ON THE USE OF THE INVERTED ABEL INTEGRAL
FOR EVALUATING SPECTROSCOPIC SOURCES

by

J. D. Algeo and M. B. Denton

Prepared for Publication
in
Applied Spectroscopy

Department of Chemistry
University of Arizona
Tucson, Arizona 85721

July, 1980

Reproduction in whole or in part is permitted for
any purpose of the United States Government

Approved for Public Release: Distribution Unlimited
ON THE USE OF THE INVERTED ABEL INTEGRAL FOR EVALUATING SPECTROSCOPIC SOURCES

J. D. ALGEO AND M. B. DENTON

Department of Chemistry
University of Arizona
Tucson, Arizona 85721

Office of Naval Research
Arlington, Virginia 22217

Inverted Abel Integral, Cubic Spline, Three Dimensional Flame Mapping.

A numerical method for evaluating the inverted Abel integral employing cubic spline approximations is described along with a modification of the procedure of Cremers and Birkebak, and an extension of the Barr method. The accuracy of the computations is evaluated at several noise levels and with varying resolution of the input data. The cubic spline method is found to be useful only at very low noise levels, but capable of providing good results with small data sets. The Barr method is computationally the simplest, and is adequate when large data sets are available. For noisy data, the method of Cremers and Birkebak gave the best results.
On the Use of the Inverted Abel Integral
for Evaluating Spectroscopic Sources

by

J. D. Algeo and M. B. Denton

Department of Chemistry
University of Arizona
Tucson, Arizona 85721
ABSTRACT

A numerical method for evaluating the inverted Abel integral employing cubic spline approximations is described along with a modification of the procedure of Cremers and Birkebak, and an extension of the Barr method. The accuracy of the computations is evaluated at several noise levels and with varying resolution of the input data. The cubic spline method is found to be useful only at very low noise levels, but capable of providing good results with small data sets. The Barr method is computationally the simplest, and is adequate when large data sets are available. For noisy data, the method of Cremers and Birkebak gave the best results.
BRIEF

Three methods for evaluating the inverted Abel integral are presented and their sensitivity to noise in the input data and resolution of the input data are evaluated.
Introduction

When spectroscopic observations are made of a flame or plasma, the quantity observed generally represents an integration of the contributions to the signal by species distributed across the source in the line of observation. Detailed knowledge of the conditions at any region within the source requires the application of special techniques. Two line atomic fluorescence may be used to obtain local temperatures within flames (1, 2). The droplet injection technique developed by Heiflje and Malmstadt (3) has been shown to be useful for making spatially resolved temperature measurements (4). Two photon excitation by pulsed lasers has been proposed by Measures as an instrumental technique for obtaining spatial resolution (5). These techniques require special instrumentation and are generally applicable only to the study of temperature profiles or distributions of species possessing good atomic fluorescence characteristics. The droplet injection technique may be more general, but may not reflect the conditions obtained with nebulizer systems.

Mathematical techniques may be used to extract information about the interior from conventional side on measurements. When applied to sources of irregular shape, mathematical techniques require that measurements be made from more than one direction relative to the orientation of the source (6, 7, 8). If the source possesses a simple and regular geometry, one set of measurements will suffice. This is a common case in analytical spectroscopy, where the source often possesses circular symmetry, and may be treated by the inverted Abel integral (9, 10, 11, 12, 13, 14).
This integral may be written as:

\[ i(r) = \frac{1}{\pi} \int_0^R \frac{I'(x)}{(x^2 - r^2)^{1/2}} \, dx \quad (1) \]

where \( i(r) \) is the value of the variable sought as a function of the radius, \( r \); \( I'(x) \) is the value of the observed variable as a function of the distance between the optical axis and the source axis, \( x \); and \( R \) is the outer radius of the source. See Figure 1.

When the inverted Abel integral is used to determine radial emission profiles, it is necessary to account for self absorption if the flame or plasma is not optically thin (15, 16, 17).

In this laboratory, we have been interested in the application of the inverted Abel integral to a variety of sources, including inductively coupled plasmas, stable analytical flames, and transient flames produced by pyrotechnic flares.

Because the transformation of a laterally observed profile into a radial profile tends to accentuate any uncertainty in the observations, it is important to evaluate the noise sensitivity of any technique used to perform the transformation. An extensive analysis of error propagation in Porter's method has been published (18), but many of the other methods have not been subjected to such scrutiny.

In this communication, we present the results of studies into the error propagation of three methods for evaluating equation (1). The methods investigated were a modification of the technique of Cremers and Birkebak (13), an extension of the method of Barr (12), and a new method, based upon Cubic Spline functions, which was developed by the authors. The methods are compared with regard to their accuracy.
under varied conditions of data resolution and noise level, and recommendations are developed for which method is most suitable for a given quality of data.

