UNIVERSITY OF ILLINOIS

DIGITAL COMPUTER

LIBRARY ROUTINE K3 - 137

TITLE Least Squares

TYPE Complete Program

PURPOSE OF ROUTINE To fit a set of N weighted experimental points by the best polynomial of the form

$$F(x) = 1/2 \sum_{s=0}^{n-1} a_s x^s$$

The criterion of excellence for the polynomial is that the sum of the squares of the deviations,

$$M = \sum_{i=0}^{N-1} [F(x_i) - f(x_i)]^2 a_w(x_i) \qquad \text{(the } f(x_i) \text{ are given experimental data)}$$

shall be a minimum with respect to arbitrary variations of the coefficients a_s. The resulting polynomial is known as a "least squares polynomial".

DURATION OF ROUTINE $10Nn^2 (n + 1) \times 10^{-3}$ seconds

METHOD USED The condition that M shall be minimal is equivalent to a set of n simultaneous linear equations for the coefficients a_s. The program produces the corresponding n x (n + 1) matrix suitable for use with the library routines L3 or L2 (linear equation solver). The former should be used if the number of coefficients n is large, or if the equations are poorly conditioned.

PROCEDURE

(1) Read in Main Tape,

(2) Insert data prepared according to specifications stated below; read it in with black switch.

(3) To start program, throw black switch. Use of white switch at this point will be described below.

(4) At end of computation and output, return to step 2 above if it is desired to process more data; otherwise proceed to step 5 below.

(5) Clear memory, and read in the appropriate version of the linear equation solver. Insert output tape from first portion of program as data here. If more than one matrix is being solved and Routine L2 (113) is used, the supplement which makes L2 a closed subroutine may be used.

(6) The solutions to the set of n equations are, in order, the desired coefficients a_s and a scale factor. (See description of linear equation solver for interpretation of the scale factor.

SPECIFICATION OF DATA

The data is to be prepared in three lists, the individual entries of which are fractions preceded by sign.

Table I (Terminated by an "L" symbol): The N observation points x_i.

Table II (Terminated by an "F" symbol): The observations $f(x_i)$, listed in the same order as the x's.

Table III (Terminated by an "N" symbol): The weight factors $w(x_i)$ in the same order as the x's.

If all of the experimental points are assigned equal weights, Table III may be omitted. The N symbol must then be replaced by a "J".

After the N or J is an integer specifying the number of coefficients n in the polynomial. This integer is terminated by spaces. Total space available in memory for storage is 874 locations. Space required for data is 2N + 1 or 3N + 1, depending on whether or not weights are specified.

USE OF WHITE SWITCH IN STEP 3:

Input of data is resumed, Tables I and II being assumed already present in the memory. This is valuable if one has a long table of data which he does not wish to repreforate, but would like to alter the single character on the end of the tape so as to change the number of variables. At step 3, a short tape Jn or Nn is inserted and the white switch thrown. At stop, throw black switch to start program.

If it is desired to process the same equally weighted data several times using different numbers of coefficients, this can be accomplished by reading in a short tape Jn (spaces) (n is the number of coefficients to be used next) following each computation, and then throwing black switch to start new computation.

SUPPLEMENTARY INFORMATION:

If programmer wishes to fit the data to a function of the form

$$G(x) = \sum_{s=0}^{n-1} b_s U_s(x)$$

($U_s(x)$ being a set of given functions), he may do so by replacing the routine at 139 by an auxiliary. This is entered from the main program with $s.2^{-39}$ in A, x in 0. It is left with $U_s(x)$ in A and in 2. Scaling required that $|U_s(x)| \leq 1/2$ for all x.

If more than 11 words are used by this routine the storage locations which start at 150 must be advanced so they will not overwrite the auxiliary. This may be done by changing the preset parameter S6 on the master tape from 00F 00 150F to the desired value.

DATE 6/15/54	RT: 1/27/60
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APPROVED BY J.P.Nash	

ns

LOCATION	ORDER	NOTES	PAGE 1	K 3
	D.0.I			
	00 3K			
3	00 F			
	00 33F	Location of least squares routine		
4	00 F			
	00 11F	number of decimal places in matrix		
5	00 F			
	00 11F	number of decimal places in solution		
6	00 F			
	00 150F	storage		
7	00 F			
	00 84F	Code N2 (110 = Code P1)		
8	00 F			
	00 139F	Auxiliary		
9	00 F			
	00 12F	input routine		
	26 999N			
	00 33K			
	Program			
	00 84K			
	Code N2			
	00 110K			
	Code P1			
	00 139K			
	Auxiliary	computes $1/2\ x^s \rightarrow U_s$		
	00 12K			
	Input routine			
	24 12N			

Temporary Store: 0, 1, 2, 3, 5, 6, 7, 8, 10, 11

Auxiliary entered with x in 0, $s \cdot 2^{-39}$ in A.

Exit with x in 0, $U_s(x)$ in A, 2.

