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# INVERSION OF ABEL'S INTEGRAL EQUATION BY MEANS OF ORTHOGONAL POLYNOMIALS\*

GERALD N. MINERBO† AND MAURICE E. LEVY‡

**1. Introduction.** The inversion of the Abel integral equation is a widely used technique in the study of extended radiation sources by means of which external measurements of the radiance (watts per  $\text{cm}^2$  per sr) produced by the source are used to deduce the radial distribution of the emission coefficient (watts per  $\text{cm}^3$  per sr) and hence the radial distribution of such parameters as temperature and density of the emitting matter. In the simplest case the source is optically thin and has cylindrical or spherical symmetry. The measurement of the radiance emitted by the extended radiation source along the edge of a circular slab in a cross section taken perpendicular to the axis of symmetry is denoted by  $Y(y)$ . A simple geometric argument can show, with the help of Fig. 1, that the radiance  $Y(y)$  is related to the emission coefficient  $R(r)$  in the following manner:

$$(1.1) \quad Y(y) = \int_{-(a^2 - y^2)^{1/2}}^{(a^2 - y^2)^{1/2}} R([x^2 + y^2]^{1/2}) dx$$

The function  $R(r)$  is assumed to vanish beyond a finite radius  $a$ . A change of variable from  $x$  to  $r$  gives the basic integral equation

$$(1.2) \quad Y(y) = 2 \int_y^a \frac{R(r)r}{(r^2 - y^2)^{1/2}} dr.$$

This is a form of Abel's integral equation. Although an exact inverse is known,

$$(1.3) \quad R(r) = -\frac{1}{\pi} \int_r^a \frac{Y'(y)}{(y^2 - r^2)^{1/2}} dy,$$

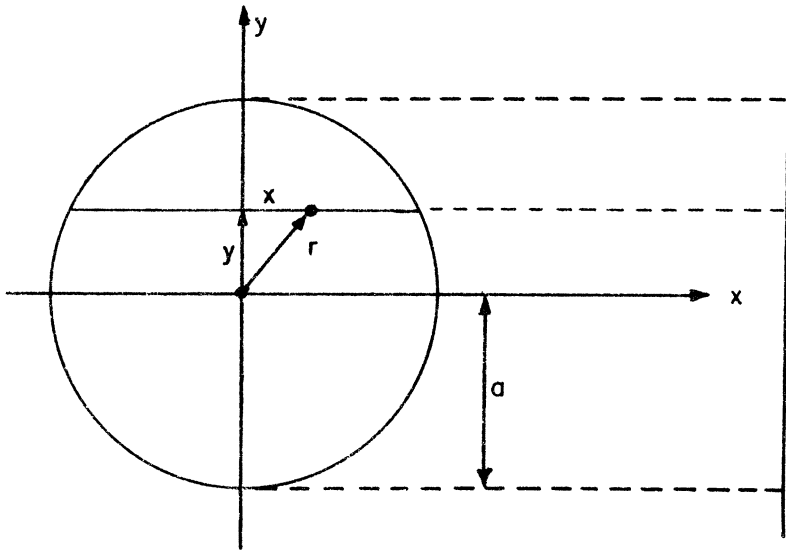
in practice the inversion procedure necessary to obtain  $R(r)$  presents many problems, particularly in the presence of experimental fluctuations.

A variety of numerical methods for performing the inversion are now available [1]–[11]. The widely used methods of Nestor–Olsen [1] and Bockasten [3] give accurate results when applied to smooth theoretical curves, but it has been found in this study that a small error in the input data can be amplified ten times or more after processing by the inversion procedure (see §4). The integral transform (1.3) is equivalent to half order differentiation [11] and therefore some noise amplification is unavoidable. It is now recognized [10], [11] that error amplification is the chief difficulty in performing reliable inversions of experimental data which usually contain short range fluctuations that are not physically meaningful but are difficult to avoid. In a number of recent papers [9]–[11] error amplification has been studied heuristically by introducing rounding errors in the input data. With some methods [5], [11] theoretical estimates of various sources of error are available. However, there has been no detailed study of noise amplification and stability.

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### Projected Image

FIG. 1. Cross section of an extended radiation source circularly symmetric with respect to the  $z$ -axis which is normal to the paper

The methods of Nestor and Olsen [1], Frie [7], and Bockasten [3] are essentially methods for the numerical integration of (1.3) which use interpolation formulas of low order (1, 2, and 3 respectively). Edels et al. [5] have given a general error analysis applicable to low order interpolation methods which provides estimates of the absolute accuracy of the method and bounds for the effect of observational errors in the data. Gaussian integration [6] provides an elegant way of avoiding the difficulties produced by the denominator in the integrand of (1.3) but it requires the value of  $Y$  at oddly spaced abscissas which moreover depend on the value of  $r$  at which  $R$  is to be computed. An obvious way of making the inversion less sensitive to experimental fluctuations is to approximate the data by smooth functions. Freeman and Katz [2] were the first to suggest a least squares fit of all the data for  $Y$  by a polynomial of fixed degree (degree 6) whose inverse is known exactly. In the method devised by Cremers and Birkebak [10] least squares fit of low degree (3 or 4) is applied piecewise to subsets of the data followed by numerical integration. The same idea is found in the paper of Barr [4]. Cremers and Birkebak performed a comparative study of the effect of rounding errors and

showed that their method is less sensitive to this type of error than previous methods [1], [7]. They suggest that their sliding fit should be superior to the fitting of all data points by a single polynomial, but actual tests showed that complete smoothing affords greater stability. Also methods which use presmoothing followed by numerical integration have the practical drawback that it is impossible to distinguish the errors introduced by each of the two operations. The method of Freeman and Katz does not have this drawback.

Methods which do not depend directly on (1.3) have been given by Herlitz [8], Maldonado et al. [9], Gorenflo and Kovetz [10]. The idea common to these papers is to use transform pairs

$$(1.4) \quad \eta_m(y) = 2 \int_y^a \frac{\rho_m(r)r}{(r^2 - y^2)^{1/2}} dr,$$

where the  $\rho_m$  form a complete set of functions and the  $\eta_m$  are orthogonal,

$$(1.5) \quad (\eta_l, \eta_m) = N_m \delta_{lm},$$

with respect to some scalar product

$$(1.6) \quad (\psi, \varphi) = \int_0^a \psi(y)\varphi(y) d\alpha(y).$$

Then if  $R$  is assumed to have the expansion

$$(1.7) \quad R(r) = \sum_m a_m \rho_m(r),$$

the coefficients  $a_m$  can be determined by evaluating the scalar products

$$(1.8) \quad a_m = \frac{1}{N_m}(\eta_m, Y).$$

Orthogonal functions provide an efficient way of performing a least squares fit, and have other advantages discussed in §2 and §3. With these methods the inversion is exact but numerical integration is still required to evaluate the scalar products in (1.8) even though these integrals are better conditioned than (1.3). Also the special functions involved, Hermite polynomials in [9] and Gegenbauer polynomials in [11] are complicated, and considerable computer time is required to generate them.

