

AD-A 145 058

AD

MEMORANDUM REPORT ARBRL-MR-03369

TECHNICAL  
LIBRARY

METHODS FOR NUMERICAL DIFFERENTIATION

Ceslovas Masaitis

July 1984



US ARMY ARMAMENT RESEARCH AND DEVELOPMENT CENTER  
**BALLISTIC RESEARCH LABORATORY**  
ABERDEEN PROVING GROUND, MARYLAND

Approved for public release; distribution unlimited.

DTIC QUALITY INSPECTED 3

Destroy this report when it is no longer needed.  
Do not return it to the originator.

Additional copies of this report may be obtained  
from the National Technical Information Service,  
U. S. Department of Commerce, Springfield, Virginia  
22161.

The findings in this report are not to be construed as an official  
Department of the Army position, unless so designated by other  
authorized documents.

The use of trade names or manufacturers' names in this report  
does not constitute indorsement of any commercial product.

Errata Sheet  
for  
ARBRL-MR-03369 "Methods for Numerical Differentiation (AD )"

p. 9 Line 17

Change  $h_o = (3.5\sigma/2a)^{1/2}$  to  $h_o = (3.5\sigma/a\sqrt{2})^{1/2}$ .

p. 9 Equation (2.16)

Replace  $\sqrt{10a\frac{\sigma}{3.5}}$  with  $\sqrt{(25.5/\sqrt{2})a\frac{\sigma}{3.5}}$ .

p. 9 Line 19

Replace 20-percent with 60-percent.

p. 11 Equation (2.17)

Move the power of 2 outside right bracket.

p. 13 Line 12

Add  $dr$  to right side of equation for  $N(g,x)$ .

p. 16 Second equation

Add the explanatory comment "where  $w$  is spectral frequency."

p. 16 Third equation

Change  $\sum_{i=1}^k$  to  $\sum_{i=1}^k$ .

p. 17 Equation (4.2)

Change  $\frac{1}{2}$  to  $\frac{1}{\alpha}$  in second term.

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER MEMORANDUM REPORT ARBRL-MR-03369	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle)  METHODS FOR NUMERICAL DIFFERENTIATION	5. TYPE OF REPORT & PERIOD COVERED	
	6. PERFORMING ORG. REPORT NUMBER	
7. AUTHOR(s)  C. Masaitis *	8. CONTRACT OR GRANT NUMBER(s)	
9. PERFORMING ORGANIZATION NAME AND ADDRESS US Army Ballistic Research Laboratory ATTN: DRXBR-SECAD Aberdeen Proving Ground, Maryland 21005-5066	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS  1L162618AH80	
11. CONTROLLING OFFICE NAME AND ADDRESS US Army Ballistic Research Laboratory ATTN: DRXBR-OD-ST Aberdeen Proving Ground, MD 21005-5066	12. REPORT DATE  July 1984	
	13. NUMBER OF PAGES  22	
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)	15. SECURITY CLASS. (of this report)  UNCLASSIFIED	
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE	
16. DISTRIBUTION STATEMENT (of this Report)		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES  *Dr. C. Masaitis P.O. Box 442 Thompson, CT 06277		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number)  Numerical differentiation Approximation Smoothing		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Divided differences, Berstein polynomials, moving polynomial arc, spline approximation, regularization, and autoregressive procedures for estimating derivative of a tabular function are compared and their common features as well as differences are discussed. It is shown that these methods can be arranged in a sequence of increasing refinement.		

DD FORM 1473  
1 JAN 73

EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

## TABLE OF CONTENTS

	<i>Page</i>
1. INTRODUCTION .....	5
2. POLYNOMIAL AND REGRESSION METHODS .....	7
3. REGULARIZATION .....	12
4. AUTOREGRESSIVE APPROACH .....	16
REFERENCES .....	18
DISTRIBUTION LIST .....	19

## 1. INTRODUCTION

The derivative of a function can be defined as the limit of a sequence of divided differences. Consequently, it is independent of any finite number of values of this sequence, i.e., it cannot be obtained from a finite set of observed functional values without additional assumptions. For instance, suppose we compute

$$R(k) = \frac{y(2^{-k}) - y(0)}{2^{-k}}$$

and obtain  $R(k) = 0$  for  $k = 1, 2, \dots, n$  for an arbitrary but finite  $n$ . Can we conclude that  $y'(0) = 0$ ? Certainly not, since  $y(t) = \sin 2^m \pi t$  with integer  $m > n$  would also yield  $R(k) = 0$  for  $k = 1, 2, \dots, n$ . Yet we have  $y'(0) = 2^m \pi$  which we can make as large as we please by selecting a sufficiently large integer  $m$ .

However, we can approximate the derivative of a tabular function if we make certain assumptions about the derivative or the tabular function. Different assumptions lead to a variety of numerical methods. Until the 1960's little research was done on this problem.<sup>1</sup> However, during the last two decades quite a few research papers on the subject have been published. The purpose of this report is to discuss certain classical and recently developed methods for estimating derivatives from discrete data. The methods range from divided differences, through smoothing by splines and by regularization procedures, to the autoregressive approach. Another purpose is to show that these methods can be arranged in the order of subsequent refinements or generalizations, although most of them were developed from independently selected assumptions. Such an arrangement can be used as an indication of improved ability to approximate unknown derivatives at the cost of increasing complexity of the method.