Description of the Methods

Application of the inverted Abel integral to spectroscopic data requires the construction of a suitable function, $I(x)$, giving the observed quantity in terms of the distance between the source axis and optical axis. A suitable function will possess the following properties: its derivative will be integrable in (1), its first derivative will have a value of zero at the source axis (i.e., $I'(0) = 0$), and it will reject noise in the observed data. The requirement that $I'(0) = 0$ is dictated by the assumption of circular symmetry, and a failure to adhere to this constraint will generally cause a large error in the computed value of $i(0)$. If the function follows noise in the input data, the resulting large values of $|I''(x)|$ will cause significant errors.

Several workers have used polynomial approximations to the unknown function, $I(x)$ (11, 12, 13). Such functions are easily generated from the observed data, and their derivatives yield an integratable representation of Equation (1).

To allow treatment of a variety of curve shapes, the data are generally broken into several segments, each covering a portion of the range of $x$, and a separate polynomial is generated for each segment. These polynomials are spliced together to obtain $I(x)$. For the $j^{th}$ segment, the polynomial representation of $I(x)$ may be written:

$$I_j(x) = A_{0j} + A_{1j}x + A_{2j}x^2 + A_{3j}x^3 + ... \quad (2)$$
with the corresponding derivative

\[ I_j'(x) = A_{1j} + 2A_{2j}x + 3A_{3j}x^2 + \ldots \quad (3) \]

For an approximation of this form, \( i(r) \) is obtained by a summation of Equation (1) over the appropriate segments. The following equation may be used for polynomials of fourth or lower order:

\[
i(r) = \sum_{j} \frac{1}{\pi} \left[ A_{1j} \ln \frac{R_{j+1} + S_{j+1}}{R_j + S_j} + 2A_{2j} (S_{j+1} - S_j) + \frac{3}{2} A_{3j} \left( R_{j+1} S_{j+1} - R_j S_j + r^2 \ln \frac{R_{j+1} + S_{j+1}}{R_j + S_j} \right) + 4A_{4j} \left( \frac{S_{j+1}^3 - S_j^3}{3} + r^2 (S_{j+1} - S_j) \right) \right] \quad (4)
\]

where \( R_j \) is the inner radius of the \( j \)th data segment, or \( r \), whichever is greater; and \( S_j = (R_j^2 - r^2)^{1/2} \).

**Development of the Spline Method**

Cubic Spline functions consist of a series of third order polynomials, each one covering an interval between two points. These polynomials are determined so that the composite function produced by joining them end-to-end has the following properties: the function passes through all of the points, and is therefore continuous; the first derivative is continuous; and the rate of change of the slope is minimized, that is:

\[
\int f''(x)^2 dx \quad (5)
\]

is minimized over the range of \( x \).

Cubic Splines have been used for interpolating data \((18,19,20)\); however, their properties of having a simple, continuous first derivative and a minimized rate of change of slope make them attractive as
approximations of $I(x)$. Reinsch (21) has addressed the problem of fitting Cubic Splines to noisy data by introducing a smoothing parameter, $S$, and allowing the function to pass outside of the data points, subject to the condition

$$\sum_{i=1}^{N} \frac{(y_i - f(x_i))^2}{(dy_i)^2} \leq S \quad (6)$$

Here $y_i$ is the input value, $f(x_i)$ is the value computed from the spline function, and $dy_i$ is the weight of the $i^{th}$ point. $N$ is the number of data points. Reinsch suggests using the standard deviations of the data points as the weights, $dy_i$, and values of $S$ in the range

$$N - \sqrt{2N} \leq S \leq N + \sqrt{2N}$$

Smoothing values well in excess of the recommended range have been explored, and, while good results were sometimes obtained, performance tended to be erratic when smoothing values larger than those recommended were used.

The spline method is implemented by first normalizing the $x$ values to an outer radius of 1.0. Reinsch's algorithm is then applied to generate a smoothed Cubic Spline function having $N-1$ segments. A transformation of the function is performed to give it coordinates compatible with Equation (4). Values of $i(r)$ are computed by evaluating the first three terms of Equation (4) over each segment from $r$ to $R$.

Details of the transformation are given below.

Reinsch's algorithm produces the Cubic Spline in terms of offsets, $h_j$, so that each segment starts at zero:

$$f_j(x - h_j) = A_{0j} + A_{1j}(x - h_j) + A_{2j}(x - h_j)^2 + A_{3j}(x - h_j)^3 \quad (7)$$
where $h_j$ is the value of $x$ at the inner end of the $j^{th}$ segment.

To simplify the application of Equation (4), the spline equations are converted into functions of $x$ as follows:

$$A_{0j}^* = A_{0j} - A_{1j}h_j + A_{2j}h_j^2 + A_{3j}h_j^3 \quad (8)$$

$$A_{1j}^* = A_{1j} - 2A_{2j}h_j + 3A_{3j}h_j^2 \quad (9)$$

$$A_{2j}^* = A_{2j} - 3A_{3j}h_j \quad (10)$$

$$A_{3j}^* = A_{3j} \quad (11)$$

This yields functions of the form:

$$f_j^*(x) + A_{0j}^* + A_{1j}^*x + A_{2j}^*x^2 + A_{3j}^*x^3, \quad (12)$$

where the $h_j$'s have been removed.

