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APPROXIMATE DIFFERENTIATION
BY CUBIC SPLINE FITTING

Jonathan D. Young

June 12, 1967

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UCRL-17659
UC-32 Math
and Computing
TID-4500 (50th Ed.)

U N I V E R S I T Y O F C A L I F O R N I A

Lawrence Radiation Laboratory
Berkeley, California

AEC Contract No. W-7405-eng-48

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Printed in the United States of America
Available from
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U.S. Department of Commerce
Springfield, Virginia 22151
Price: Printed Copy $3.00; Microfiche $0.65

APPROXIMATE DIFFERENTIATION BY CUBIC SPLINE FITTING

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ABSTRACT

Cubic spline fitting of a discrete function, $\{x_i, y_i\}$ with a new technique for terminal derivatives is used for estimating first derivatives at the points x_i.

INTRODUCTION

Let $y(x)$ be a function known only in the discrete form as a table of values:

$$x_i \ , \ y_i \ ; \ i = 1, I,$$

with the x_i distinct and monotonically increasing. Various methods exist for approximating $y'(x)$ at the points x_i. References 1 and 2 describe the use of cubic spline functions. The references cited differ in the manner in which the terminal derivatives $y'(x_1)$ and $y'(x_I)$ are computed. We present here a technique which we believe is an improvement over either.

CUBIC SPLINE FITTING

The cubic spline function f which fits y for the table (x_i, y_i) has the following properties:

(1) Over any interval $[x_{i-1}, x_i]$; $i = 2, I$, the function f is a cubic in x,

(2) $f(x_i) = y_i$; $i = 1, I$.

(3) For the whole interval $[x_1, x_I]$ f has continuous first and second derivatives.

(4) $\int_{x_1}^{x_I} [f''(x)]^2 \, dx$ is minimized.

From (2) we note that f is an exact fit for the table (x_i, y_i). By (3) we mean that for any i; $i = 2, I-1$, with $f = f_-$ on $[x_{i-1}, x_i]$ and $f = f_+$ on $[x_i, x_{i+1}]$, f_- and f_+ are cubics in x with $f'_-(x_i) = f'_+(x_i)$ and $f''_-(x_i) = f''_+(x_i)$. By (4) we mean that for any function $g(x)$ satisfying (2) and (3) we have

$$\int_{x_1}^{x_I} [f''(x)]^2 \, dx \leq \int_{x_1}^{x_I} [g''(x)]^2 \, dx.$$

COMPUTATION

Let f_1' denote the derivative of the spline function f at x_i, where $i = 1, I$. If $y_1' \equiv y'(x_1)$ and $y_I' \equiv y'(x_I)$ are known, then the f_i' can be computed by setting

$$f_1' = y_1'$$

and (1)

$$f_I' = y_I'$$

and solving the system

$$(x_{i+1} - x_i) f_{i-1}' + 2(x_{i+1} - x_{i-1}) f_i' + (x_i - x_{i-1}) f_{i+1}' =$$

$$3\{(x_{i+1} - x_i)(y_i - y_{i-1})/(x_i - x_{i-1}) + (x_i - x_{i-1})(y_{i+1} - y_i)/(x_{i+1} - x_i)\} \quad (2)$$

for f_i' ; $i = 2, I - 1$.

In the (usual) case that terminal derivatives are not known, some additional requirement must be imposed at x_1 and x_I. Reference 1 requires that

$$f''(x_1) = 0 \text{ and } f''(x_I) = 0$$

which gives

$$2f_1' + f_2' = 3(y_2 - y_1)/(x_2 - x_1)$$

and (3)

$$f_{I-1}' + 2f_I' = 3(y_I - y_{I-1})/(x_I - x_{I-1}).$$

Equations (2) and (3) give a system of I equations that can be readily solved for the f_i' ; $i = 1, I$.