The present method combines the simplicity of the discrete methods and the advantages of orthogonal expansions. A least squares polynomial of degree  $K$  is fitted to all the data points for  $Y$  by using polynomials which are orthogonal over a discrete range [12]–[15]. This is an efficient procedure for performing polynomial fits on a high speed digital computer [13], [15], particularly if different degrees  $K$  are to be tried. The process is completely discrete since the integrals in (1.8) are replaced by finite sums. The inversion of the orthogonal polynomials is carried out exactly. Thus the fitting process itself is the only appreciable source of error since the other operations are purely algebraic and performed with great accuracy by the computer. Statistical analysis can be applied to the residuals to determine the best value of  $K$  and the significance of fit, as described in §3. In the case of purely random noise, error amplification factors can be calculated. Thus

for each calculated value of  $R$  the program will predict the associated probable error on the assumption that random noise is dominant.

**2. Inversion method.** We suppose that  $Y$  is specified by data  $Y_n$  at abscissas  $y_n$ ,  $n = 0, 1, \dots, N$  with  $y_0 = 0$  and  $y_N = a$ . The abscissas do not have to be equally spaced. The data will be fitted by the polynomial  $Y_K(y)$  that minimizes the expression

$$(2.1) \quad E_1 = \sum_{n=0}^N |Y_K(y_n) - Y_n|^2.$$

$Y_K$  is chosen to be a polynomial of degree  $K$  in  $y^2$  that vanishes at  $y = a$ . This choice deserves comment because experimental  $Y$  curves usually have some asymmetry about the center and seldom approach zero precisely at the tails. Asymmetry in  $Y$  indicates departure from cylindrical symmetry in  $R$  in which case (1.2) is not strictly applicable. The recommended procedure with the present method is to take the average of the two sides of an asymmetric  $Y$  curve before inversion. If  $Y(a) \neq 0$  the solution of (1.2) would be

$$(2.2) \quad R(r) = \frac{1}{\pi} \frac{Y(a)}{(a^2 - r^2)^{1/2}} - \frac{1}{\pi} \int_r^a \frac{Y'(y)}{(y^2 - r^2)^{1/2}} dy$$

instead of (1.3). Thus an error in the determination of  $a$  is likely to be magnified regardless of the inversion method used. One should ensure that the  $Y$  data approach zero smoothly by manual fitting of the  $y$ -axis to the tail, and by subtraction of any background that may be present.<sup>1</sup> It is felt that since these corrections require judgement, they are best left to the experimenter and should not be part of the numerical inversion program.

The polynomial  $Y_K$  will be expressed in powers of  $v = 1 - (y/a)^2$  as in Freeman and Katz [2]. If powers of  $y^2$  were used the inversion would require considerable reshuffling of the coefficients of the polynomial [11], with consequent loss of numerical accuracy. The change of variables

$$(2.3) \quad \begin{aligned} u &= 1 - \frac{r^2}{a^2}, & v &= 1 - \frac{y^2}{a^2}, \\ R(r) &= \frac{1}{a} U\left(1 - \frac{r^2}{a^2}\right), & Y(y) &= V\left(1 - \frac{y^2}{a^2}\right), \end{aligned}$$

in (1.2), (1.3) yields

$$(2.4) \quad V(v) = \int_0^v U(u)(v - u)^{-1/2} du,$$

and

$$(2.5) \quad U(u) = \frac{1}{\pi} \int_0^u V'(v)(u - v)^{-1/2} dv.$$

<sup>1</sup> Part of the discussion in §3 depends on the assumption that the errors in the data are normally distributed with equal variance. The corrections at the tail envisaged here involve a shift of origin and a change of scale and thus should not affect the probability distribution of the errors.

Powers of  $v$  are transformed into powers of  $u$  (see [2]). If

$$V(v) = v^j,$$

then

$$U(u) = \lambda_j u^{j-1/2},$$

where

$$(2.6) \quad \lambda_j = \frac{j! \Gamma(\frac{1}{2})}{\pi \Gamma(j + \frac{1}{2})} = \frac{j(j-1) \cdots 1}{\pi(j - \frac{1}{2})(j - \frac{3}{2}) \cdots \frac{1}{2}}, \quad j = 1, 2, \dots,$$

$$\lambda_0 = 0.$$

An efficient way of determining the least-squares polynomial  $V_K = Y_K$  on a digital computer [12], [13] is to generate polynomials  $p_m(v)$  of degree  $m$  in  $v$  which are orthogonal over the discrete points  $v_n = 1 - (y_n/a)^2$ ,

$$(2.7) \quad [p_l, p_m] = N_m \delta_{lm},$$

where

$$(2.8) \quad [\psi, \varphi] = \sum_{n=0}^N \psi(v_n) \varphi(v_n).$$

The polynomials  $p_m$  correspond to the orthogonal set  $\eta_m$  in (1.5) but now the weight function  $\alpha$  is a step function and (2.8) serves as the scalar product. They have the usual extremal property of orthogonal functions [12], namely if we take

$$(2.9) \quad a_m = \frac{1}{N_m} [p_m, Y]$$

as in (1.8), then

$$(2.10) \quad V_K(v) = \sum_{m=0}^K a_m p_m(v)$$

is the polynomial of degree  $K$  that minimizes  $E_1$  in (2.1). The minimum value of  $E_1$  is

$$(2.11) \quad E_1 = [Y - V_K, Y - V_K] = [Y, Y] - \sum_{m=0}^K a_m^2 N_m.$$

The polynomials  $p_m(v)$  are generated from the given values of  $y_n$  by using the recurrence relations

$$p_{m+1}(v) = (v - \alpha_m) p_m(v) - \beta_m p_{m-1}(v),$$

$$p_0 = 1, \quad p_{-1} = 0,$$

with

$$(2.12) \quad \alpha_m = \frac{1}{N_m} [p_m, v p_m],$$

$$\beta_m = \frac{N_m}{N_{m-1}}.$$

These relations can be derived [12], [14, Chap. 8] from the orthogonality conditions (2.7). The polynomials are standardized so that the leading coefficient in  $p_m(v)$  is always unity. The computer program used was that of Rank [15], similar to that described by Forsythe [13]. The coefficients of  $p_m(v)$

$$(2.13) \quad p_m(v) = \sum_{j=0}^m c_j^m v^j$$

are obtained recursively from the following relations:

$$(2.14) \quad \begin{aligned} c_j^{m+1} &= c_{j-1}^m - \alpha_m c_j^m - \beta_m c_j^{m-1}, \\ c_0^0 &= 1, \quad c_j^m = 0 \quad \text{if } j > m \quad \text{or } m < 0 \quad \text{or } j < 0. \end{aligned}$$

