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INVERSE INTERPOLATING SPLINES WITH APPLICATIONS TO THE EQUATION SOLVING

C. IANCU, T. OPROIU and I. PĂVĂLOIU

1. INTRODUCTION

Let f be the function:

(1) $$f:[a,b]\to\mathbb{R},$$

and:

(2) $$\Delta_x : a = x_0 < x_1 < \dots < x_{n-1} < x_n = b,\quad n \geq 2,\ n\in\mathbb{N},$$

a partition of the interval $[a,b]$.

We assume that the function f is twice derivable on the interval $[a,b]$, and $f'(x)\neq 0$ for all $x\in[a,b]$. We denote $F = f([a,b])$.

From the above assumption it results that the function f is a bijection; hence there exists $f^{-1}:F\to[a,b]$.

Since we have assumed that the function f is twice derivable on the interval $[a,b]$, and $f'(x) \neq 0$, $\forall x \in [a,b]$, it results that the function f^{-1} will also be twice derivable on the set F, and:

$$(f^{-1}(f_i))' = 1/f'(x_i),$$

$$(3) \qquad (f^{-1}(f_i))'' = -f''(x_i)/(f'(x_i))^3, \quad i = \overline{0,n}.$$

Next, we deal with the elaboration of a numerical method for solving certain equations of the form:

$$(4) \qquad f(x) = 0, \quad x \in [a,b],$$

using the inverse interpolating cubic splines.

Assuming that the equation (4) admits a root $\overline{x} \in [a,b]$, then from $f(\overline{x}) = 0$ it follows that $f^{-1}(0) = \overline{x}$, while from $f'(x) \neq 0$ for all $x \in [a,b]$ it follows the uniqueness of $\overline{x}$.

We shall remark the following two cases for solving the equation (4):

A. The values $f_i = f(x_i)$, $i = \overline{0,n}$, of the function f on the knots of the partition (2) are given, and $f'(x_o) = m_o$, $f''(x_o) = M_o$, where $m_o, M_o \in \mathbb{R}$, $m_o \neq 0$, are also given.

B. The values of the function f on every point of the interval $[a,b]$ are known.

In order to solve the equation (4) in each case (A or B), we shall construct an inverse interpolating spline.

2. INVERSE INTERPOLATING SPLINES

Let $[\alpha,\beta] \subseteq F$ be the shortest interval containing the

values $f_i = f(x_i)$, $i = \overline{0,n}$, of the function f on the knots of the partition (2).

Since f is bijective on $[a,b]$, it is either increasing or decreasing on this interval.

We shall consider further that f is increasing, and we shall denote by:

$$(5) \qquad \Delta_f : \alpha = f_o < f_1 < \ldots < f_{n-1} < f_n = \beta$$

the partition of the interval $[\alpha,\beta]$ determined by the points f_i, $i = \overline{0,n}$.

We shall construct the inverse interpolating cubic spline associated to the function f.

Using the partitions (2) and (5), we construct the function $\overline{H}$, whose restrictions have the following form:

$$(6) \qquad \overline{H}_i(y) = a_i y^3 + b_i y^2 + c_i y + d_i, \quad i = \overline{0,n-1},$$

for all $y \in [f_i, f_{i+1}]$. These restrictions are uniquely determined from the conditions:

$$(7) \qquad \begin{aligned} \overline{H}_i(f_i) &= x_i, \\ \overline{H}_i'(f_i) &= D_i', \\ \overline{H}_i''(f_i) &= D_i'', \\ \overline{H}_i(f_{i+1}) &= x_{i+1}, \quad i = \overline{0,n-1}, \end{aligned}$$

where:

$$(8) \qquad \begin{aligned} D_o' &= 1/f'(x_o) = 1/m_o, \\ D_o'' &= -f''(x_o)/(f'(x_o))^3 = -M_o/m_o^3; \\ D_i' &= \overline{H}_{i-1}'(f_i), \quad D_i'' = \overline{H}_{i-1}''(f_i), \quad i = \overline{1,n}. \end{aligned}$$

From (6) and (7) one obtains:

(9) $a_i = (1 - D'_i[x_i,x_{i+1};f] - (D''_i/2)[x_i,x_{i+1};f]^2(x_{i+1} - x_i))([x_i,x_{i+1};f]^3(x_{i+1} - x_i)^2)^{-1}$,

(10) $b_i = D''_i/2 - 3a_if_i$,

(11) $c_i = D'_i - D''_if_i + 3a_if_i^2$,

(12) $d_i = x_i - D'_if_i + (D''_i/2)f_i^2 - a_if_i^3, \quad i = \overline{0,n-1}$,

where $[x_i,x_{i+1};f]$ denotes the first order divided difference of the function f on the knots x_i, x_{i+1}.