On the other hand, reference 2 requires that the f at x_1 have the slope of a circle passing through (x_1,y_1) and (x_2,y_2) and having a slope f_2' at x_2. A similar requirement is imposed at x_I. We have then

$$f_1' = (2r_1 + f_2' r_1^2 - f_2')/(1 + f_2')^2$$

and (4)

$$f_I' = (2r_{I-1} + f_{I-1}' r_{I-1}^2 - f_{I-1}')/(1 + f_{I-1}^2)^2 ,$$

where $r_1 = (y_2 - y_1)/(x_2 - x_1)$

and $r_{I-1} = (y_I - y_{I-1})/(x_I - x_{I-1})$.

Since (4) is not linear in f_2' and f_{I-1}', an iterative procedure is proposed for solving (4) and (2) alternately after a first guess for f_2' and f_{I-1}'. The authors assure us the process converges rapidly.

We use in lieu of Eqs. (3) or (4) the requirement that the slope of f at x_1 be that of a cubic passing through (x_1,y_1), (x_2,y_2), and (x_3,y_3) with the slope f_2' at x_2. The resulting equation,

$$f_1' + a_1 f_2' = b_1 y_1 + c_1 y_2 + d_1 y_3 , \tag{5}$$

where

$$d = (x_2-x_1)^2/\{(x_3-x_1)^3 - 2(x_2-x_1)(x_3-x_1)^2 + (x_2-x_1)^2(x_3-x_1)\},$$

$$c = d\{2x_3-x_1)^3 - 3(x_2-x_1)(x_3-x_1)^2\}/(x_2-x_1)^3 ,$$

$$b = -c - d,$$

and $e = d(x_3-x_1) + c(x_2-x_1) - 1,$

relates f_1' and f_2' in a somewhat complicated but nonetheless linear manner.

Applying a similar process at x_I we get

$$f_I' + a_I f_{I-1}' = b_I y_I + c_I y_{I-1} + d_I y_{I-2} , \tag{6}$$

with appropriate definitions of a_I, b_I, c_I, and d_I. Equations (2), (5), and (6) are solved for f_i'; i = 1, I.

COMPUTER PROGRAM

A CHIPPEWA FORTRAN subroutine, SPLYND, has been written for the CDC 6600 which will perform the prescribed computation to approximate y_i' ; $i = 1, I$, given x_i, y_i. This routine is described in detail and listed in the Appendix.

ACKNOWLEDGMENT

This work was done under the auspices of the U. S. Atomic Energy Commission.

APPENDIX

SPLYND

ABSTRACT

SPLYND is a CHIPPEWA FORTRAN subroutine for the CDC 6600 which approximates derivatives y_i' ; $i = 1, I$ by cubic spline fit of a data set (x_i, y_i) ; $i = 1, I$ for $3 \leq I \leq 100$.

USAGE

The routine is called by

CALL SPLYND(X,Y,I,D).

The arrays X, Y, and D have dimension 100. Prior to the call, X contains the values x_i, Y contains the corresponding y_i, and I is the number of such points. The approximate derivative y_i' at each x_i is returned in the array D.

METHOD

The computation of the derivatives except at the terminal points x_1 and x_I is as described in reference 1. Special formulas are used at the terminal points whereby the derivatives are based on cubics that fit respectively y_1, y_2, y_3, and y_2' and y_{I-2}, y_{I-1}, y_I, and y_{I-1}'.

The linear algebraic system which results is solved by the subroutine SOLVYR. Listings of SPLYND and SOLVYR are attached.

RESTRICTIONS

With the present coding, the number of points I cannot exceed 100. The method can not be used for I less than 3. The diagonal dominance required by SOLVYR is assured.

REFERENCES

1. G. Birkhoff and C. R. de Boor, "Piecewise Polynomial Interpolation and Approximation," in Approximation of Functions, Henry L. Garabedian, Ed. (Elsevier Publishing Co., Amsterdam, 1965), pp. 164-168.