Once the  $c_j^m$  have been computed, the inverse of  $p_m$  can be obtained with the aid of (2.6).

$$(2.15) \quad \begin{aligned} q_m(u) &= \frac{1}{\pi} \int_0^u p'_m(v)(u-v)^{-1/2} dv \\ &= \sum_{j=1}^m \lambda_j c_j^m u^{j-1/2}. \end{aligned}$$

If  $V$  is approximated by  $V_K$ , (2.10), then the corresponding expression for  $U$  is

$$(2.16) \quad U_K(u) = \sum_{m=0}^K a_m q_m(u).$$

Therefore for a fit of degree  $K$  the inversion is represented by a matrix  $T_{in}^K$

$$(2.17) \quad R_K(r_i) = \frac{1}{a} \sum_{n=0}^N T_{in}^K Y_n,$$

where

$$(2.18) \quad T_{in}^K = \sum_{m=0}^K q_m(u_i) \frac{1}{N_m} p_m(v_n).$$

One of the advantages of the orthogonal decomposition is that the quantities  $a_m, p_m, q_m$  do not depend on  $K$ . Thus different values of  $K$  can be tried by merely changing the upper limit of the sum in (2.16), (2.18).

Fitting  $Y$  by  $V_K$  is the only appreciable source of error in practice because the quantities  $T_{in}^K$  are calculated very accurately by the computer. As  $K$  increases the error  $E_1$  in (2.1) will decrease and would vanish (except for computer rounding errors) when  $K = N$  since  $V_N$  is the interpolating polynomial that passes through all the data points. In tests on analytic functions we chose the value of  $K$  that minimizes the standard deviation  $\sigma_2$

$$(2.19) \quad \sigma_2 = \left( \frac{E_2}{N} \right)^{1/2},$$

where

$$E_2 = \sum_{i=0}^N |R(r_i) - R_K(r_i)|^2$$

For experimental data, on the assumption of random noise, the best value of  $K$  can be determined by statistical tests on the residuals in (2.11) as described in the next section.

**3. Amplification of random noise.** One of the advantages of expansions in orthogonal functions is that, in the presence of random noise, the coefficients  $a_m$  in (2.9) act as independent stochastic variables. Thus a simple statistical test can be applied to each new  $a_m$  to determine whether it significantly increases the accuracy. The basic statements (i)–(iv) are proved in Guest [14] or Birge and Weinberg [12]. In (v)–(vii) the same type of analysis is applied to the inverted function  $R$ . It is shown that noise amplification depends on factors  $A, A_i$  which are easily computed from the coefficients  $T_{in}^K$  of (2.18). For each computed value  $R_K(r_i)$  one can predict a probable error, (3.17), on the assumption that random noise is dominant.

The observations  $Y_n$  are assumed to be independent stochastic variables distributed about true values  $\bar{Y}_n$  with equal variance  $\sigma^2$ . Statement (iv) requires the further assumption that the  $Y_n$  are normally distributed.

(i) The coefficients  $a_m$  of (2.9) are independent stochastic variables, i.e.,

$$(3.1) \quad \text{cov}(a_l, a_m) = 0, \quad l \neq m,$$

and are distributed about true values

$$(3.2) \quad \bar{a}_m = \frac{1}{N_m} [p_m, \bar{Y}],$$

with variance

$$(3.3) \quad \text{var } a_m = \frac{\sigma^2}{N_m}.$$

(ii) The variance of the fitted value is

$$(3.4) \quad \text{var } V_K(v_n) = \sigma^2 \sum_{m=0}^K \frac{p_m^2(v_n)}{N_m}.$$

(iii) The expectation value of  $E_1^K$  in (2.11) is

$$(3.5) \quad \langle E_1^K \rangle = (N - K)\sigma^2.$$

With experimental data  $\sigma$  is usually unknown. By means of this statement it can be estimated from the residuals. The quantity

$$(3.6) \quad \mu = \left[ \frac{E_1^K}{N - K} \right]^{1/2}$$

will be an unbiased estimate of  $\sigma$ .

If the true curve is a polynomial of degree  $L$  the errors  $E_1^K$  and  $E_2^K$  will decrease rapidly as  $K$  increases up to  $K = L$  after which  $E_1^K$  will decrease slowly but  $E_2^K$  will



start increasing again due to noise amplification. The following statement provides a test of significance for each new coefficient  $a_m$ .

(iv) If the variables  $Y_n$  follow a normal probability distribution, the ratio

$$(3.7) \quad t = \frac{(a_m - \bar{a}_m)\sqrt{N_m}}{\mu}$$

will follow a  $t$ -distribution with  $N - K$  degrees of freedom. To determine whether a coefficient  $a_{K+1}$  is significant, one makes the null hypothesis that  $\bar{a}_{K+1} = 0$  and applies the  $t$ -test to

$$(3.8) \quad t = \frac{a_{K+1}\sqrt{N_{K+1}}}{\mu}.$$

For example with  $N = 20$  points and  $K + 1 = 9$  one can state with 95% confidence that  $a_9 \neq 0$  if  $t$  falls outside the interval

$$-2.20 \leq t \leq 2.20.$$

If  $t$  falls inside this interval no strict inference can be made but  $a_9$  is rejected on the grounds that it will not significantly improve the accuracy of the fit. Numerical tests of the suitability of this criterion are described in § 4.

Considering now the errors in the inverted function  $R$ , if we define

$$(3.9) \quad \bar{R}_K(r_i) = \frac{1}{a} \sum_{n=0}^N T_{in}^K \bar{Y}_n,$$

we can obtain a statement analogous to (ii) and (iii).