One further modification is necessary, since the condition $I'(0) = 0$ is not met by the Cubic Spline function. The innermost segment's coefficients are recomputed so that $I'(0) = 0$ while the original values at the ends of the segments are preserved, along with the continuity of the first derivative. This is accomplished by Equations (13-16):

$$A_{00}^# = A_{00}^* \quad (13)$$

$$A_{10}^# = 0 \quad (14)$$

$$A_{20}^# = \frac{3(A_{11}^* + A_{01}^* - A_{00}^*)(N-1)}{3} - A_{11}^*(N-1) + A_{31} \quad (15)$$

$$A_{30}^# = (A_{01}^* - A_{00}^*)(N-1)^3 - A_{30}^*(N-1) \quad (16)$$

These yield the inner segment equation:

$$f_0^#(x) = A_{00}^# + A_{20}^#x^2 + A_{30}^#x^3 \quad (17)$$
Note that the value $A_{01}$ in Equation (16) is the coefficient from Equation (7), while all other A's in the right hand sides of Equations (13-16) are from Equation (12).

The transformed polynomials $f_0^*(x)$ and $f_1^*(x)$ through $f_{N-1}^*(x)$ are used in Equation (4) to compute the values of $i(r)$.

It was found that this method produced large errors in the values of $i(0)$ due to a sharp change in curvature in the inner segment of the spline function. The following modification was found to reduce the error, and was incorporated into the method: The point next to the center, i.e. at $r = \frac{1}{N-1}$, is reflected across the center to $r = \frac{-1}{N-1}$. The spline curve is then fitted to the $N+1$ points from $r = \frac{-1}{N-1}$ to $r = 1.0$. The segment of this spline function covering $r = \frac{-1}{N-1}$ to $r = 0.0$ is discarded, and the procedure is continued beginning at Equation (8). The inclusion of this extra point appears to steady the function near $r = 0$. Reflection of 2 or 3 points was also tried, but showed no benefit relative to reflecting 1 point.

A further attempt at reducing the error in $i(0)$ was made by reducing the statistical weight, $dy$, of the points at $r = \frac{-1}{N-1}$, $r = 0$ and $r = \frac{1}{N-1}$. This technique did not improve the results, and was not incorporated into the method.

The Cubic Spline method, with one reflected point and equal weight on all points, will be referred to as SPLINE.

Extension of the Barr Method

Barr (12) developed a method of performing the Abel inversion which, while using a multisegmented polynomial approximation to $I(x)$, differs from other methods in that the integration is performed before
the differentiation. This reversal of the order of operations is claimed to reduce the sensitivity to noise in the input data. In addition, this method greatly reduces the amount of computation required through the use of a table of coefficients from which a sum of products is used to compute \( i(r) \):

\[
k = (N-1)r
\]

\[
i(r) = \sum_{n=k-2}^{N} \beta_k n^r, \text{ for } \ N > 2
\]

\[
i(r) = \sum_{n=0}^{N} \beta_k n^r, \text{ for } \ N \leq 2 \tag{18}
\]

Note that \( i(r) \) may be obtained only for values of \( r \) which yield integral values of \( (N-1)r \), and that the function \( I(x) \) need not be generated, since only the observed values, \( I_0 \) through \( I_n \), are needed.

The table of coefficients is given in Ref. (12) for \( N = 21 \). Smaller data sets are handled by the assumption that \( I(x) = 0 \) for \( x > 1.0 \).

In order to perform a complete comparison of this method to the others studied, it was necessary to extend the table of coefficients beyond \( N = 21 \). The table has been extended to cover \( N \leq 51 \) by the use of the equations presented in the appendix.

Modification of the Cremers and Birkebak Method

A method involving multisegmented polynomials in which the segments are overlapped to provide smoothing was developed by Cremers and Birkebak (13). The method has been implemented in this laboratory with two changes:

In order to comply with the restriction that \( I'(0) = 0 \), Cremers and Birkebak changed the form of the approximation of \( I(x) \) from Equation (2) to a fit in \( x^2 \) for the innermost segment:
\[ I_0(x) = A_{00} + A_{10}x^2 + A_{20}x^4 + A_{30}x^6 + A_{40}x^8 \] \quad (19)

To avoid changing the form of Equation (4) to allow for the high orders involved in (19), we have used Equation (2) throughout, subject to the limitation that \( A_1 = 0 \) in the innermost segment. This change from the original method might also be expected to improve the results by reducing the ability of the inner segment to reproduce noise.

The amount of overlap between adjacent segments utilized in fitting the approximations to \( I(x) \), fixed at three points in Cremers and Birkebak's work, was made variable in our modification, and is expressed in percent. Thus, a 50% overlap specifies that one half of the points from the adjacent segments are to be used when fitting \( I(x) \). This modification permits some variation in the amount of smoothing performed.

It was found that double precision (64 bit) math was necessary in the least squares curve fitting computation when 51 point data sets were used.