It should, though, be emphasized that no method can be best in every case. For instance, suppose we observe two functions  $y_1(t) \equiv 0$  and  $y_2(t) = \sin 120\pi t$  at the points  $t_n = 0.2n, n=0, 1, 2, \dots, 6$  and that our observations are exact. Then the observed values are all zeros in both cases. Hence, even though a method  $M$  produces good values of  $y'(t_n)$ , i.e., all close to zero, it will give inadequate estimates of  $y_2'(t_n)$  all of which are equal to  $120\pi$ .

---

<sup>1</sup> E. Issacson and H. B. Keller, Analysis of Numerical Methods, John Wiley, New York (1966), pp 288-294.

This example shows that a good method should also provide information about the frequency components whose contributions to the derivative cannot be detected from the data. The spectral analysis method<sup>2</sup> and autoregressive approach<sup>3</sup> provide this explicitly, the first by deriving the spectrum of the underlying function, the second by determining all the frequencies compatible with the data and by indicating those for which the amplitudes can be determined from the data with sufficient accuracy.

Section 2 of this report begins with a discussion of classical methods of divided differences, polynomial interpolation, and regression methods, including their refinement by application of splines. Section 3 shows that the regularization procedure<sup>4,5</sup> can be interpreted as a refinement of the spline approach. Section 4 shows that the autoregressive method<sup>3</sup> is a refinement of the regularization procedure.

The numerical method for computing the derivative of an analytic function by J. N. Lyness and C. B. Moler<sup>6</sup> is not discussed here since it requires evaluation of the function for complex values of its argument. Although frequently an observed function may be assumed to be analytic, its continuation into a complex domain from a finite set of observed values in a real domain is even more difficult than evaluation of its derivative. Thus, this method cannot be applied to evaluate a derivative from a finite set of observed values corresponding to real values of the independent variable.

---

<sup>2</sup> R. S. Anderssen and P. Bloomfield, "A Time Series Approach to Numerical Differentiation," *Technometrics*, 16 (1) (1974), pp 69-75.

<sup>3</sup> C. Masaitis and G. Francis, "Numerical Differentiation of Noisy Data," BRL Memorandum Report 3126, Aug 81 (AD A104631).

<sup>4</sup> A. N. Tikonov, "Solution of Incorrectly Formulated Problems and the Regularization Method," *Soviet Math. Dokl.* 4 (1963), pp 1035-1038.

<sup>5</sup> J. Cullum, "Numerical Differentiation and Regularization," *SIAM J. Numer. Anal.* 8 (1971), pp 254-265.

<sup>6</sup> J. N. Lyness and C. B. Moler, "Numerical Differentiation of Analytic Functions," *SIAM J. Numer. Anal.* 4 (1966), pp 202-210.

## 2. POLYNOMIAL AND REGRESSION METHODS

Let  $x_n$  be an observed value of an unknown function  $y(t)$  at the point  $t_n = nh$  for some  $h > 0$  and  $n=1,2, \dots, N$ . Assume that  $y(t) \in C^2$  and that the error of observation is  $\epsilon_n$ , i.e.,

$$x_n = y(nh) + \epsilon_n, \quad (2.1)$$

with

$$|\epsilon_n| < \delta. \quad (2.2)$$

The simplest way of obtaining an approximation  $x_n'$  of the derivative  $y'(nh)$  is by the divided difference:

$$x_n' = \frac{(x_{n+1} - x_{n-1})}{2h}, \quad (2.3)$$

i.e., in view of (2.1)

$$x_n' = \frac{y(t_{n+1}) - y(t_{n-1})}{2h} + \frac{\epsilon_{n+1} - \epsilon_{n-1}}{2h}. \quad (2.4)$$

By Taylor's formula we have:

$$y(t_{n+1}) = y(t_{n-1}) + 2hy'(\tau_n), \quad (2.5)$$

with  $t_{n-1} < \tau_n < t_{n+1}$ .

It follows from (2.4) and (2.5) that

$$x_n' = y'(\tau_n) + \frac{\epsilon_{n+1} - \epsilon_{n-1}}{2h}. \quad (2.6)$$

If the error term  $(\epsilon_{n+1} - \epsilon_{n-1})/2h$  is negligible we get from (2.6):  $x_n' \approx y'(\tau_n)$ , i.e., this approximation equates the derivative at the midpoint between  $t_{n-1}$  and  $t_{n+1}$  to its value at a certain unknown intermediate point  $\tau_n \in I_n$  where  $I_n$  is the interval  $(t_{n-1}, t_{n+1})$ . Thus, we have

$$y'(t_n) - x_n' = y'(t_n) - y'(\tau_n) - \frac{\epsilon_{n+1} - \epsilon_{n-1}}{2h}, \quad (2.7)$$

or, in view of (2.2), the error of this estimate is bounded as follows:

$$|y'(t_n) - x_n'| \leq |y'(t_n) - y'(\tau_n)| + \frac{\delta}{h}. \quad (2.8)$$

Again, by Taylor's formula we have

$$y'(t_n) = y'(\tau_n) + (\tau_n - t_n)y''(\tau_n'), \quad (2.9)$$

where  $\tau_n'$  is an intermediate value between  $\tau_n$  and  $t_n$ , i.e.,  $t_{n-1} < \tau_n' < t_{n+1}$ . Obviously  $|\tau_n - t_n| < 2h$ . Since we assume that  $y''(t)$  is continuous it is bounded by, say,  $M_n$  on the interval  $[t_{n-1}, t_{n+1}]$ . Therefore we obtain from (2.8) and (2.9):

$$|y'(t_n) - x_n'| \leq 2hM_n + \frac{\delta}{h}. \quad (2.10)$$

If we know the bound  $M \geq M_n$  of the second derivative in the interval  $[t_1, t_N]$  and the bound  $\delta$  we can choose the step size  $h$  equal to, say,  $h_0$  which minimizes the error of the estimate (2.3). The value of  $h_0$  is obtained by minimizing the right-hand side of (2.10) with  $M_n$  replaced by  $M$ . Thus,

$$h_0 = \sqrt{\frac{\delta}{2M}}. \quad (2.11)$$

We can use this optimal step size if we know  $M$  and  $\delta$  before observations are made. If we have to differentiate already collected data then we can use (2.11) provided the step size of the observations  $h < h_0$ . In this case, we use the data with the step size  $h' = kh$  with  $k$  being a positive integer such that  $kh$  is as close as possible to  $h_0$ .

This choice of  $h_0$  minimizes the error of the estimate (2.3) in the worst case, namely when the absolute value of the second derivative is equal to its upper bound and the error is equal to its bound  $\delta$ . In a practical situation such a case may never occur since the observation errors may be relatively small where the second derivative is exceptionally large.

Furthermore, it may be much more important to have an average error, such as the root mean square error (RMSE) small, even at the expense of larger errors in an extreme

case. By assuming that observation errors are mutually independent and have zero means and that  $y''(t)$  is a stochastic process independent of observation errors we get from (2.7) and (2.9):

$$E\left[(y'(t_n) - x_n')^2\right] = E\left[(\tau_n - t_n)^2 y''^2(\tau_n')\right] + \frac{\sigma^2}{2h^2}, \quad (2.12)$$

where  $\sigma^2$  is the variance of  $\epsilon_n$ .

Since  $|\tau_n - t_n| \leq 2h$  we have

$$E\left[(y'(t_n) - x_n')^2\right] \leq 4h^2 E\left[y''^2(\tau_n')\right] + \frac{\sigma^2}{2h^2}. \quad (2.13)$$

Let  $E\left[y''^2(\tau_n')\right] = \tilde{M}_n^2$ . Then the expected value of the square of the estimated error is minimized by

$$\tilde{h}_o = 8^{-1/4} \sqrt{\frac{\sigma}{\tilde{M}_n}}. \quad (2.14)$$

Suppose now that the observed data are distance traveled by a vehicle with maximum acceleration  $a \text{ m/s}^2$  and that all values of acceleration are equally likely. Then  $\tilde{M}_n^2 = 1/2 a^2$  and, thus, by (2.13) and (2.14) the error bound is

$$\left(E\left[\left[y'(t) - x_n'\right]^2\right]\right)^{1/2} \leq \sqrt{2a\sigma}. \quad (2.15)$$

Let us assume that observation errors are normally distributed and that we make about 100 observations. Then a reasonable bound of the error is  $\delta = 3.5\sigma$ . In this case the optimal value of  $h$  given by (2.11) is  $h_o = (3.5\sigma/2a)^{1/2}$ . This value substituted in (2.13) yields

$$\left(E\left[\left[y'(t) - x_n'\right]^2\right]\right)^{1/2} \leq \sqrt{10a\frac{\sigma}{3.5}}. \quad (2.16)$$

i.e., an error bound 20-percent higher than that in (2.15). This simple case illustrates that minimizing the error of the worst case does not produce the best approximation in terms of the RMS or some other average.

The approximation (2.3) is exact for the polynomials of the first degree, provided the data are exact. A straightforward generalization is an approximation that produces exact derivatives for polynomials of degree  $k$  or less, assuming exact data. Obviously, differentiation of an interpolating polynomial is such a procedure. An interpolating polynomial is given by either Lagrange's, Newton's, Gauss's or any other polynomial interpolation formula. Instead of differentiating an interpolating polynomial we can obtain the same estimate by an iterative procedure such as that described by D. B. Hunter<sup>7</sup> or H. C. Hershey et al.<sup>8</sup>

According to Weierstrass' theorem, a continuous function can be approximated arbitrarily closely by polynomials of increasing degree. However, approximations of derivatives obtained by differentiating these polynomials may be very poor. If the data are interpolated by Bernstein polynomials  $B_k$  of increasing degree  $k$  then a uniform approximation of the function by  $B_k$  and of its derivative by  $B_k'$  is obtained.<sup>9</sup> However, even small observation errors may affect the derivatives  $B_k'$  drastically and, thus, cause large errors in the estimates of  $y'(t)$ . Besides, round-off errors in computing coefficients of these polynomials for large values of  $k$  are very substantial. Therefore, in practice, the degree of an interpolating polynomial is chosen equal two or three. Even in this case, the resulting errors may be very large.