(v) The variance of  $R_K(r_i)$  is

$$(3.10) \quad \begin{aligned} \text{var } R_K(r_i) &= \langle \{R_K(r_i) - \bar{R}_K(r_i)\}^2 \rangle \\ &= \frac{1}{a^2} \sum_{n=0}^N \sum_{r=0}^N T_{in} T_{ir} \langle (Y_n - \bar{Y}_n)(Y_r - \bar{Y}_r) \rangle \\ &= \frac{\sigma^2}{a^2} (A_i^K)^2, \end{aligned}$$

where

$$(3.11) \quad A_i^K = \left[ \sum_{n=0}^N (T_{in}^N)^2 \right]^{1/2} = \left[ \sum_{m=0}^K \frac{q_m^2(u_i)}{N_m} \right]^{1/2}.$$

The norm of a function will be denoted by

$$(3.12) \quad \|R\| = [R, R]^{1/2}.$$

The expectation value of  $\|R_K - \bar{R}_K\|^2$  can be obtained similarly.

$$(3.13) \quad \langle \|R_K - \bar{R}_K\|^2 \rangle = N \frac{\sigma^2}{a^2} (A^K)^2,$$

where

$$(3.14) \quad A^K = \left[ \frac{1}{N} \sum_{i=0}^N \sum_{n=0}^N (T_{in}^K)^2 \right]^{1/2} = \left[ \frac{1}{N} \sum_{m=0}^K \frac{\|q_m\|^2}{N_m} \right]^{1/2}.$$

(vi) The errors in the function  $R$  separate into absolute errors and errors due to noise.

$$(3.15) \quad \begin{aligned} \langle \{R(r_i) - R_K(r_i)\}^2 \rangle &= \langle \{R(r_i) - \bar{R}_K(r_i)\}^2 \rangle + \langle \{\bar{R}_K(r_i) - R_K(r_i)\}^2 \rangle \\ &= \{R(r_i) - \bar{R}_K(r_i)\}^2 + \frac{\sigma^2}{a^2} (A_i^K)^2. \end{aligned}$$

Likewise the expectation value of  $E_2^K$  is

$$(3.16) \quad \langle E_2^K \rangle = \langle \|R - R_K\|^2 \rangle = \|R - \bar{R}_K\|^2 + N \frac{\sigma^2}{a^2} (A^K)^2.$$

The first terms in (3.15) and (3.16) depend on the absolute accuracy of the method which can be determined by tests on analytic functions as in § 4. For each computed value of  $R_K(r_i)$  an estimate of the standard deviation (or probable error) due to noise alone can be obtained from

$$(3.17) \quad \begin{aligned} \sigma^*(R_i) &= \frac{\mu}{a} A_i^K, \\ \text{P.E.}^*(R_i) &= .675 \frac{\mu}{a} A_i^K, \end{aligned}$$

using  $\mu$  from (3.6). Similarly the contribution of noise to  $\sigma_2$  can be estimated from

$$(3.18) \quad \sigma_2^* = \frac{\mu}{a} A^K.$$

The factors  $A^K$ ,  $A_i^K$  increase rapidly with increasing  $K$  (see Tables 3, 4, 5). For the types of functions and the noise levels usually encountered with experimental data, it is expected that the final accuracy will be limited by the growth of noise errors rather than by the absolute accuracy of the method.

In inversions of experimental data the error  $E_2$  cannot be computed of course but the progress of the calculation can be judged by computing the norms

$$(3.19) \quad \Delta_2^K = \frac{1}{\sqrt{N}} \|R_{K+1} - R_K\| = \frac{1}{\sqrt{N}} \frac{1}{a} |a_{K+1}| \|q_{K+1}\|.$$

(vii) The maximum gain in accuracy in  $\sigma_2$  obtained by including  $a_{K+1}$  is  $\Delta_2^K$ . This follows from the triangle inequality

$$(3.20) \quad \begin{aligned} \sigma_2^K - \sigma_2^{K+1} &= \frac{1}{\sqrt{N}} \|R - R_K\| - \frac{1}{\sqrt{N}} \|R - R_{K+1}\| \\ &\leq \frac{1}{\sqrt{N}} \|R_{K+1} - R_K\| = \Delta_2^K. \end{aligned}$$

At the same time the contribution to  $\sigma_2$  due to noise will increase by a component

$$(3.21) \quad \frac{1}{\sqrt{N}} \frac{\mu}{a} \frac{\|q_{K+1}\|}{\sqrt{N_{K+1}}}.$$

A natural criterion would be to reject  $a_{K+1}$  when  $\Delta_2^K$  becomes comparable to (3.21).

However, the ratio of these quantities is

$$(3.22) \quad \frac{|a_{K+1}|\sqrt{N_{K+1}}}{\mu}.$$

Therefore if  $a_{K+1}$  was rejected on the basis of the  $t$ -test it is not likely to improve the accuracy in  $\sigma_2$ .

(viii) If one removes the assumption of random noise, the factors  $A, A_i$  still provide absolute bounds for error amplification. We have

$$(3.23) \quad |R(r_i) - R_K(r_i)| \leq |R(r_i) - \bar{R}_K(r_i)| + |R_K(r_i) - \bar{R}_K(r_i)|$$

from the triangle inequality, and

$$(3.24) \quad |R_K(r_i) - \bar{R}_K(r_i)| \leq \frac{1}{a} A_i^K \|Y - \bar{Y}\|$$

from the Schwarz inequality. Similarly

$$(3.25) \quad \sigma_2^K = \frac{1}{\sqrt{N}} \|R - R_K\| \leq \frac{1}{\sqrt{N}} \|R - \bar{R}_K\| + \frac{1}{a} A^K \|Y - \bar{Y}\|.$$

These bounds hold for any type of error in the data.

The above discussion has emphasized the effect of experimental errors. Regarding the absolute accuracy of the method, it does not seem possible to give an analytical treatment. In addition to the differences  $|\bar{Y}_n - \bar{Y}_K(y_n)|$  one would like to know how far the true curve  $\bar{Y}_K$  deviates at intermediate points and what effect this will have on the differences  $|R(r_i) - \bar{R}_K(r_i)|$ . In the mathematical literature various error bounds are available for expansions in infinite series of polynomials, but for the case of a small finite  $K$  it seems that very little can be said in general [12], [14].