LOCATION	ORDER		NOTES PAGE 2 K 3
	00 12K		
0	L5 4L		Plant address a
	46 1L		
1	50 S6		Enter data input
	50 1L	From 12L	
2	26 S7		
	L4 18L		
3	42 5L		Switch after data is read in
	L5 1L		
4	50 S6		Leaves first location of previously
	10 20F		read in data in A.
5	50 19L		
	26 F		
6	42 49S3		N end of weights
	50 20L		put order in Q.
7	S5 F		J store Q at 14S3
	26 13L		end data
8	42 48S3		F
	27 12L		end of f_i
9	L5 8S7		
	46 11L		L end of x_i
10	50 15L		Store -1 after last x_i
	09 1F		
11	40 F		
	L5 19S3		Plant address of next data storage.
12	L4 8S7		
	22 L		
13	40 14S3		
	00 40F		read in constant
14	81 4F		
	74 41S7		n
15	00 4F		
	91 4F		
16	32 14L		
	S5 F		

LOCATION	ORDER	NOTES	PAGE 3 K 3
17	42 50S3	to main program	store n.
	24 S3		
18	26 1L		
	00 6L		
19	27 18S3		use without weight table
	75 F		
20	40 2F		use with weight table
	75 F		

Punches out matrix $A_{rs} = \sum_{i=0}^{N-1} 1/4\ U_r(x_i)U_s(x_i)$

$$A_{rn} = -\sum_{i=0}^{N-1} 1/2\ U_r(x_i)\ f(x_i)$$

r = 0,1,2,...,n-1

s = 0,1,2,...,n-1

r = 0,1,...,n-1

Each row is scaled to < 1/2 but greater than ~ 1/8

0	92 993F		Print spaces
	27 2L		r → 0
1	92 770F	from	Print N (End of row)
	F5 6F	29L	r → r + 1
2	42 6F	From 0L	
	L0 50L		
3	36 6L		r-n
	41 8F		< 0 Clear store.
4	L5 26L		
	42 18L		Plant address of shift orders
5	42 19L		
	23 33L		s → 0
6	L7 48L	From 3L	Print character at end of matrix
	00 16F		
7	82 4F		
	92 1021F		Spaces
8	24 S9		On to next data

LOCATION	ORDER		NOTES PAGE 4
	L1 50L	From 31L	
9	L4 7F		
	32 44L		s - n
10	L5 7F		< 0
	50 10L		
11	26 S8		Calculate U_s.
	40 3F		Store U_s at 3.
12	L5 6F		
	50 12L		
13	26 S8		Calculate U_r
	50 3F		
14	40 2F		Store U_r at 2
	75 F	By 7L,	. w
15	40 10F	23L	Calculate U_s . w
	S5 S6		
16	40 11F		Double Precision
	50 11F		
17	7J 2F		
	50 10F		
18	74 2F		
	10 F	By 4L,	$U_r U_s \cdot 2^{-p} \cdot 2^{u} \cdot w$
19	40 1F	5L, 25L,	
	00 F	43L	
20	L4 5F		Store accumulated sum
	40 5F		$\Sigma\, U_r(x_i)\, U_s(x_i)\, w(x_i) \cdot 2^{-p} \cdot 2^{u}$
21	F5 27L		
	42 27L		Prepare to treat next experimental
22	F5 44L		points.
	42 44L		
23	F5 14L		
	42 14L		
24	LL 5F		Test scaling of matrix element
	32 27L		
25	F5 18L		Scale down on next run
	42 18L		

LOCATION	ORDER		NOTES PAGE 5
26	L5 5F	By 21L, 35L	
	10 1F		
27	40 5F	From 38L	
	L5 F		Bring down next $x_i \rightarrow 0$
28	40 F	From 24L	
	L7 8F		Test for maximum of terms in above
29	L2 5F		sum.
	36 31L		
30	L5 5F		Store new maximum value
	40 8F		
31	L7 F	From 29L	Test for end of data
	32 8L		
32	L1 48L		Switch to print every other
	32 45L		time
33	F5 7F		
	42 7F	From 5L	$s \rightarrow s + 1$
34	F0 50L		
	32 38L		$s - n$
35	L5 15L		< 0
	42 27L		Store address first x_i
36	L7 48L		Store address first f_i
	42 44L		
37	L5 49L		Store address first w_i
	42 14L		
38	27 27L		$N(5) \rightarrow 0$
	L1 48L	From 34L	Try switch again, and
39	40 48L		
	36 1L		change it.
40	L3 8F		Scale
	L2 8F	From 44L	up every other time through
41	32 5L		the row of matrix
	00 1F		
42	32 5L		
	40 8F		
43	F5 19L		Scale up on next run by factor 2

LOCATION	ORDER	NOTES	PAGE 6
	42 19L		
44	23 40L	By 22L, 36L	N(A) = 0
	L1 F	From 9L	$-f_i$ goes to A
45	22 11L		
	L5 5F	From 32L	Print
46	50 S4		out
	50 46L		A_{rs}
47	26 26S7		
	26 33L		back for next matrix element
48	00 S5		
	00 F		
49	00 S6		storage of constants
	00 F		
50	00 F		
	00 F		(number of variables)