This modification of the method of Cremers and Birkebak will be referred to as C & B 3 when third order approximations to \( I(x) \) are used, and as C & B 4 when fourth order fits are employed. Except for a limited set of experiments intended for direct comparison to Ref. (9), all work with this method involved a 50% overlap.
Procedures

Three functions describing different shapes of \( i(r) \) vs. \( r \) were used to generate test data:

\[ i(r) = 1 - 3r^2 + 2r^3, \quad (20) \]

the bell-shaped curve from Ref. (13),

\[ i(r) = 0.75 + 32r^3 \text{ over the range } 0 \leq r \leq 0.25 \text{ and } i(r) = 16/27(1 + 6r - 15r^2 + 8r^3) \text{ over the range } 0.25 \leq r \leq 1.0, \quad (21) \]

the off axis distribution from Ref. (13), and

\[ i(r) = 0.79788e^{-8r^2}, \quad (22) \]

a Gaussian curve with \( \mu = 0 \) and \( \sigma = 1/4. \)

"True" inverted data were prepared for comparison with the various inversion methods by evaluation of these functions. "Exact" input data for the inversion calculations were prepared by integration of

\[ I(x) = 2 \int_{x}^{R} \frac{i(r)r}{(r^2 - x^2)^{1/2}} \, dr \quad (23) \]
using (20), (21) or (22) as \( i(r) \). These data were rounded to \( \pm 5 \times 10^{-5} \), corresponding to a residual peak to peak noise level of approximately 0.02 \( \% \), and were assigned weights of \( 5 \times 10^{-5} \) for use by SPLINE. Various amounts of noise were added from a normal distribution by a pseudorandom number generator. The noise was expressed in percent as a peak to peak value referred to the largest observation in the exact data. The standard deviation of noisy data for use by SPLINE was considered to be \( 1/4 \) of the peak to peak noise. Data sets having 11, 21, 31, 41 and 51 points each were prepared and noise was added at 0.1, 0.25, 0.5, 1, 2, 5, and 10 \( \% \). Several replicate data sets were prepared at all added noise levels.

To provide a direct comparison with the results of Cremers and Birkebak, data sets were prepared by rounding the exact values to \( \pm 0.005 \).

The accuracy of the inversion calculations was evaluated by computing the standard deviation of the errors between the computed inversion and the true inversion. This was expressed as a percentage noise in the inverted data relative to the largest value in the true inversion, again using the criterion that four standard deviations define the peak to peak noise. Two factorial design experiments were performed, and the data were subjected to Analyses of Variance.

All computations were programmed in FORTRAN and performed on a Data General NOVA computer.

Results

The modified Cremers and Birkebak method was compared to the original using the off axis distribution of Equation (21). Both
exact data and data rounded to ± 0.005 were used, as in Ref. (13). The results are presented in Table I. The modified method performed much better than the original with 11 point data sets. Above 11 points, the original method was better when exact data were used.

The first factorial experiment used all three distributions, 11 through 41 point data sets, and from 1 through 10 percent added noise. C & B 3 was the best overall, followed by SPLINE and then BARR, with all differences significant (p < 0.05). The three distributions produced significantly (p < 0.05) different results, with the normal curve (Eq. 22) being the easiest to reproduce, followed by the polynomial bell (Eq. 20) and the more difficult off axis curve (Eq. 21).

Some trends are evident in the data from the first experiment (see Table II). The most striking is the failure of BARR at 11 points. Plots of the inverted output from all three curve shapes, of which Figure 2b is representative, show an overdamped appearance when compared to the output of the other methods (Figures 2a and c). Both SPLINE and BARR appear underdamped in the presence of noise when a large number of points are used, as depicted in Figures 3a and b. At the lower noise levels (1 to 2 %), BARR with 31 points worked well, as did C & B 3 with 31 or 41 points. At higher noise levels (5 to 10 %), C & B 3 was clearly superior to both SPLINE and BARR. All three distributions gave qualitatively similar results.

A second factorial experiment was undertaken to elucidate the behavior of the methods at lower noise levels. This experiment used only one distribution, Equation (21), and covered the 0.1 to 0.5 % noise range. Statistical analysis grouped SPLINE and C & B 3 together, with BARR significantly (p < 0.05) worse, due again to the failure of BARR at 11
points. The results of this experiment are shown in Table III. All data collected on the Equation (21) distribution are summarized in Table IV and Figures 4 through 8.

These figures show that SPLINE provided the best results when the input data contained less than 0.25% noise, and that C & B 3 was best with data containing over 0.25% noise. BARR was very poor with 11 point data sets, becoming better as the resolution of the data increased. With small amounts of noise and 41 or 51 data points, BARR approached C & B 3, but both were less precise than SPLINE. As the noise level increased, BARR provided results intermediate to the other two methods.

As seen in Figures 4 and 7, C & B 4 was inferior to C & B 3.