The statement was made that in applications to experimental data the accuracy of the inversion will be limited by the noise errors rather than by the absolute accuracy of the method. In other words, with a suitable  $K$ ,  $\|R - R_K\|^2$  could be made much smaller than the lowest value of  $\langle E_2^K \rangle$  that can be reached in the presence of noise. For a given noise level specified by  $\sigma$ , this statement is obviously not true if we allow  $\bar{Y}$  to be an arbitrary function with a continuous derivative that passes through the true values  $\bar{Y}_n$ . What the statement expresses is the circumstance that the functions encountered in practice have a very simple shape with a slowly varying derivative and a small number of inflection points. It is difficult to formulate in a quantitative way conditions on the function that will ensure the truth of this statement. In §4 we present two examples with curve shapes and noise levels that are representative of those encountered in practice.

If our statement is true then the value of  $K$  that minimizes  $E_2^K$  will lie in a range where the absolute errors are still decreasing and the noise errors increasing steadily with  $K$ . Thus the question of how well the true curve  $\bar{Y}$  can be represented by a polynomial, i.e., how small  $\|R - \bar{R}_K\|$  can be made for any  $K$ , becomes

unimportant.<sup>2</sup> The important precaution is to stop increasing  $K$  as soon as the incremental gain in absolute accuracy is offset by the increase in the noise contribution to the error. If our statement is false, i.e., if the input function is too complicated to be represented by a polynomial or if the noise level is too low, this situation could be detected by the failure of the  $t$ -test to indicate a good fit. This was found to be the case in tests on analytic functions with very low noise levels (see § 4.2).

**4. Numerical results.** The numerical examples described in this section were designed to test first the absolute accuracy of the method of this paper, second the usefulness and applicability of the results of § 3 relating to random noise, third the stability against small localized perturbations introduced at different points along the input curve. The polynomial method was compared to the techniques of Nestor and Olsen [1], Bockasten [3], and Maldonado et al. [9].

**4.1. Absolute accuracy.** The accuracy tests were carried out with theoretical curves having known inverses. Two pairs were chosen, labelled A and B. Curve A corresponds to the following choice for  $Y$  and  $R$ :

$$(4.1) \quad Y(y) = \begin{cases} -\frac{2}{3}(\frac{1}{4} - y^2)^{1/2}(1 + 8y^2) + \frac{4}{3}(1 - y^2)^{1/2}(1 + 2y^2) \\ \quad - 4y^2 \log\{[1 + (1 - y^2)^{1/2}]/[\frac{1}{2} + (\frac{1}{4} - y^2)^{1/2}]\}, & 0 \leq y \leq \frac{1}{2}, \\ \frac{4}{3}(1 - y^2)^{1/2}(1 + 2y^2) - 4y^2 \log\{[1 + (1 - y^2)^{1/2}]/y\}, & \frac{1}{2} \leq y \leq 1. \end{cases}$$

$$R(r) = \begin{cases} 1 - 2r^2, & 0 \leq r \leq \frac{1}{2}, \\ 2(1 - r)^2, & \frac{1}{2} \leq r \leq 1. \end{cases}$$

Several authors have published inversion tests on this curve [1], [9], [10] and it is a convenient basis for comparison. Table 1 shows the difference between calculated and theoretical values of  $R(r)$  for  $N = 20$  equally spaced points. Judging from the standard deviation  $\sigma_2$  the methods of Bockasten, Maldonado et al. and the polynomial method are close in accuracy. However, the polynomial method is more accurate near the center of the distribution which is usually the important region in experimental inversions.

A distribution with a Gaussian tail was used for the second case shown in Table 2.

$$(4.2) \quad Y(y) = \frac{\sqrt{\pi}}{\beta} (1 - y^2)^{-1/2} \exp \left[ \beta^2 \left( 1 - \frac{1}{1 - y^2} \right) \right].$$

$$R(r) = (1 - r^2)^{-3/2} \exp \left[ \beta^2 \left( 1 - \frac{1}{1 - r^2} \right) \right].$$

Curve B stands for (4.2) with  $\beta = 1.1$ . In this case  $R(r)$  has an off axis peak at  $r \simeq .44$ . The order of increasing accuracy is now Nestor–Olsen, Maldonado, Bockasten, and polynomial. Because curve B has a fairly complicated shape a large value of  $K$ ,  $K = 11$ , was needed for best results, whereas for most test curves tried the optimum

<sup>2</sup> It may be helpful to apply another test of polynomial behavior to the  $Y$  data, for example divided differences. In the presence of noise, however, the higher order differences would be uncertain and this test would not necessarily be more conclusive.

TABLE 1  
Accuracy test of four inversion methods applied to curve A, (4.1)

Position ( $y$ or $r$ )	$Y(y)$ (Input)	$R(r)$ (Theor.)	Differences $R_{\text{calc.}} - R_{\text{theor.}}$			
			Nestor-Olsen	Bockasten	Maldonado et al.	Polynomial ( $K = 8$ )
.00	1.0000	1.0000	+.0006	+.0016	+.0016	+.0012
.05	.9931	.9950	+.0005	+.0020	+.0013	+.0009
.10	.9724	.9800	-.0027	-.0009	-.0016	+.0000
.15	.9384	.9550	-.0049	-.0034	-.0032	-.0007
.20	.8915	.9200	-.0007	+.0009	-.0013	-.0006
.25	.8327	.8750	-.0012	+.0015	-.0003	+.0001
.30	.7631	.8200	-.0033	+.0002	-.0000	+.0010
.35	.6842	.7550	-.0049	-.0007	-.0005	+.0008
.40	.5979	.6800	-.0050	+.0002	-.0008	-.0006
.45	.5069	.5950	-.0065	+.0002	-.0014	-.0020
.50	.4151	.5000	-.0093	-.0005	-.0010	+.0003
.55	.3292	.4050	-.0096	-.0012	+.0004	+.0022
.60	.2527	.3200	-.0067	+.0008	+.0003	-.0001
.65	.1861	.2450	-.0072	-.0002	+.0005	-.0015
.70	.1300	.1800	-.0056	+.0006	+.0002	-.0004
.75	.0845	.1250	-.0073	-.0017	-.0004	+.0011
.80	.0495	.0800	-.0041	+.0003	+.0001	+.0007
.85	.0247	.0450	-.0030	+.0008	+.0006	-.0011
.90	.0092	.0200	-.0036	-.0007	+.0004	-.0002
.95	.0017	.0050	-.0009	+.0008	+.0010	+.0023
1.00	.0000	.0000	.0000	.0000	.0000	.0000
Standard Deviation $\sigma_2$			.00517	.00123	.00112	.00110

value was in the range  $K = 7$  to  $9$ . For  $K = 8$  with curve  $B$  a standard deviation  $\sigma_2 = .00452$  was obtained, which still compares favorably with the other methods. Similar comparisons were made with a number of other test curves. The conclusion was that the polynomial method is at least as good and usually better than the other three in absolute accuracy. It is relatively more accurate at the center of the distribution than at the tail.