In view of this, instead of differentiating interpolating polynomials, derivatives are estimated by differentiating a low degree polynomial that is obtained by a least squares approximation of a sequence of data points located symmetrically on both sides of the point where the value of derivative is estimated.<sup>10</sup> This is a common procedure of moving polynomial arcs and it provides a degree of smoothing of the observation errors by averaging their effects over several data points. This averaging becomes more effective as the number of data points fitted by a single polynomial increases. However, the larger the span the less accurate is the representation of the data. Hence we must choose a compromise between the degree of smoothing and the faithfulness to the data.

---

<sup>7</sup> D. B. Hunter, "An Iterative Method of Numerical Differentiation," *Comp. J.* 3 (1960), pp 270-271.

<sup>8</sup> H. C. Hershey, J. L. Lakin, and R. Simha, "Numerical Differentiation of Equally Spaced and Not Equally Spaced Experimental Data," *Ind. Eng. Chem. Found.* 6 (1967), pp 413-421.

<sup>9</sup> P. J. Davis, "Interpolation and Approximation," Blaisdell Publishing Company (1963), p. 113.

<sup>10</sup> S. Wold, "Spline Functions in Data Analysis," *Technometrics*, 16 (1974), pp 1-11.

A polynomial fitted to a span of the data is a linear combination of the powers of the independent variable. This procedure can be refined in two ways. First, we may transform the data and then fit by a polynomial.<sup>9</sup> For instance, if we observe  $y(t) = ce^{-kt}$  then  $\log y(t)$  can be fitted by a first degree polynomial. Second, we can fit the data by a linear combination of functions other than powers of the independent variable, such as exponentials, trigonometric functions and others.<sup>11</sup> Such fits are called linear regression models and a polynomial fit is a special case of such a representation.

Since a spline function can be represented as a linear combination of so-called B-splines an approximation by a spline function can be interpreted as a refinement of the linear regression approach. The refinement is obtained by adding a condition to the approximation criterion, namely, a requirement to minimize certain combinations of approximation errors and the  $L_2$  norm of the second derivative of the approximating function. This added condition is included by the following considerations. It can be shown that, of all the functions interpolating the data, a cubic spline has second derivatives with the minimal  $L_2$  norm. Consequently, when data are fitted instead of interpolated, it is natural to select a function  $f(t)$  that represents the data with sufficient accuracy and at the same time minimizes

$$J = \int_{t_1}^{t_N} [f''(t)]^2 dt ,$$

i.e., to minimize  $J$  subject to the constraint

$$\frac{1}{N} \sum_{n=1}^N [f(t_n) - x_n]^2 \leq S , \quad (2.17)$$

where  $S$  is a measure of desired accuracy. C. M. Reinsch<sup>12</sup> has shown that the solution of this minimization problem is a cubic spline with the nodes  $t_1, t_2, \dots, t_N$ . This function is obtained by minimizing

$$\int_{t_1}^{t_N} [f''(t)]^2 dt + p \left\{ \frac{1}{N} \sum_{n=1}^N [f(t_n) - x_n]^2 + z - S \right\} ,$$

---

<sup>11</sup>R. S. Anderssen and P. Bloomfield, "Numerical Differentiation Procedures for Non Exact Data," *Numer. Math.* 22 (1974), pp 157-182.

<sup>12</sup>C. H. Reinsch, "Smoothing by Spline Functions," *Numer. Math.* 10 (1967), pp 177-183.

where  $z$  is a slack variable and  $p$  is a Lagrange multiplier. By the method of calculus of variations it can be shown that  $z=0$ . Thus, the problem is to minimize

$$A(f,p) = \int_{t_1}^{t_N} [f''(t)]^2 dt + p \left\{ \sum_{n=1}^N [f(t_n) - x_n]^2 - S \right\} \quad (2.18)$$

and the solution to this problem is a cubic spline, as stated above.

### 3. REGULARIZATION

Minimization of (2.18) by the standard methods of calculus of variations expresses  $p$  as a monotone function of  $S$ . Thus, we can choose  $S$  and determine the corresponding  $p$  or choose  $p$  and compute  $S$ . We may do the latter since, in practice, we do not know how closely the data can be fitted. With  $p = 0$  const and  $\alpha = 1/p$  the function,  $f$ , that minimizes  $A(f,P)$  is obtained by minimizing

$$\frac{1}{N} \sum_{n=1}^N [f(t_n) - x_n]^2 - S + \alpha \int_{t_1}^{t_N} [f''(t)]^2 dt .$$

When  $\alpha$  (and hence  $p$ ) is specified in advance,  $S$  is constant (dependent on  $\alpha$ ). Hence it can be omitted from the expression to be minimized. Therefore for a fixed  $\alpha$ ,  $f$  is obtained by minimizing

$$B(f,\alpha) = \frac{1}{N} \sum_{n=1}^N [f(t_n) - x_n]^2 + \alpha \int_{t_1}^{t_N} [f''(t)]^2 dt . \quad (3.1)$$

The integral in this relation can be interpreted as the square of a seminorm in a Banach space of functions with square integrable second derivatives. If this seminorm is replaced by another seminorm involving first and second derivatives we obtain  $f$  by minimizing

$$\tilde{B}(f,\alpha) = \frac{1}{N} \sum_{n=1}^N [f(t_n) - x_n]^2 + \alpha \left\{ \int_0^1 [f'(t)]^2 dt + \int_0^1 [f''(t)]^2 dt \right\} . \quad (3.2)$$

Here the integration limits have been changed to 0 and 1 which we can always do by rescaling the independent variable  $t$ .