Conclusions

The choice among these methods of performing the Abel Inversion depends upon the situation at hand. If a noise level of over 0.25 is present in the data, the best results may be expected from the modified Cremers and Birkebak method, and a large number of data points should be used. Where precise data are available, the Cubic Spline method should provide the best results, if a reliable estimate of the standard deviation of the data is also available. A small set will suffice in this case. The Barr method may be chosen when simplicity of computation is important, and a large number of data points are available.
Acknowledgements

This research was partially supported by the Office of Naval Research, by an Alfred P. Sloan Foundation Research Fellowship awarded to M. B. Denton, and partially by a contract from Naval Air Systems Command.
References


<table>
<thead>
<tr>
<th>Number of Degree Points</th>
<th>EXACT DATA</th>
<th>ROUNDED DATA</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>This work,</td>
<td>This work,</td>
</tr>
<tr>
<td></td>
<td>Ref&lt;sup&gt;a&lt;/sup&gt;</td>
<td>50 % Overlap</td>
</tr>
<tr>
<td></td>
<td>This work,</td>
<td>3 Points</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Third</td>
<td>(12)</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>154</td>
<td>1.33</td>
</tr>
<tr>
<td>21</td>
<td>4.04</td>
<td>1.48</td>
</tr>
<tr>
<td>31</td>
<td>1.84</td>
<td>1.34</td>
</tr>
<tr>
<td>41</td>
<td>1.06</td>
<td>1.24</td>
</tr>
<tr>
<td>51</td>
<td>0.73</td>
<td>0.66</td>
</tr>
<tr>
<td>Fourth</td>
<td>(12)</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>83</td>
<td>1.08</td>
</tr>
<tr>
<td>21</td>
<td>1.38</td>
<td>1.73</td>
</tr>
<tr>
<td>31</td>
<td>0.74</td>
<td>1.64</td>
</tr>
<tr>
<td>41</td>
<td>0.53</td>
<td>1.53</td>
</tr>
<tr>
<td>51</td>
<td>0.44</td>
<td>1.15</td>
</tr>
</tbody>
</table>

Table I. Comparison of the Modified Cremers and Birkebak method to Cremers and Birkebak's results for the curve given by Eq. 21. All data are peak to peak noise as a percent of the largest value in the true inversion.

<sup>a</sup>Values have been converted to percent noise.

<sup>b</sup>Three point overlaps were produced by the following overlap percentages: 11 points - 100 %; 21 points - 75 %; 31 points - 50 %, 41 points - 37.5 % and 51 points - 30 %. Note that the maximum overlap available with 11 point data sets is only 2 points.
<table>
<thead>
<tr>
<th>Curve Shape Method</th>
<th>Number of Points</th>
<th>0.02</th>
<th>1&lt;sup&gt;a&lt;/sup&gt;</th>
<th>2&lt;sup&gt;a&lt;/sup&gt;</th>
<th>5&lt;sup&gt;a&lt;/sup&gt;</th>
<th>10&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPLINE</td>
<td>11</td>
<td>0.4</td>
<td>2.0</td>
<td>4.5</td>
<td>12.0</td>
<td>13.5</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>0.3</td>
<td>3.3</td>
<td>5.6</td>
<td>8.9</td>
<td>19.2</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>0.4</td>
<td>3.0</td>
<td>4.9</td>
<td>6.9</td>
<td>16.2</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>0.4</td>
<td>2.8</td>
<td>4.8</td>
<td>24.0</td>
<td>23.4</td>
</tr>
<tr>
<td>Eq. 20 BARR</td>
<td>11</td>
<td>6.4</td>
<td>6.0</td>
<td>6.6</td>
<td>11.4</td>
<td>17.9</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>1.3</td>
<td>1.2</td>
<td>3.1</td>
<td>6.8</td>
<td>15.4</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>0.6</td>
<td>1.9</td>
<td>6.0</td>
<td>6.3</td>
<td>16.2</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>0.4</td>
<td>1.7</td>
<td>6.1</td>
<td>27.1</td>
<td>26.7</td>
</tr>
<tr>
<td>C &amp; B 3 Spline</td>
<td>11</td>
<td>0.7</td>
<td>2.2</td>
<td>7.5</td>
<td>13.3</td>
<td>17.7</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>0.6</td>
<td>1.6</td>
<td>6.5</td>
<td>4.4</td>
<td>15.4</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>0.8</td>
<td>1.0</td>
<td>2.9</td>
<td>3.6</td>
<td>12.6</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>0.5</td>
<td>1.5</td>
<td>2.7</td>
<td>4.7</td>
<td>12.1</td>
</tr>
<tr>
<td>Eq. 21 BARR</td>
<td>11</td>
<td>0.7</td>
<td>6.4</td>
<td>5.1</td>
<td>8.8</td>
<td>20.0</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>0.1</td>
<td>2.9</td>
<td>4.1</td>
<td>19.9</td>
<td>22.4</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>0.1</td>
<td>3.9</td>
<td>6.0</td>
<td>13.4</td>
<td>21.0</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>0.1</td>
<td>4.3</td>
<td>5.6</td>
<td>17.9</td>
<td>27.9</td>
</tr>
<tr>
<td>C &amp; B 3 Spline</td>
<td>11</td>
<td>1.4</td>
<td>4.8</td>
<td>3.4</td>
<td>7.3</td>
<td>15.5</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>1.6</td>
<td>2.2</td>
<td>3.0</td>
<td>11.4</td>
<td>10.3</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>1.6</td>
<td>2.2</td>
<td>6.0</td>
<td>5.1</td>
<td>8.9</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>1.3</td>
<td>2.1</td>
<td>3.0</td>
<td>17.9</td>
<td>15.5</td>
</tr>
<tr>
<td>Eq. 22 BARR</td>
<td>11</td>
<td>0.9</td>
<td>1.9</td>
<td>5.9</td>
<td>8.0</td>
<td>8.9</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>0.7</td>
<td>2.7</td>
<td>2.7</td>
<td>5.8</td>
<td>9.8</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>0.6</td>
<td>1.6</td>
<td>3.2</td>
<td>8.3</td>
<td>25.3</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>0.7</td>
<td>2.3</td>
<td>3.5</td>
<td>12.3</td>
<td>19.1</td>
</tr>
<tr>
<td>C &amp; B 3 Spline</td>
<td>11</td>
<td>17.8</td>
<td>18.1</td>
<td>18.6</td>
<td>15.1</td>
<td>20.4</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>2.8</td>
<td>2.8</td>
<td>2.3</td>
<td>4.8</td>
<td>11.8</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>1.0</td>
<td>1.2</td>
<td>2.1</td>
<td>8.5</td>
<td>19.4</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>0.6</td>
<td>2.1</td>
<td>4.7</td>
<td>5.6</td>
<td>13.7</td>
</tr>
<tr>
<td>Eq. 20 BARR</td>
<td>11</td>
<td>2.8</td>
<td>2.8</td>
<td>2.7</td>
<td>6.5</td>
<td>12.9</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>2.2</td>
<td>2.5</td>
<td>3.0</td>
<td>8.1</td>
<td>7.9</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>2.1</td>
<td>2.2</td>
<td>2.6</td>
<td>3.7</td>
<td>6.6</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>2.0</td>
<td>2.4</td>
<td>1.9</td>
<td>4.7</td>
<td>7.6</td>
</tr>
</tbody>
</table>