**4.2. Random noise amplification.** The amplification of random noise is summarized by the factors  $A_i$  of (3.11) and  $A$  of (3.14). These were computed from the inversion matrix for  $N = 20$  equally spaced points. Table 3 shows the results for three frequently used values of  $K$ . The same factors were computed from the inversion matrices of the Nestor-Olsen and Bockasten methods but are not available for the method of Maldonado et al. since it is not a discrete method. Comparison of the amplification factors  $A_i$  shows the superiority of the polynomial method not only at the center where the difference is striking, but also in the range  $i = 5$  to  $15$  where the response is flat and close to unity. The factors  $A_i$  increase again towards the tail with the polynomial method but remain at a tolerable level.

In order to study the applicability of the  $t$ -test, rounding errors were introduced in curves  $A$  and  $B$ . The correct application of the  $t$ -test requires the presence of normally distributed errors. Rounding errors were chosen because they are so easily generated and also to facilitate comparison with similar tests in other

TABLE 2  
*Accuracy test of four inversion methods applied to curve B using twenty unperturbed data points for Y(y) as input*

Position (y or r)	Y(y) (Input)	R(r) (Theor.)	Differences $R_{calc} - R_{theor}$			
			Nestor-Olsen	Bockasten	Maldonado et al.	Polynomial ( $K = 11$ )
.00	1.6113	1.0000	+.0001	+.0007	+.0051	-.0003
.05	1.6085	1.0007	+.0003	+.0002	+.0124	-.0002
.10	1.5998	1.0029	+.0005	+.0001	+.0058	+.0001
.15	1.5850	1.0063	+.0007	.0000	-.0025	+.0002
.20	1.5637	1.0109	+.0010	.0000	-.0059	+.0001
.25	1.5352	1.0163	+.0014	+.0001	-.0116	-.0001
.30	1.4986	1.0220	+.0019	-.0001	+.0069	-.0001
.35	1.4528	1.0275	+.0024	+.0001	+.0113	+.0001
.40	1.3962	1.0315	+.0030	+.0001	-.0008	+.0002
.45	1.3270	1.0327	+.0036	-.0001	-.0034	+.0001
.50	1.2430	1.0286	+.0043	-.0002	-.0059	-.0001
.55	1.1416	1.0157	+.0047	+.0001	-.0029	+.0001
.60	1.0198	.9889	+.0048	+.0003	+.0009	+.0002
.65	.8749	.9402	+.0037	+.0005	+.0034	+.0001
.70	.7055	.8585	+.0004	+.0010	+.0026	-.0000
.75	.5141	.7293	-.0074	+.0015	-.0050	+.0003
.80	.3125	.5387	-.0210	+.0007	-.0122	+.0003
.85	.1310	.2930	-.0396	-.0053	-.0064	+.0001
.90	.0213	.0694	-.0250	-.0022	+.0217	+.0014
.95	.0001	.0004	-.0003	+.0070	+.0054	+.0031
1.00	.0000	.0000	.0000	.0000	.0000	.0000
Standard deviation $\sigma_2$			.0118	.00281	.00822	.00078

papers [9], [10]. If data is rounded to  $n$  digits beyond the decimal point, the probability distribution for the errors is a constant function of width  $10^{-n}$  and standard deviation  $\sigma = 12^{-1/2} \times 10^{-n}$ . The input data for curves A and B were rounded to two decimal places which corresponds to  $\sigma \simeq .00289$ . The results for A and B are shown in Tables 4 and 5 respectively.  $\mu$  is an estimate for  $\sigma$  defined in (3.6). The standard deviation  $\sigma_1$  for the  $Y$  function decreases monotonically with  $K$  but  $\sigma_2$  for the  $R$  function has a minimum at an intermediate value of  $K$ . The last two columns give the value of  $\sigma_2$  obtained with accurate input data and the theoretical estimate  $A^K\sigma$  of the contribution to  $\sigma_2$  due to noise. The former decreases and the latter increases with increasing  $K$  in the region of interest. The table also shows the computed absolute value of  $t$ , (3.8), and the length of the interval corresponding to a 95 % confidence level (double tail test).

Fur curve B the  $t$ -test predicts that the contributions from values of  $K$  above 7 are not significant. It is seen that  $K = 7$  does give the smallest  $\sigma_2$ . In the case of curve A the  $t$ -test indicates that  $K = 5$  is optimal but better results are obtained with  $K = 6$  and 7. However this circumstance can be regarded as accidental since in this case the computed  $\sigma_2$  is smaller than the theoretical noise component  $A^K\sigma$ . The  $t$ -test will not always yield the smallest  $\sigma_2$  but it gives a sound compromise between absolute errors and noise errors. The constancy of  $\mu$ , computed from (3.6),

TABLE 3  
Error amplification factors for three inversion methods

Noise amplification factors $A_i$					
$i$	Nestor-Olsen	Bockasten	Polynomial		
			$K = 7$	$K = 8$	$K = 9$
0	15.4	19.2	2.89	3.48	4.10
1	8.72	9.39	2.64	3.09	3.52
2	6.71	6.77	1.99	2.13	2.20
3	5.66	5.56	1.26	1.27	1.40
4	4.98	4.83	.98	1.26	1.64
5	4.50	4.33	1.13	1.40	1.55
6	4.13	3.95	1.15	1.20	1.21
7	3.85	3.66	.96	1.02	1.27
8	3.61	3.43	.85	1.12	1.27
9	3.41	3.23	.94	1.10	1.10
10	3.25	3.07	.95	.95	1.19
11	3.10	2.92	.84	1.02	1.18
12	2.97	2.80	.86	1.06	1.07
13	2.86	2.69	.96	.96	1.21
14	2.76	2.59	.89	1.11	1.14
15	2.67	2.51	.91	1.10	1.36
16	2.58	2.43	1.09	1.14	1.29
17	2.51	2.35	1.03	1.33	1.60
18	2.43	2.32	1.55	1.70	1.70
19	2.04	1.41	1.18	1.79	3.25
$A =$	5.33	5.88	1.38	1.61	1.91

TABLE 4  
Standard deviations and  $t$ -test for curve A

$K$	$\sigma_1$	$\mu$	$ d $	95 % Point	$\sigma_2$	$\sigma_2$ (Absolute)	$A^k \sigma$
	$\times 10^{-3}$	$\times 10^{-3}$			$\times 10^{-3}$	$\times 10^{-3}$	$\times 10^{-3}$
3	5.00	5.42	19.4	2.11	13.7	14.3	1.81
4	4.40	4.92	2.14	2.12	10.3	10.6	2.27
5	3.12	3.60	3.86	2.13	3.53	3.11	2.81
6	2.89	3.46	1.52	2.15	3.17	3.24	3.38
7	2.88	3.57	.390	2.16	<u>2.61</u>	2.27	3.98
8	2.62	3.38	1.58	2.18	2.95	<u>1.10</u>	4.65
9	2.60	3.51	.333	2.20	2.97	1.21	5.53

for different values of  $K$  is fairly good. As an estimate of  $\sigma$ ,  $\mu$  tends to err on the high side, which means that the estimates (3.17) for the errors in  $R$  are generally conservative.