Taking into account the equalities:

$$\bar{H}'_i(f_{i+1}) = D'_{i+1},$$
(13)
$$\bar{H}''_i(f_{i+1}) = D''_{i+1}, \quad i = \overline{0,n-1},$$

one obtains from (6), (9), (10) and (11) the following recurrence formulae:

$$D'_{i+1} = D'_i + D''_i[x_i,x_{i+1};f](x_{i+1} - x_i) + 3a_i[x_i,x_{i+1};f]^2(x_{i+1} - x_i)^2,$$
(14)
$$D''_{i+1} = D''_i + 6a_i[x_i,x_{i+1};f](x_{i+1} - x_i),$$

for the calculation of the values D'_i and D''_i, $i = \overline{0,n-1}$.

Knowing the restrictions $\bar{H}_i$ for $i = \overline{0,n-1}$, if we have determined an interval (x_j, x_{j+1}) in which the root $\bar{x}$ of the given equation (4) is lying, since $\bar{H}_j$ approaches the function f^{-1} for $x \in (x_j, x_{j+1})$, it results the following approximation for the root $\bar{x}$:

(15) $$\bar{H}_j(0) = d_j \cong \bar{x}.$$

3. ANOTHER FORM FOR THE INVERSE INTERPOLATING SPLINE

In this section we shall give a new form for the inverse interpolating spline (6). For this purpose, using the model proposed in [5], we shall construct the cubic interpolating spline for f^{-1} on the knots of the partition (5), whom restriction on the interval $[f_{i-1}, f_i]$ has the following form:

(16) $$\bar{H}_{i-1}(y) = ((D''_i - D''_{i-1})/(6k_i))(y - f_{i-1})^3 + (D''_{i-1}/2)\cdot(y - f_{i-1})^2 + D'_{i-1}(y - f_{i-1}) + x_{i-1},$$

where:

$$y \in [f_{i-1}, f_i], \quad D''_i \neq D''_{i-1}, \quad k_i = f_i - f_{i-1}, \quad i = \overline{1,n},$$

and:

$$D'_i = \bar{H}'_i(f_i), \quad D''_i = \bar{H}''_i(f_i), \quad i = \overline{0,n}.$$

Denoting by $H(3, \Delta_f)$ the set of all the cubic interpolating splines corresponding to the partition (5), the following proposition holds:

<u>Proposition 1</u>. <u>Every spline $\bar{H} \in H(3, \Delta_f)$ which has the form (16) is uniquely determined if it satisfies the following conditions:</u>

$$\bar{H}_{i-1}(f_i) = x_i,$$
(17)
$$\bar{H}'_{i-1}(f_i) = D'_i,$$
$$D'_0 = a_1, \quad D''_0 = a_2,$$

<u>where $a_1, a_2 \in \mathbb{R}$ are given.</u>

Proof. Using the formula (16), the first two conditions (17) can be written as follows:

$$(18)\quad \begin{aligned} D_i'' &= (6/k_i^2)(x_i - x_{i-1}) - (6/k_i)D_{i-1}' - 2D_{i-1}'' , \\ D_i' &= (3/k_i)(x_i - x_{i-1}) - 2D_{i-1}' - (k_i/2)D_{i-1}'' , \quad i = \overline{1,n} . \end{aligned}$$

Since, in the problem we have studied, we have $D_0' = a_1 = 1/f'(x_0)$ and $D_0'' = a_2 = -f''(x_0)/(f'(x_0))^3$ are known, it follows that the system (18) is compatible determined and provides the values $D_1', D_2', \ldots, D_n', D_1'', D_2'', \ldots, D_n''$ which determine the cubic spline whose restrictions are of the form (16).

Note. If the function f is decreasing, one proceeds analogously, performing a rearrangement of the knots from right to left and taking the values D_n' and D_n'' instead of D_0' and D_0'', respectively.

4. SOLUTION OF THE EQUATION $f(x) = 0$

The sign of the values f_i, $i = \overline{0,n}$, of the partition (5) points out the interval $(x_j, x_{j+1}) \subset (a,b)$ in which the root $\bar{x}$ of the equation (4) is lying.