Table II. Noise in the computed inversion for levels of noise in the input data of up to 10%. Each value is the mean of 2 replicates.
Table III. Percent noise in the computed inversion for three methods with input noise of up to 0.5%. All data are for the off-axis distribution of Eq. 21.

Each value is the mean of 5 replicates.
<table>
<thead>
<tr>
<th>Method</th>
<th>Number of Points</th>
<th>0</th>
<th>0.1</th>
<th>0.25</th>
<th>0.5</th>
<th>1</th>
<th>2</th>
<th>5</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SPLINE</td>
<td>11</td>
<td>0.66</td>
<td>0.89</td>
<td>1.52</td>
<td>2.59</td>
<td>6.4</td>
<td>5.1</td>
<td>8.8</td>
<td>20.0</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>0.10</td>
<td>0.49</td>
<td>1.10</td>
<td>1.86</td>
<td>2.9</td>
<td>4.1</td>
<td>19.9</td>
<td>22.4</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>0.14</td>
<td>0.79</td>
<td>1.17</td>
<td>1.92</td>
<td>3.9</td>
<td>6.0</td>
<td>13.4</td>
<td>21.0</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>0.13</td>
<td>0.55</td>
<td>1.43</td>
<td>1.50</td>
<td>4.3</td>
<td>5.6</td>
<td>17.9</td>
<td>27.9</td>
</tr>
<tr>
<td></td>
<td>51</td>
<td>0.14</td>
<td>0.58</td>
<td>1.75</td>
<td>2.87</td>
<td>5.4</td>
<td>5.3</td>
<td>17.2</td>
<td>24.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>25.57</td>
<td>25.60</td>
<td>25.61</td>
<td>25.64</td>
<td>26.8</td>
<td>24.9</td>
<td>21.8</td>
<td>20.4</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>5.53</td>
<td>5.46</td>
<td>5.56</td>
<td>5.66</td>
<td>6.0</td>
<td>6.8</td>
<td>9.6</td>
<td>14.2</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>2.40</td>
<td>2.33</td>
<td>2.53</td>
<td>2.77</td>
<td>2.6</td>
<td>3.7</td>
<td>10.5</td>
<td>22.5</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>1.37</td>
<td>1.36</td>
<td>1.54</td>
<td>2.14</td>
<td>4.2</td>
<td>4.3</td>
<td>17.4</td>
<td>20.4</td>
</tr>
<tr>
<td></td>
<td>51</td>
<td>0.88</td>
<td>0.93</td>
<td>1.46</td>
<td>1.94</td>
<td>5.3</td>
<td>4.1</td>
<td>18.5</td>
<td>21.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>1.40</td>
<td>1.42</td>
<td>1.57</td>
<td>2.09</td>
<td>4.8</td>
<td>3.4</td>
<td>7.3</td>
<td>15.5</td>
</tr>
<tr>
<td></td>
<td>21</td>
<td>1.56</td>
<td>1.45</td>
<td>1.62</td>
<td>1.78</td>
<td>2.2</td>
<td>3.0</td>
<td>11.4</td>
<td>10.3</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>1.58</td>
<td>1.37</td>
<td>1.46</td>
<td>1.57</td>
<td>2.2</td>
<td>6.0</td>
<td>5.1</td>
<td>8.9</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>1.25</td>
<td>1.25</td>
<td>1.20</td>
<td>1.35</td>
<td>2.1</td>
<td>3.0</td>
<td>17.9</td>
<td>15.5</td>
</tr>
<tr>
<td></td>
<td>51</td>
<td>0.90</td>
<td>0.89</td>
<td>0.94</td>
<td>1.05</td>
<td>2.2</td>
<td>2.3</td>
<td>5.5</td>
<td>12.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>1.46</td>
<td>1.70</td>
<td>1.95</td>
<td>2.76</td>
<td>5.1</td>
<td>4.9</td>
<td>18.3</td>
<td>36.8</td>
</tr>
<tr>
<td></td>
<td>41</td>
<td>2.82</td>
<td>2.88</td>
<td>3.04</td>
<td>2.87</td>
<td>3.4</td>
<td>4.3</td>
<td>13.8</td>
<td>22.2</td>
</tr>
</tbody>
</table>