2. A. H. Fowler and C. W. Wilson, Cubic Spline, A Curve Fitting Routine, Report Y-1400, Union Carbide Nuclear Company, Oak Ridge, Tenn., 1963, pp. 9-25 (unpublished).

```
      SUBROUTINE SPLYND(X,Y,N,D)
      DIMENSION X(100),Y(100),D(100),A(100,4)
  100 DO 150 I=1,N
      IF(I.NE.1)GO TO 110
      YI=Y(1)  $YM=Y(2)  $YL=Y(3)  $DL=X(2)-X(1)  $RL=(YM-YI)/DL
      DI=X(3)-X(2)  $SI=DL+DI  $RI=(YL-YM)/DI  $J=1  $K=3  $GO TO 140
  110 IF(I.EQ.N)GO TO 130
      IF(I.EQ.2)GO TO 120
      DL=DI  $RL=RI  $DI=X(I+1)-X(I)  $RI=(Y(I+1)-Y(I))/DI  $SI=DL+DI
  120 CONTINUE
      A(I,1)=DI  $A(I,2)=2.*SI  $A(I,3)=DL  $A(I,4)=3.*(DI*RL+DL*RI)
      GO TO 150
  130 CONTINUE
      DL=-DI  $SI=-SI  $YI=Y(N)  $YM=Y(N-1)  $YL=Y(N-2)  $J=3  $K=1
  140 DD=DL*DL  $SS=SI*SI  $SC=SS*SI  $DS=DL*SS  $DC=DD*DL  $A(I,J)=0.
      CC=DD/(SC-2.*DS+DD*SI)  $BB=CC*(2.*SC-3.*DS)/DC  $AA=-BB-CC
      A(I,K)=BB*DL+CC*SI-1.  $A(I,2)=1.  $A(I,4)=AA*YI+BB*YM+CC*YL
  150 CONTINUE
      K=1
      CALL SOLVYR(A,D,N,K)
      RETURN
      END
```

```
      SUBROUTINE SOLVYR(A,P,N,K)
      DIMENSION A(100,4),P(100),S(100),D(100),F(100),B(100),R(100)
  100 M=N-1  $IT=1  $A(1,1)=0.  $A(N,3)=0.  $BJ=0.
      DO 120 I=1,N
      S(I)=A(I,4)  $P(I)=0.  $R(I)=S(I)  $FI=0.
      D1=A(I,1)  $D2=A(I,2)  $D(I)=D2  $IF(D1.EQ.0.)GO TO 106
      D(I)=D1  $FI=D2/D1-BJ  $IF(FI.EQ.0.)GO TO 400
  106 F(I)=FI
      DI=D(I)  $IF(DI.EQ.0.)GO TO 400
      BI=A(I,3)/DI  $IF(FI.EQ.0.)GO TO 112
      BI=BI/FI
  112 B(I)=BI
  120 BJ=BI
  130 SJ=0.
      DO 140 I=1,N
      SI=S(I)  $DI=D(I)  $FI=F(I)  $SI=SI/DI  $IF(FI.EQ.0.)GO TO 134
      SI=(SI-SJ)/FI
  134 S(I)=SI
  140 SJ=SI
      I=N  $SJ=0.
      DO 160 L=1,N
      SI=S(I)  $BI=B(I)  $SI=SI-BI*SJ  $S(I)=SI  $SJ=SI
  160 I=I-1
      DO 170 I=1,N
  170 P(I)=P(I)+S(I)
      IF(K.LE.1)GO TO 300
      WRITE(3,501)IT
      DO 180 I=1,N
  180 WRITE(3,503)S(I),P(I)
      IF(IT.GE.K)GO TO 300
```

```
      IT=IT+1  $SJ=0.  $SI=S(1)
      DO 200 I=1,N
      SK=0. $IF(I.NE.N) SK=S(I+1) $RI=A(I,1)*SJ+A(I,2)*SI+A(I,3)*SK-R(I)
      S(I)=RI  $R(I)=RI  $SJ=SI  $SI=SK
  200 CONTINUE
      GO TO 130
  300 RETURN
  400 WRITE(3,505)
      STOP
  501 FORMAT(26H0 CORRECTION, SOLUTION IT=,I2)
  503 FORMAT(1H ,2E15.7)
  505 FORMAT(26H1***MATRIX NOT SUITABLE***)
      END
```

XBL 679-4875

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