Let

$$f(t) = \int_0^t g(\tau) d\tau = \int_0^1 h(t - \tau)g(\tau) d\tau ,$$

where  $h(t)$  is the Heaviside step function. Then  $f'(t) = g(t)$  and  $f''(t) = g'(t)$ . Thus, (3.2) can be written as follows:

$$\tilde{B}(f, \alpha) = \frac{1}{N} \sum_{n=1}^N \left[ \int_0^1 h(t_n - \tau)g(\tau) d\tau - x_n \right]^2 + \alpha \left\{ \int_0^1 [g(\tau)]^2 d\tau + \int_0^1 [g'(\tau)]^2 d\tau \right\} \quad (3.3)$$

and  $g(t)$  is obtained by minimizing (3.3). Thus, replacing the seminorm

$$\left[ \int_0^1 [f''(t)]^2 dt \right]^{1/2}$$

by

$$\left[ \int_0^1 [f''(t)]^2 dt + \int_0^1 [f'(t)]^2 dt \right]^{1/2}$$

reduces the spline approximation to the computation of a derivative by the regularization procedures of A. N. Tikhonov,<sup>4</sup> provided we represent his functional

$$N(g, x) = \int_0^1 \left[ \int_0^1 h(t - \tau)g(\tau) - x(t) \right]^2 dt$$

in a discrete form, as we must since  $x(t)$  is given only at a set of discrete values of  $t$ . If we replace the first term of (3.3) by  $N(g, x)$ , we get Tikhonov's regularizing functional:

$$C(g, \alpha) = \int_0^1 \left[ \int_0^1 h(t - \tau)g(\tau) d\tau - x(t) \right]^2 dt + \alpha \left\{ \int_0^1 [g(\tau)]^2 d\tau + \int_0^1 [g'(\tau)]^2 d\tau \right\} . \quad (3.4)$$

By equating the variation of  $C(g, \alpha)$  with respect to  $g$  to zero we obtain the following necessary condition on  $g$  for the minimum of  $C(g, \alpha)$ :

$$\int_0^1 \int_0^1 h(\theta - \tau)h(\theta - t)g(\tau) d\tau d\theta - \int_0^1 h(\theta - t)x(\theta) d\theta + \alpha g(t) - \alpha g''(t) = 0 . \quad (3.5)$$

Transversality conditions yield:

$$g'(0) = g'(1) = 0 . \quad (3.6)$$

(3.5) can be written in the form:

$$g''(t) = g(t) + \frac{1}{\alpha} \int_t^1 \int_0^\tau g(\theta) d\theta d\tau - \frac{1}{\alpha} \int_t^1 x(\theta) d\theta . \quad (3.7)$$

Substituting  $t=1$  in (3.7) gives:

$$g''(1) = g(1) + \frac{1}{\alpha} \int_0^1 g(\theta) d\theta . \quad (3.8)$$

We differentiate (3.7) with respect to  $t$  and obtain:

$$g'''(t) = g'(t) + \frac{1}{\alpha} x(t) - \frac{1}{\alpha} \int_0^t g(\theta) d\theta . \quad (3.9)$$

When  $t=1$  (3.9) yields:

$$g'''(1) = g'(1) + \frac{1}{\alpha} x(1) - \frac{1}{\alpha} \int_0^1 g(\theta) d\theta . \quad (3.10)$$

We eliminate the integral from (3.8) and (3.10) and obtain:

$$g'''(1) + g''(1) = g(1) + \frac{1}{\alpha} x(1) . \quad (3.11)$$

In view of (3.6), substitution of  $t=0$  in (3.9) gives

$$g'''(0) = \frac{1}{\alpha} x(0) . \quad (3.12)$$

By differentiating (3.9) with respect to  $t$  we get:

$$g^{iv}(t) - g''(t) + \frac{1}{\alpha} g(t) = \frac{1}{\alpha} x'(t) . \quad (3.13)$$

Thus, the optimizing function  $g(t)$  satisfies differential equation (3.13) with the boundary conditions (3.6), (3.11), and (3.12). Eigenvalues of (3.13) can be easily expressed in terms of  $\alpha$ . Denote these eigenvalues by  $\pm\lambda$  and  $\pm\mu$ . Then Green's function of (3.13) is

$$G(t, \tau) = \frac{1}{2\lambda\mu(\lambda^2 - \mu^2)} \left[ \mu e^{\lambda(t-\tau)} - \mu e^{-\lambda(t-\tau)} - \lambda e^{\mu(t-\tau)} + \lambda e^{-\mu(t-\tau)} \right] . \quad (3.14)$$

