. Second panel shows the Fourier deconvolution (that incorrectly assumed a constant PSF), bottom panel shows the Jansson, iterative solution.
Figure 1: Relaxation function vs. solution range.