The method we present in this paper is given by the formulae (15) and (16), obtaining the following approximation for the root $\bar{x}$:

$$(19)\quad \bar{x} \cong \bar{H}_j(0) = ((D_{j+1}'' - D_j'')/(6k_{j+1}))(-f_j)^3 + (D_j''/2)(-f_j)^2 + D_j'(-f_j) + x_j .$$

5. ESTIMATE OF THE ERROR

Theorem 1. Let the function (1) be increasing. If the inverse function f^{-1} is approximated on the interval $[f_{i-1}, f_i]$, $i = \overline{1,n}$, by a cubic spline of the form (16), observing the conditions (17) and $D_i'' - D_{i-1}'' > 0$, then the following inequalities hold:

$$(20)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < \begin{cases} \delta_x, & \text{for } D_{i-1}'' > 0,\ D_{i-1}' > 0 ; \\ \delta_x - 2D_{i-1}'k_i, & \text{for } D_{i-1}'' > 0,\ D_{i-1}' < 0 ; \\ \delta_x - D_{i-1}''k_i^2, & \text{for } D_{i-1}'' < 0,\ D_{i-1}' > 0 ; \\ \delta_x - 2D_{i-1}'k_i - D_{i-1}''k_i^2, & \text{for } D_{i-1}'' < 0,\ D_{i-1}' < 0 , \end{cases}$$

where $\delta_x = x_i - 2x_{i-1} + x$, $x \in [x_{i-1}, x_i]$, $i = \overline{1,n}$.

Proof. It results from (16):

$$\bar{H}_{i-1}(y) - f^{-1}(y) = ((D_i'' - D_{i-1}'')/(6k_i))(y - f_{i-1})^3 + (D_{i-1}''/2)(y - f_{i-1})^2 + D_{i-1}'(y - f_{i-1}) + x_{i-1} - f^{-1}(y) ,$$

and then:

$$(21)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < |(D_i'' - D_{i-1}'')/(6k_i)|\,|y - f_{i-1}|^3 + |D_{i-1}''/2|\,|y - f_{i-1}|^2 + |D_{i-1}'|\,|y - f_{i-1}| + |x_{i-1} - x| .$$

From the conditions of the theorem we have $|y - f_{i-1}| <$

$< |f_i - f_{i-1}| = k_i$, and then the inequality (21) can be put in the form:

$$(22)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < ((D''_i - D''_{i-1})/(6k_i))k_i^3 + |D''_{i-1}/2|k_i^2 + |D'_{i-1}|k_i + x - x_{i-1} .$$

If $D''_{i-1} > 0$, one obtains from (22):

$$(23)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < (D''_i/6)k_i^2 - (D''_{i-1}/6)k_i^2 + (D''_{i-1}/2)k_i^2 + |D'_{i-1}|k_i + x - x_{i-1} = (D''_i/6)k_i^2 + 2(D''_{i-1}/6)k_i^2 + |D'_{i-1}|k_i + x - x_{i-1} .$$

Taking into account the first equality (18), the inequality (23) will acquire the form:

$$(24)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < (k_i^2/6)(D''_i + 2D''_{i-1}) + |D'_{i-1}|k_i + x - x_{i-1} = (k_i^2/6)(6(x_i - x_{i-1})/k_i^2 - 6D'_{i-1}/k_i) + |D'_{i-1}|k_i + x - x_{i-1} = x_i - x_{i-1} - D'_{i-1}k_i + |D'_{i-1}|k_i + x - x_{i-1} = x_i - 2x_{i-1} + x - D'_{i-1}k_i + |D'_{i-1}|k_i .$$

For $D'_{i-1} > 0$, we obtain from the inequality (24):

$$(25)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < x_i - 2x_{i-1} + x = \delta_x ,$$

while for $D'_{i-1} < 0$ we have:

$$(26)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < \delta_x - 2D'_{i-1}k_i .$$

If $D''_{i-1} < 0$, then we obtain from (22):

$$(27)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < (D''_i/6)k_i^2 - (D''_{i-1}/6)k_i^2 - (D''_{i-1}/2)k_i^2 + |D'_{i-1}|k_i + x - x_{i-1} = (D''_i/6)k_i^2 - 4(D''_{i-1}/6)k_i^2 + |D'_{i-1}|k_i + x - x_{i-1} .$$

Taking into account the first equality (18), the inequality (27) will acquire the following form:

$$(28)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < (k_i^2/6)(6(x_i - x_{i-1})/k_i^2 - 6D'_{i-1}/k_i - 2D''_{i-1}) - 4(D''_{i-1}/6)k_i^2 + |D'_{i-1}|k_i + x - x_{i-1} = x_i - x_{i-1} - D'_{i-1}k_i - 2(D''_{i-1}/6)k_i^2 - 4(D''_{i-1}/6)k_i^2 + |D'_{i-1}|k_i + x - x_{i-1} = \delta_x - D''_{i-1}k_i^2 - D'_{i-1}k_i + |D'_{i-1}|k_i .$$

For $D'_{i-1} > 0$, the inequality (28) provides the following result:

$$(29)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < \delta_x - D''_{i-1}k_i^2 ,$$

while for $D'_{i-1} < 0$ we obtain from the same inequality (28) the result:

$$(30)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < \delta_x - 2D'_{i-1}k_i - D''_{i-1}k_i^2 .$$

So, theorem 1 is proved.