The general solution of (3.13) is:

$$g(t) = A_1 e^{\lambda t} + A_2 e^{-\lambda t} + A_3 e^{\mu t} + A_4 e^{-\mu t} + \int_0^t G(t, \tau) x'(\tau) d\tau .$$

We integrate the last integral by parts and obtain:

$$g(t) = A_1 e^{\lambda t} + A_2 e^{-\lambda t} + A_3 e^{\mu t} + A_4 e^{-\mu t} + \int_0^t G_t(t, \tau) x(\tau) d\tau , \quad (3.15)$$

where  $G_t(t, \tau)$  is the derivative of  $G(t, \tau)$  with respect to  $t$  and

$$G_t(t, \tau) = \frac{1}{\lambda^2 - \mu^2} \left[ \cosh \lambda(t - \tau) - \cosh \mu(t - \tau) \right] .$$

The constants of integration  $A_1, A_2, A_3,$  and  $A_4$  are determined by the boundary conditions (3.6), (3.11), and (3.12). The integral in (3.15) can be approximated by a numerical quadrature formula such as trapezoidal or Simpson's rule and with the observed values  $x_n = x(t_n)$ . Thus, (3.15) determines an approximation of the derivative  $g(t_n)$  for a given  $\alpha$ . With the exact values of  $x(t)$ ,  $g(t)$  given by (3.15) converges to  $x'(t)$  as  $\alpha \rightarrow 0$ . When only a finite number of values  $x_n = x(t_n)$  are available and when these values contain observation errors the best approximation of  $x'(t)$  is obtained from  $\alpha > 0$  as shown by examples of the artificial data with exact values  $x'(t)$  obtainable by direct analytic differentiation.<sup>5</sup> In the case of real data, i.e., when  $x'(t)$  is not known, the "best" value of  $\alpha$  must be selected by an empirical criterion. Wahba proposes a cross-validation procedure,

by which approximation  $g(t)$  and hence

$$f(t) = \int_0^t g(t) dt$$

is determined from part of the data, say, with every 10th point omitted.<sup>13</sup> The resulting values of  $f(t)$  for omitted points are compared with the omitted data. The value of alpha that produces the least RMS of these differences is defined as the "best"  $\alpha$ .

An alternative procedure was proposed by R. S. Anderssen and P. Bloomfield.<sup>11</sup> It is based on the assumption that the spectrum of observations is in the form

$$b + b/\left\{\alpha \left[ (w/I)^2 + (w/I)^4 \right]\right\}$$

where  $I = (t_N - t_1)/N$ . The parameter  $\alpha$  can be determined by approximating the spectrum of the data obtained from the Fourier transform. This process is based on the assumption that  $x(t)$  is a stochastic process and that spectra of  $x(t)$  and observation errors  $\epsilon_n$  do not overlap.

#### 4. AUTOREGRESSIVE APPROACH

As stated in the preceding section, the regularization procedure is a refinement of the spline approximation. A further refinement of these methods is provided by an autoregressive approach.<sup>3</sup> This approach is based on the assumptions which imply that an approximating derivative satisfies a linear homogeneous differential equation with constant coefficients:<sup>3</sup>

$$\sum_{i=1}^k a_i g^{(i)}(t) = 0.$$

For any  $\alpha \neq 0$  this equation can be written in the form:

$$\sum_{i=1}^k a_i g^{(i)}(t) + \frac{1}{\alpha} g(t) = \frac{1}{\alpha} g(t). \quad (4.1)$$

Since  $g(t)$  approximates  $x'(t)$ , (4.1) is approximated by

---

<sup>13</sup>G. Wahba, "Period Splines for Spectral Density Estimation: The Use of Cross Validation for Determining the Degree of Smoothing," *Commun. in Statistics* 4 (1975), pp 125-141.

$$\sum_{i=1}^k a_i g^{(i)} + \frac{1}{2}g(t) = \frac{1}{\alpha}x'(t) \quad (4.2)$$

which is a generalization of (3.13). Thus, the autoregressive approach is a refinement of regularization that corresponds to  $k = 4$ ,  $a_1 = a_3 = 0$ ,  $a_2 = -1$ , and  $a_4 = 1$ . Instead of using a fixed order ( $k = 4$ ) and fixed coefficients, the autoregressive approach determines the order  $k$  and the coefficient  $a_i$  from the observations. Usually the data allow more than one choice of  $k$  and  $a_i$ 's. An empirical criterion is selected to assign relative weights to every set of allowable values of  $k$  and  $a_i$ 's. These weights express a compromise between the faithfulness of the data representation and the stability of the corresponding autoregressive model. The approximation of the derivative is the weighted average of these approximations. Since this approach selects an approximation on the basis of the data instead of an a priori model as indicated by (3.13), the approximation of the derivative obtained by this approach is more accurate, in most cases, than that of any of the other methods described above.