Table IV. Summary of data collected for the distribution given by Eq. 21.
Figure 1. Top view of the experiment, showing the relationship of $x$, $r$, and $R$. 
Figure 2. Comparison of some computed inversions with the true inversion of the Equation 21 distribution. Inversions computed from 11 point data sets without added noise. Solid line = true inversion; broken line = computed inversion.

2a. Inversion computed by Spline.
$l(r)$

RADIUS

2c. Inversion computed by C & B 3.
Figure 3. Comparison of some computed inversions with the true inversion of the Equation 21 distribution. Inversions computed from 51 point data sets having 5% noise added. Solid line = true inversion; broken line = computed inversion.

3a. Inversion computed by SPLINE.
Figure 4. Noise level in the computed inversion as a function of the noise level in the input data for 11 point data sets from Equation 21.
Figure 5. Noise in the computed inversion as a function of the noise level in the input data for 21 point data sets from Equation 21.
Figure 6. Noise in the computed inversion as a function of the noise level in the input data for 31 point data sets from Equation 21.
Figure 7. Noise in the computed inversion as a function of the noise level in the input data for 41 point data sets from Equation 21.
Figure 8. Noise in the computed inversion as a function of the noise level in the input data for 51 point data sets from Equation 21.
Appendix - Computation of $S_{kn}$

The table of coefficients, $S_{kn}$, used in the Barr method may be computed for a system having $N + 1$ points by the following algorithm (22). The table is general, and may be used for any smaller data set. Copies of the table for $N=51$ are available from the authors.