Theorem 2. In the conditions of theorem 1, if the function f is decreasing, then the following inequalities hold:

$$(31)\quad |\bar{H}_{i-1}(y) - f^{-1}(y)| < \begin{cases} \alpha_x, & \text{for } D''_i < 0,\ D'_i < 0; \\ \alpha_x - 2D'_i \cdot k_i, & \text{for } D''_i < 0,\ D'_i > 0; \\ \alpha_x + D''_i \cdot k_i^2, & \text{for } D''_i > 0,\ D'_i < 0; \\ \alpha_x + D''_i \cdot k_i^2 - 2D'_i \cdot k_i, & \text{for } D''_i > 0,\ D'_i > 0, \end{cases}$$

where:

(32) $\alpha_x = 2x_i - x - x_{i-1} \leq 2h_i$, $i = \overline{1,n}$.

The proof of theorem 2 is similar to that of theorem 1.

We notice that:

(33) $\delta_x = x_i - x_{i-1} + x - x_{i-1} \leq 2h_i$, $i = \overline{1,n}$.

Using the formulae (32) and (33), one obtains from theorems 1 and 2 the following results:

Theorem 3. In the conditions of theorem 1, the following estimate holds:

(34) $\| \bar{H} - f^{-1} \| \leq \max_{1 \leq i \leq n} \{2h_i, 2h_i + p_1, 2h_i + p_2, 2h_i + p_1 + p_2\}$,

where:

$p_1 = -2 \min_{1 \leq i \leq n} D'_{i-1} k_i$,

$p_2 = - \min_{1 \leq i \leq n} D''_{i-1} k_i^2$.

Theorem 4. In the conditions of theorem 2, the following estimate holds:

(35) $\| \bar{H} - f^{-1} \| \leq \max_{1 \leq i \leq n} \{2h_i, 2h_i + \bar{p}_1, 2h_i + \bar{p}_2, 2h_i + \bar{p}_1 + \bar{p}_2\}$.

6. NUMERICAL APPLICATION

Based on the theory of Section 3, a calculation program written in BASIC (accuracy: 11 significant digits) was elaborated. This program allows to determine the root of an equation $f(x) = 0$, where the analytical expression of $f(x)$ is known (case B, Section 1).

As input data one considers: n = the number of knots, and the knots $x_o, x_1, \ldots, x_n$. The values $y_i = f(x_i)$, $i = \overline{0,n}$, and those of the first and second order derivatives of these ones are computed by means of the numerical-type functions FNA(X), FNB(X), FNC(X), defined by the programmer for $f(x)$, $f'(x)$ and $f''(x)$, respectively.

The values $f(x_i)$, $i = \overline{0,n}$, are increasingly ordered (the lines 230-310 of the program); after that, the values $D'_o = 1/f'(x_o)$ and $D''_o = -f''(x_o)/(f'(x_o))^3$ are calculated. Then one determines D'_i and D''_i , $i = \overline{1,n}$, with the recurrent relations (18).

After these calculations, the interval $[y_i, y_{i+1}]$, $i = \overline{0,n-1}$, in which the root is lying, is tested, and then, by means of the formula (19), one estimates the value of the root $\bar{x} \cong \bar{H}(0)$ and $f(\bar{x})$.

The program was especially applied to the case when only three knots, x_o, x_1, x_2, are given (see Table 1), the root lying into one of the intervals (x_o, x_1), (x_1, x_2).

In order to determine as accurately as possible the value of the root, the program contains a sequence which restricts the interval in which the knots are lying, as follows: if $f(x_o) \cdot f(\bar{x}) > 0$, then one removes x_o , while in the opposite case x_n is removed; in both cases the value $\bar{x}$ found at the previous step is inserted instead of the removed knot. This successive removal process stops when $|f(\bar{x})|$

becomes smaller than 10^{-10} (this restriction being imposed by the restriction of the microcomputer we used).

Table 1 lists the results obtained by means of this program in the case of five equations. The listing of the program is given further down.