## REFERENCES

1. E. Issacson and H. B. Keller, Analysis of Numerical Methods, John Wiley, New York (1966), pp 288-294.
2. R. S. Anderssen and P. Bloomfield, "A Time Series Approach to Numerical Differentiation," Technometrics, 16 (1) (1974), pp 69-75.
3. C. Masaitis and G. Francis, "Numerical Differentiation of Noisy Data," BRL Memorandum Report 3126, Aug 81 (AD A104631).
4. A. N. Tikonov, "Solution of Incorrectly Formulated Problems and the Regularization Method," Soviet Math. Dokl. 4 (1963), pp 1035-1038.
5. J. Cullum, "Numerical Differentiation and Regularization," SIAM J. Numer. Anal. 8 (1971), pp 254-265.
6. J. N. Lyness and C. B. Moler, "Numerical Differentiation of Analytic Functions," SIAM J. Numer. Anal. 4 (1966), pp 202-210.
7. D. B. Hunter, "An Iterative Method of Numerical Differentiation," Comp. J. 3 (1960), pp 270-271.
8. H. C. Hershey, J. L. Lakin, and R. Simha, "Numerical Differentiation of Equally Spaced and Not Equally Spaced Experimental Data," Ind. Eng. Chem. Found. 6 (1967), pp 413-421.
9. P. J. Davis, "Interpolation and Approximation," Blaisdell Publishing Company (1963), p. 113.
10. S. Wold, "Spline Functions in Data Analysis," Technometrics, 16 (1974), pp 1-11.
11. R. S. Anderssen and P. Bloomfield, "Numerical Differentiation Procedures for Non Exact Data," Numer. Math. 22 (1974), pp 157-182.
12. C. H. Reinsch, "Smoothing by Spline Functions," Numer. Math. 10 (1967), pp 177-183.
13. G. Wahba, "Period Splines for Spectral Density Estimation: The Use of Cross Validation for Determining the Degree of Smoothing," Commun. in Statistics 4 (1975), pp 125-141.

DISTRIBUTION LIST

<u>No. of Copies</u>	<u>Organization</u>	<u>No. of Copies</u>	<u>Organization</u>
12	Administrator Defense Technical Info Center ATTN: DTIC-DDA Cameron Station Alexandria, VA 22314	1	Commander US Army Materiel Development and Readiness Command ATTN: DRCDMD-ST 5001 Eisenhower Avenue Alexandria, VA 22333
1	Director Defense Advanced Research Projects Agency ATTN: Mr. C. Lehner 1400 Wilson Boulevard Arlington, VA 22209	1	Commander US Army Materiel Development and Readiness Command ATTN: DRCLDC, Mr. T. Shirata 5001 Eisenhower Avenue Alexandria, VA 22333
1	Deputy Assistant Secretary of the Army (R&D) Washington, DC 20310	1	Commander US Army Materiel Development and Readiness Command ATTN: DRCPM-GCM-WF 5001 Eisenhower Avenue Alexandria, VA 22333
1	HQDA (DAMA-ZD/H. Woodall) WASH, DC 20310	1	Commander US Army Armament Materiel Readiness Command ATTN: DRSMC-LEP-L(R) Rock Island, IL 61299
1	HQDA (DAMA-RAA) WASH, DC 20310	1	Commander Armament R&D Center US Army AMCCOM ATTN: DRSMC-TDC(D) Dover, NJ 07801
1	HQDA (DAMA-WSW) WASH, DC 20310	2	Commander Armament R&D Center US Army AMCCOM ATTN: DRSMC-TSS(D) Dover, NJ 07801
1	HQDA (DAMA-CSS) WASH, DC 20310	1	Commander Armament R&D Center & US Army AMCCOM ATTN: DRSMC-CG(D) Dover, NJ 07801
1	HQDA (DAMA-RQD) WASH, DC 20310		
1	Commander in Chief, USAREUR & 7A ATTN: AEAGB-PDN-SE APO New York 09403		
1	Commander US Army Concepts Analysis Agency ATTN: MOCA-FDS 8120 Woodmont Avenue Bethesda, MD 20014		
1	Commander US Army Operational Test and Evaluation Agency ATTN: DACS-TEM-G Fort Belvoir, VA 22060		