For $k: = 0$, step 1 until $N$

do begin

$k_0 = 4430k^6 - 704k^4 + 3532k^2 + 37.6$

$C_0 = (-448k^5 - 1088k^4 + 96k^3 + 819.2k^2 + 426.4k - 2.4)/K_k$

$C_1 = (-224k^5 + 544k^4 - 1920k^3 - 212.8k^2 - 158.8k + 38.4)/K_k$

$C_2 = (1088k^4 - 1212.8k^2 - 72)/K_k$

$C_3 = (224k^5 + 544k^4 + 1920k^3 - 212.8k^2 + 158.8k + 38.4)/K_k$

$C_4 = (448k^5 - 1088k^4 - 96k^3 + 819.2k^2 - 426.4k - 2.4)/K_k$

end

For $n: = 0$, step 1 until $N$

do begin

IF $k < 2$ or $n - k \geq 2$

$S_{kn} = \sum_{i=0}^{4} C_i n^i$

ELSE IF $n - k \geq -2$

$S_{kn} = \sum_{i=0}^{n-k+2} C_i k^{n-k+2} + 1, n$

end

end
## TECHNICAL REPORT DISTRIBUTION LIST, GEN

<table>
<thead>
<tr>
<th>Office of Naval Research</th>
<th>Attn: Code 472</th>
<th>Copies</th>
</tr>
</thead>
<tbody>
<tr>
<td>Attn: Code 472</td>
<td>800 North Quincy Street</td>
<td>Arlington, Virginia 22217</td>
</tr>
<tr>
<td>U.S. Army Research Office</td>
<td>Attn: CRD-AA-IP</td>
<td></td>
</tr>
<tr>
<td>P.O. Box 1211</td>
<td>Research Triangle Park, N.C. 27709</td>
<td>1</td>
</tr>
<tr>
<td>Naval Ocean Systems Center</td>
<td>Attn: Mr. Joe McCartney</td>
<td>San Diego, California 92152</td>
</tr>
<tr>
<td>Naval Weapons Center</td>
<td>Attn: Dr. A. B. Amster, Chemistry Division</td>
<td>China Lake, California 93555</td>
</tr>
<tr>
<td>Naval Civil Engineering Laboratory</td>
<td>Attn: Dr. R. W. Drisko</td>
<td>Port Hueneme, California 93401</td>
</tr>
<tr>
<td>Department of Physics &amp; Chemistry</td>
<td>Naval Postgraduate School</td>
<td>Monterey, California 93940</td>
</tr>
<tr>
<td>Dr. L. H. Peebles</td>
<td>Building 114, Section D</td>
<td>666 Summer Street</td>
</tr>
<tr>
<td>ONR Area Office</td>
<td>Attn: Scientific Dept.</td>
<td>715 Broadway</td>
</tr>
<tr>
<td>Onr Western Regional Office</td>
<td>1030 East Green Street</td>
<td>Pasadena, California 91106</td>
</tr>
<tr>
<td>ONR Eastern/Central Regional Office</td>
<td>Attn: Dr. A. L. Slafkosky</td>
<td>Scientific Advisor</td>
</tr>
<tr>
<td>Attn: Dr. A. L. Slafkosky</td>
<td>Building 114, Section D</td>
<td>666 Summer Street</td>
</tr>
<tr>
<td>Director, Naval Research Laboratory</td>
<td>Attn: Code 6100</td>
<td>Washington, D.C. 20390</td>
</tr>
<tr>
<td>The Assistant Secretary of the Navy (RE6S)</td>
<td>Department of the Navy</td>
<td>Room 4E706, Pentagon</td>
</tr>
<tr>
<td>Commander, Naval Air Systems Command</td>
<td>Attn: Code 310C (H. Rosenwasser)</td>
<td>Department of the Navy</td>
</tr>
<tr>
<td>Defense Technical Information Center</td>
<td>Building 5, Cameron Station</td>
<td>Alexandria, Virginia 22314</td>
</tr>
<tr>
<td>Dr. Fred Saalfeld</td>
<td>Chemistry Division, Code 6100</td>
<td>Naval Research Laboratory</td>
</tr>
<tr>
<td>Office of Naval Research</td>
<td>Attn: Dr. Richard S. Miller</td>
<td>800 N. Quincy Street</td>
</tr>
<tr>
<td>Naval Ship Research and Development Center</td>
<td>Attn: Dr. G. Bosmajian, Applied Chemistry Division</td>
<td>Annapolis, Maryland 21401</td>
</tr>
<tr>
<td>Naval Ocean Systems Center</td>
<td>Attn: Dr. S. Yamamoto, Marine Sciences Division</td>
<td>San Diego, California 91232</td>
</tr>
<tr>
<td>Mr. John Boyle</td>
<td>Materials Branch</td>
<td>Naval Ship Engineering Center</td>
</tr>
</tbody>
</table>
| Dr. M. B. Denton  
Department of Chemistry  
University of Arizona  
Tucson, Arizona 85721 | 1 | Dr. John Duffin  
United States Naval Postgraduate School  
Monterey, California 93940 | 1 |
| Dr. R. A. Osteryoung  
Department of Chemistry  
State University of New York at Buffalo  
Buffalo, New York 14214 | 1 | Dr. G. M. Hieftje  
Department of Chemistry  
Indiana University  
Bloomington, Indiana 47401 | 1 |
| Dr. B. R. Kowalski  
Department of Chemistry  
University of Washington  
Seattle, Washington 98105 | 1 | Dr. Victor L. Rehn  
Naval Weapons Center  
Code 3813  
China Lake, California 93555 | 1 |
| Dr. S. P. Ferone  
Department of Chemistry  
Purdue University  
Lafayette, Indiana 47907 | 1 | Dr. Christie G. Enke  
Michigan State University  
Department of Chemistry  
East Lansing, Michigan 48824 | 1 |
| Dr. D. L. Venezky  
Naval Research Laboratory  
Code 6130  
Washington, D.C. 20375 | 1 | Dr. Kent Eisenraut, MBT  
Air Force Materials Laboratory  
Wright-Patterson AFB, Ohio 45433 | 1 |
| Dr. H. Freiser  
Department of Chemistry  
University of Arizona  
Tucson, Arizona 85721 | 1 | Walter G. Cox, Code 3632  
Naval Underwater Systems Center  
Building 148  
Newport, Rhode Island 02840 | 1 |
| Dr. Fred Saalfeld  
Naval Research Laboratory  
Code 6110  
Washington, D.C. 20375 | 1 | Professor Isiah M. Warner  
Texas A&M University  
Department of Chemistry  
College Station, Texas 77840 | 1 |
| Dr. R. Chernoff  
Department of Mathematics  
Massachusetts Institute of Technology  
Cambridge, Massachusetts 02139 | 1 | Professor George H. Morrison  
Cornell University  
Department of Chemistry  
Ithaca, New York 14853 | 1 |
| Dr. K. Wilson  
Department of Chemistry  
University of California, San Diego  
La Jolla, California | 1 | Dr. Rudolph J. Marcus  
Office of Naval Research  
Scientific Liaison Group  
American Embassy  
APO San Francisco 96503 | 1 |
| Dr. A. Zipino  
Naval Undersea Center  
San Diego, California 92132 | 1 | Mr. James Kelley  
DTNSRDC Code 2803  
Annapolis, Maryland 21402 | 1 |