Table 1

Equation $f(x) = 0$	Interval in which the root is lying	Knots used at start	Root ($\bar{x}$) at every step	$\lvert f(\bar{x}) \rvert$
$4x^3 + 3x^2 + 3x - 1 = 0$	(0.2, 0.4)	0.2, 0.3, 0.4	0.2499800875 0.2500000081 0.2500000000	1.05E-04 4.23E-08 0.00E+00
$x^2 - 10 \ln x - 3 = 0$	(4, 6)	4, 5, 6	4.1512952567 4.1514567631 4.1514567195	9.52E-04 2.57E-07 0.00E+00
$\ln x - 4 + x^2 = 0$	(1, 3)	1, 2, 3	1.8448743194 1.8412032474 1.8411000557 1.8410971431 1.8410970608 1.8410970585 1.8410970585	1.60E-02 4.49E-04 1.27E-05 3.58E-07 1.01E-08 2.84E-10 7.28E-12
$x - (1/10) \cdot \sin x - 1 = 0$	(0.5, 2)	0.5, 1.5, 2	1.0890477291 1.0885982411 1.0885977529 1.0885977524	4.29E-04 4.66E-07 5.06E-10 1.82E-12
$x - 0.2 \cdot \sin x - 5 = 0$	(4.5, 6.5)	4.5, 5.5, 6.5	4.8006851220 4.8007808072 4.8007808029	8.05E-05 4.28E-09 7.28E-09


```
100 REM Inverse interpolating cubic spline for eq. solving.
110 DEF FNA(X)=4.*X^3+3.*X^2+3.*X-1.
120 DEF FNB(X)=12.*X^2+6.*X+3.
130 DEF FNC(X)=24.*X+6.
140 LPRINT:LPRINTSPC(10)"  Input Data":LPRINT
150 READ N
160 DIM X(N+1),F(N+1),DP(N+1),DS(N+1)
170 FOR I=0 TO N:READ X(I):NEXT I
180 FOR I=0 TO N:AA=FNA(X(I)):F(I)=AA
190 LPRINT USING"    x(##)=+##.####";I,X(I);
200 LPRINT USING"      f(##)=+##.####";I,F(I)
210 NEXT I
220 LPRINT:LPRINT SPC(4)"H(o)";SPC(12)"f(H(o))"
230 REM Increasing arrangement of the values y(i).
240 IV=0
250 FOR I=0 TO N-1
260 IF F(I)<=F(I+1)THEN GOTO 300
270 TT=F(I):F(I)=F(I+1):F(I+1)=TT
280 TT=X(I):X(I)=X(I+1):X(I+1)=TT
290 IV=IV+1
300 NEXT I
310 IF IV<>0 THEN GOTO 240
320 REM Values of DS(i) and DP(I).
330 DP(0)=1./FNB(X(0))
340 DS(0)=-FNC(X(0))/(FNB(X(0))^3)
350 FOR I=0 TO N-1
360 K=F(I+1)-F(I):H=X(I+1)-X(I)
370 DS(I+1)=6.*H/(K*K)-2.*DS(I)-6.*DP(I)/K
380 DP(I+1)=3.*H/K-K*DS(I)/2.-2.*DP(I)
390 NEXT I
400 FOR I=0 TO N-1
410 IF F(I)*F(I+1)<0. THEN GOTO 430
420 NEXT I
430 Y=0.
440 AA=Y-F(I)
450 BB=(DS(I+1)-DS(I))*AA^3/(F(I+1)-F(I))/6.
460 CC=DS(I)*AA^2/2.+DP(I)*AA+X(I)
470 HY=BB+CC
480 LPRINT USING"#.##########";HY;
490 LPRINT USING"        +#.##^^^^";FNA(HY)
500 IF ABS(FNA(HY))<1.E-10 THEN GOTO 540
510 IF F(0)*F(1)<0. THEN X(N)=HY ELSE X(0)=HY
520 FOR I=0 TO N:AA=FNA(X(I)):F(I)=AA:NEXT I
530 GOTO 230
540 LPRINT:LPRINT USING"  Root:    H(o)=+#.##########";HY
550 LPRINT USING"         f(H(o))=  +#.##^^^^";FNA(HY)
560 STOP
570 DATA 2.
580 DATA 0.2,0.3,0.4
```

Note. We mention that a program was elaborated also for the inverse interpolating spline presented in Section 2, but in many concrete cases, when the knots got near to the root (in the meaning of the above removal), undeterminacies appeared because of the small values of the denominator in formula (9). That is why the inverse interpolating spline proposed in Section 3 (which has not created such problems) has been chosen.

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