DISTRIBUTION LIST

<u>No. of Copies</u>	<u>Organization</u>	<u>No. of Copies</u>	<u>Organization</u>
2	Commander Armament R&D Center & US Army AMCCOM ATTN: DRSMC-SCF(D) DRSMC-SCF-C(D), Mr. Baumgarthe Dover, NJ 07801	1	Commander US Army Missile Command ATTN: DRSMI-R Redstone Arsenal, AL 35898
2	Commander Armament R&D Center & Development Command ATTN: DRSMC-LCS-A(D), Mr. Hauptman DRSMC-LCS(D), Mr. Killen Dover, NJ 07801	1	Commander US Army Missile Command ATTN: DRSMI-YDL Redstone Arsenal, AL 35898
1	Commander Benet Weapons Laboratory Armament R&D Center ATTN: DRSMC-LCB-TL(D) Watervliet, NY 12189	3	Commander US Army Tank Automotive Command ATTN: DRSTA-TSL DRDTA-TWL, Dr. J. Parks M551 PIP Office Warren, MI 48090
1	Commander US Army Aviation Research and Development Command ATTN: DRDAV-E 4300 Goodfellow Boulevard St. Louis, MO 63120	3	Commander US Army Tank Automotive Command ATTN: DRSTA-R DRSTA-ZED, Mr. T. Puuri, Mr. Ron Beck Warren, MI 48090
1	Director US Army Air Mobility Research and Development Laboratory Ames Research Center Moffett Field, CA 94035	1	Project Manager M1 Abrams Tank Systems 28150 Dequindre Street Warren, MI 48090
1	Commander US Army Communications Research and Development Command ATTN: DRSEL-ATDD Fort Monmouth, NJ 07703	1	Commander US Army Harry Diamond Labs ATTN: DELHD-TA-L 2800 Powder Mill Road Adelphi, MD 20783
1	Commander US Army Electronics Research and Development Command ATTN: DELSD-L Technical Support Activity Fort Monmouth, NJ 07703	4	Commander US Army Training & Doctrine Command ATTN: Library ATCD-CM-AR, COL Kelly ATCD-A, BG Clarke COL J. Broden Fort Monroe, VA 23651

DISTRIBUTION LIST

<u>No. of Copies</u>	<u>Organization</u>	<u>No. of Copies</u>	<u>Organization</u>
2	Director US Army TRADOC Systems Analysis Activity ATTN: ATAA-SL ATAA-T, Mr. Shook White Sands Missile Range NM 88002	2	Commander US Army Combined Arms Combat Developments Activity ATTN: ATCACC-MA ATCA-CAT-D Fort Leavenworth, KS 66027
2	Commander US Army Armor Center & Fort Knox ATTN: ATSB-CD COL DeMont ATSB-DCG Fort Knox, KY 40121	1	Commander David W. Taylor Naval Ship Research and Development Center Bethesda, MD 20084
2	President US Army Armor & Engineer Board ATTN: ATZK-AE-PD COL Shrader Mr. W. Hahn Fort Knox, KY 40121	1	Commander US Naval Surface Weapon Ctr ATTN: G31 Dahlgren, VA 22448
1	Commander US Army Field Artillery School ATTN: Combat & Training Div Fort Sill, OK 73503	1	Commander US Naval Surface Weapon Ctr Silver Spring, MD 20910
2	Commandant US Army Infantry School ATTN: ATSH-CD-CSO-OR ATSH-MV Fort Benning, GA 31905	2	Superintendent US Naval Postgraduate School ATTN: Dr. Sam Parry Dr. R. Stolfi Monterey, CA 93940
1	Director DARCOM-MSA-ADEA ATTN: DRXTB-T, MAJ Martin Fort Lewis, WA 98433	1	Commander Marine Corps Development and Education Command ATTN: Plans & Studies Div Quantico, VA 22134
1	Commander HQ, TCATA Fort Hood, TX 76544	1	Director Battelle Advanced Concepts Lab Columbus Division ATTN: Dr. R. Stein Warren, MI 48090
1	Dr. Ceslovas Masaitis P.O. Box 442 Thompson, CT 06277	1	AFWL/SUL Kirtland AFB, NM 87117

DISTRIBUTION LIST

No. of  
Copies                      Organization

Aberdeen Proving Ground

Dir, USAMSAA  
ATTN: DRXSY-D  
          DRXSY-MP, Mr. H. Cohen  
          Mr. B. Siegel

Cdr, USATECOM  
ATTN: DRSTE-TO-F  
Cdr, CRDC, AMCCOM  
ATTN: DRSMC-CLB-PA  
          DRSMC-CLN  
          DRSMC-CLJ-L

Dir, USAHEL  
ATTN: Mr. A. J. Eckles III

USER EVALUATION SHEET/CHANGE OF ADDRESS

This Laboratory undertakes a continuing effort to improve the quality of the reports it publishes. Your comments/answers to the items/questions below will aid us in our efforts.

1. BRL Report Number \_\_\_\_\_ Date of Report \_\_\_\_\_
2. Date Report Received \_\_\_\_\_
3. Does this report satisfy a need? (Comment on purpose, related project, or other area of interest for which the report will be used.) \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_
4. How specifically, is the report being used? (Information source, design data, procedure, source of ideas, etc.) \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_
5. Has the information in this report led to any quantitative savings as far as man-hours or dollars saved, operating costs avoided or efficiencies achieved, etc? If so, please elaborate. \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_
6. General Comments. What do you think should be changed to improve future reports? (Indicate changes to organization, technical content, format, etc.) \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

CURRENT ADDRESS

\_\_\_\_\_  
Name  
\_\_\_\_\_  
Organization  
\_\_\_\_\_  
Address  
\_\_\_\_\_  
City, State, Zip

7. If indicating a Change of Address or Address Correction, please provide the New or Correct Address in Block 6 above and the Old or Incorrect address below.

OLD ADDRESS

\_\_\_\_\_  
Name  
\_\_\_\_\_  
Organization  
\_\_\_\_\_  
Address  
\_\_\_\_\_  
City, State, Zip

(Remove this sheet along the perforation, fold as indicated, staple or tape closed, and mail.)