The  $t$ -test was applied to several different test curves with varying amounts of rounding error. As expected it works best when the noise standard deviation  $\sigma$  is large compared to the lowest  $\sigma_2$  that can be obtained in the absence of noise. However the  $t$ -test and the estimates in (3.6) were still reliable with  $\sigma$  as low as

TABLE 5  
Standard deviations and *t*-test for curve B

<i>K</i>	$\sigma_1$	$\mu$	$ t $	95 % Point	$\sigma_2$	$\sigma_2$ (Absolute)	$A^E\sigma$
	$\times 10^{-3}$	$\times 10^{-3}$			$\times 10^{-3}$	$\times 10^{-3}$	$\times 10^{-3}$
5	9.56	11.0	4.47	2.13	22.9	21.8	2.81
6	3.88	4.64	8.42	2.15	8.81	9.16	3.38
7	2.80	3.47	3.47	2.16	<u>5.27</u>	4.61	3.98
8	2.53	3.27	1.62	2.18	6.72	4.53	4.65
9	2.51	3.38	.451	2.20	5.54	2.94	5.53
10	2.10	2.97	2.06	2.23	11.3	1.06	7.08
11	1.82	2.71	1.73	2.26	8.83	<u>.778</u>	10.9

$2.9 \times 10^{-4}$ . Below this level *t* behaves erratically and does not consistently fall within a given confidence interval, i.e., the *t*-test continues to indicate that some of the  $a_K$  are significant for large values of *K* up to *K* = *N*. For low noise levels one has no automatic criterion for selecting *K* ; however, adequate accuracy can always be obtained by using the following degrees of fit : *K* = 4 for *N* = 10 data points, *K* = 8 for *N* = 20, and *K* = 11 for *N* = 30.

The procedure followed here may be criticized because the *t*-test is not strictly applicable to rounding errors. The use of normally distributed errors would be more desirable and in addition these are more likely to be encountered with experimental data. However, in these tests only one set of 20 error values was used for each curve, and the difference between these two distributions is hardly detectable for such a small set. A thorough check of the validity of the *t*-test could be obtained by using a reasonably large sample of normally distributed error sets and determining the reliability of the *t*-test over this sample. However, since the results were so favorable in the few cases tested, there seems to be little justification in undertaking such a program.

**4.3. Stability against localized perturbations.** In addition to amplification of random errors, it is useful to know the response to small, localized perturbations. This test is more stringent than tests on rounded data because the effect of rounding errors may be averaged out. By contrast the present test will indicate the worst effect that can be expected if systematic errors are present in different portions of the input curve.

The stability analysis applied to curve A is shown in Table 6. A perturbation of + 1 % is applied to one of the input data values  $Y(y_p)$  and the others left unchanged. The four inversion methods are applied to this perturbed data and the standard deviations  $\sigma_2$  computed in the usual way from (2.19). With the polynomial method the degree of fit was kept fixed at *K* = 8. When  $Y(y_p)$  is replaced by  $(1.01) \times Y(y_p)$  the point most strongly affected is usually  $R(r_p)$  where  $r_p = y_p = p/20$ . In Table 6 we report the percentage error in  $R(r_p)$  and its nearest neighbors  $R(r_{p-1})$  and  $R(r_{p+1})$ . Thus  $D_p$  is the percentage error

(4.3) 
$$D_p = \frac{R^{cal}(r_p) - R^{th}(r_p)}{R^{th}(r_p)} \times 100,$$

where  $R^{cal}$  and  $R^{th}$  denote calculated and theoretical values respectively. As *p*



TABLE 6  
Stability test of four different methods applied to curve A

Nestor—Olsen				Bockasten			Maldonado et al.			Polynomial		
Percent errors			Standard deviation	Percent errors			Standard deviation	Percent errors			Standard deviation	
$p$	$D_{p-1}$	$D_p$	$D_{p+1}$	$\sigma_2$	$D_{p-1}$	$D_p$	$D_{p+1}$	$\sigma_2$	$D_{p-1}$	$D_p$	$D_{p+1}$	$\sigma_2$
0	—	12.8	.047	.029	—	15.4	1.14	.035	—	5.09	2.90	.0131
1	-8.37	7.38	-.276	.025	-11.3	7.38	.564	.030	2.00	2.63	1.78	.0084
2	-4.41	5.37	-.512	.017	-5.55	5.16	.178	.017	-1.41	1.59	1.24	.0101
3	-3.59	4.21	-.075	.013	-4.04	3.97	.565	.012	-1.17	1.14	1.26	.0056
4	-3.22	4.04	-.143	.012	-3.46	3.81	.587	.011	-1.07	1.16	1.23	.0051
5	-2.38	3.51	-.404	.010	-2.49	3.44	.402	.0086	-.696	1.12	1.17	.0044
6	-2.14	2.88	-.648	.0086	-2.05	2.95	.254	.0069	-.480	.939	.993	.0035
7	-2.16	2.33	-.742	.0076	-1.90	2.55	.347	.0057	-.402	.914	.838	.0030
8	-2.19	1.97	-1.09	.0070	-1.80	2.45	.408	.0050	-.424	.750	.672	.0024
9	-2.11	1.40	-1.85	.0062	-1.48	2.33	.188	.0040	-.441	.555	.680	.0020
10	-2.29	.459	-2.37	.0056	-1.23	1.96	-.005	.0030	-.504	.540	.938	.0020
11	-2.93	-.214	-2.09	.0055	-1.28	1.62	.525	.0024	-.420	.790	.906	.0017
12	-3.35	-.079	-2.93	.0055	-1.34	2.01	.057	.0022	-.099	.719	.939	.0015
13	-2.97	-1.07	-3.12	.0053	-.716	1.59	.617	.0016	-1.125	.816	.833	.0016
14	-3.70	-1.41	-5.83	.0053	-.918	1.87	1.14	.0015	.041	.667	.320	.0012
15	-3.77	-4.30	-5.08	.0052	-.311	.096	.591	.0012	-.056	.160	.875	.0011
16	-6.37	-3.70	-6.75	.0052	-1.97	1.59	2.10	.0013	-.480	.625	2.00	.0012
17	-5.49	-5.56	-18.1	.0052	-.164	3.13	-3.37	.0013	.125	1.78	3.00	.0011
18	-7.00	-17.2	-18.4	.0052	1.56	-2.78	17.5	.0012	1.11	2.50	20.0	.0011

TABLE 7  
*Stability test of four different methods applied to Curve B*

$p$	Nestor-Olsen				Bockasten				Maldonado et al.				Polynomial			
	Percent errors			Standard deviation	Percent errors			Standard deviation	Percent errors			Standard deviation	Percent errors			Standard deviation
	$D_{p-1}$	$D_p$	$D_{p+1}$		$D_{p-1}$	$D_p$	$D_{p+1}$		$D_{p-1}$	$D_p$	$D_{p+1}$		$D_{p-1}$	$D_p$	$D_{p+1}$	
0	—	20.5	.025	.047	—	24.5	1.51	.055	—	8.46	5.67	.024	—	3.31	2.98	.012
1	-13.6	11.8	.046	.042	-18.64	11.55	1.04	.049	3.49	5.25	3.64	.018	2.67	2.43	1.77	.010
2	-7.26	9.13	.072	.029	-9.36	8.42	.835	.029	-1.29	3.40	2.21	.018	1.04	.893	.696	.0065
3	-5.42	7.65	1.03	.025	-6.52	6.95	.715	.022	-1.08	2.11	1.57	.010	-.131	.336	.693	.0065
4	-4.43	6.67	.141	.022	-5.16	5.92	.633	.018	-1.47	1.50	.790	.0093	-.061	.634	.981	.0087
5	-3.76	5.94	.185	.020	-4.37	5.24	.545	.016	-1.53	.702	2.41	.010	.260	.713	.856	.0083
6	-3.24	5.36	.234	.019	-3.76	4.63	.509	.014	-1.90	2.16	2.64	.012	.119	.498	.716	.0062
7	-2.80	4.88	.291	.018	-3.31	4.14	.461	.013	-.004	2.64	1.26	.011	.012	.545	.830	.0054
8	-2.42	4.47	.353	.017	-2.92	3.83	.398	.012	.480	1.24	.882	.0090	.223	.675	.762	.0061
9	-2.06	4.11	.415	.016	-2.58	3.33	.351	.010	-.634	.853	.526	.0084	.256	.485	.496	.0061
10	-1.73	3.77	.467	.015	-2.29	2.98	.341	.0090	-.793	.497	.715	.0088	.039	.295	.488	.0060
11	-1.41	3.45	.482	.014	-2.00	2.65	.329	.0079	-.962	.666	.994	.0088	-.024	.342	.618	.0060
12	-1.11	3.11	.395	.013	-1.70	2.35	.327	.0068	-.614	.924	1.14	.0094	-.026	.361	.660	.0052
13	-.849	2.68	.043	.013	-1.42	2.07	.359	.0058	-.219	1.12	1.02	.0097	-.046	.463	.749	.0045
14	-.690	1.98	-1.01	.012	-1.12	1.83	.436	.0047	.139	.927	-.025	.0086	.156	.554	.406	.0047
15	-.792	.603	-3.90	.012	-.792	1.63	.343	.0037	.125	-.162	-1.65	.0078	.152	.070	-.082	.0050
16	-1.59	-2.62	-1.35	.012	-.414	1.26	-1.59	.0026	-.793	-1.85	-1.51	.0081	-.275	-.343	1.81	.0050
17	-4.22	-12.6	-36.0	.012	-.215	-.976	-2.83	.0018	-2.33	-1.89	32.3	.0083	-.685	1.15	4.43	.0045
18	-13.6	-35.4	-68.0	.012	-1.91	-2.66	1572	.0021	-2.23	31.5	1236	.0083	.867	3.30	-4290	.0045

increases the percentage deviations  $D_p$  decrease in magnitude at first but eventually increase again as the perturbation approaches the tail of the distribution. This is partly due to the fact that the percentage errors are large at the tail in the absence of any perturbation. The standard deviations, however, decrease monotonically with increasing  $p$ .

Comparison of the four methods shows that the order of increasing stability is Nestor-Olsen, Bockasten, Maldonado, and polynomial. The differences are even more pronounced than in Table 3. The polynomial method is the only one where the percentage errors remain at an acceptable level. The same operations were applied to curve B; the results are shown in Table 7. For the polynomial method,  $K$  was again kept fixed at  $K = 8$ . The errors are larger on the whole but trends are the same. For applications to experimental data that contain appreciable random errors or short range fluctuations, the polynomial method is clearly preferable.

The polynomial method does not perform well for values of  $r$  close to  $a$ . For the majority of applications accuracy at the tail of the distribution is of no importance. This defect could be improved upon by including a weight function  $v^{-1} = (1 - y^2/a^2)^{-1}$  in the expression for  $E_1$ , (2.1), to emphasize the errors at the tail. The minimization would then lead to a different set of orthogonal polynomials. The polynomials would have to be of the form  $\mu_m(v) = v\pi_m(v)$  where  $\pi_m$  satisfy (2.7) with a weight function  $v$  inserted in the scalar product. However, it is felt that any method which fits all the data points simultaneously is likely to sacrifice accuracy at the tail. The methods that use piecewise polynomial fits [4], [10] would probably still be superior in this respect.

**5. Conclusions.** The four inversion methods tested in this paper, Nestor and Olsen, Bockasten, Maldonado et al. and polynomial all give adequate accuracy when applied to smooth test functions. However the polynomial method is superior with regard to amplification of random noise and stability against localized perturbations. In addition the polynomial method has several practical advantages: (a) it is a discrete method, (b) data points do not have to be equally spaced, (c) significance of fit can be tested by a simple automatic criterion, and (d) an estimate of the probable error in the radial function due to random noise can be computed. The method presented here is not suited for applications where great accuracy is required for values of  $r$  close to  $a$ .

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