



DECUS

PROGRAM LIBRARY

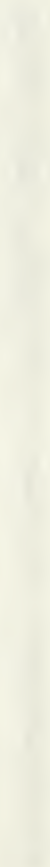
DECUS NO.	8-134
TITLE	LSQ (LEAST SQUARES SUBROUTINE)
AUTHOR	Kenneth B. Wiberg
COMPANY	Department of Chemistry Yale University New Haven, Connecticut
DATE	June 11, 1968
SOURCE LANGUAGE	

DECEMBER

PROGRAM



10



LSQ (LEAST SQUARES SUBROUTINE)

DECUS Program Library Write-up

DECUS No. 8-134

This subroutine calculates the slope and intercept for

$$y_i = mx_i + b$$

by the method of least squares. The rms deviation of y , the correlation coefficient and an estimate of the percent error in the slope are also calculated.

Specifications : The program requires 1.5 pages of memory and the following page 0 locations:

10-13 temporary storage
100-113;156-160 data return from subroutine
117-123 data for subroutine
114-116;153-155;161-177 temporary storage

The page zero locations may be changed as desired by changing the list which precedes the program on the symbolic tape. The subroutine calls the subroutine FLOAT, and uses the floating point interpreter, version C.

Description: Before calling the subroutine, the following locations are set up:

117 N = the number of data points
120 LX = starting location for X array.
121 LY = starting location for Y array
122 LCALC = starting location of YCALC array
 into which the calculated values of y are
 to be placed
123 LDIF = starting location of DIF array into
 which the differences between Y and $YCALC$
 are to be placed.

The subroutine is called by an effective JMS I LSQ. On return to the calling program, the following will be available:

100 S = slope
103 B = intercept
106 R = correlation coefficient
111 ERROR = rms deviation in y
156 TEM2 = % error in slope

Method of Calculation :

The slope and intercept are obtained using the usual expressions:

$$\text{SLOPE} = (\text{SUMX} * \text{SUMY} - \text{G} * \text{SUMXY}) / (\text{SUMX} ** 2 - \text{G} * \text{SUMXX})$$

$$\text{B} = (\text{SUMX} * \text{SUMXY} - \text{SUMY} * \text{SUMXX}) / (\text{SUMX} ** 2 - \text{G} * \text{SUMXX})$$

where G is the number of points in floating point form. The correlation coefficient is calculated from:

$$\text{R} = (\text{SUMX} * \text{SUMY} - \text{G} * \text{SUMXY}) / \text{SQRT}((\text{SUMY} ** 2 - \text{G} * \text{SUMYY}) * (\text{SUMX} ** 2 - \text{G} * \text{SUMXX}))$$

and the % error in the slope is estimated from:

$$\% \text{ERROR} = \text{G} * \text{SQRT}(\text{SUM}(((\text{X}_i - \bar{\text{X}}) * \text{DIF}_i) ** 2)) / (\text{SUMX} * \text{SUMY} - \text{G} * \text{SUMXY})$$

The quantity $\text{SUM}(((\text{X}_i - \bar{\text{X}}) * \text{DIF}_i) ** 2)$ is collected as SUMXY on pg. 2 of the subroutine. SUMX is set equal to $\bar{\text{X}}$, and TEM3 contains the numerator from the slope calculation. The above method of estimating the error in slope makes the error independent of translation of the x axis and was suggested by E. C. Lupton, Jr.

/LEAST SQUARES SUBROUTINE

IX=10
 IY=11
 ICALC=12
 IDIF=13
 S=100
 B=103
 R=106
 ERROR=111
 G=114
 N=117
 LX=120
 LY=121
 LCALC=122
 LDIF=123
 SUMYY=153
 TEM2=156
 TEM3=161
 SUMX=164
 SUMY=167
 SUMXY=172
 SUMXX=175
 CALL=4400
 RETURN=5400
 FLOAT=4355
 FSQRT=2
 FLPT=4407
 *3400

3400	0000	LSQ,	0	
3401	7200		CLA	
3402	1117		TAD N	
3403	7041		CIA	
3404	3366		DCA NEGN	/INDEX
3405	1120		TAD LX	/SET UP REGISTERS
3406	3010		DCA IX	
3407	1121		TAD LY	
3410	3011		DCA IY	
3411	4407		FLPT	
3412	5361		FGET ZERO	
3413	6164		FPUT SUMX	
3414	6167		FPUT SUMY	
3415	6175		FPUT SUMXX	
3416	6172		FPUT SUMXY	
3417	6153		FPUT SUMYY	
3420	0000		FEXT	
3421	4407	BEGIN,	FLPT	
3422	5167		FGET SUMY	
3423	1411		FADD I IY	
3424	6167		FPUT SUMY	/STORE SUM Y
3425	5410		FGET I IX	/GET X
3426	1164		FADD SUMX	
3427	6164		FPUT SUMX	/STORE SUM X
3430	5410		FGET I IX	
3431	3410		FMPY I IX	
3432	1175		FADD SUMXX	

3433	6175	FPUT SUMXX	/STORE SUM X*X
3434	5410	FGET I IX	
3435	3411	FMPY I IY	
3436	1172	FADD SUMXY	
3437	6172	FPUT SUMXY	/STORE SUM X*Y
3440	5411	FGET I IY	
3441	3411	FMPY I IY	
3442	1153	FADD SUMYY	
3443	6153	FPUT SUMYY	/STORE SUM Y*Y
3444	0000	FEXT	/FINISHED SUMMATIONS
3445	2011	ISZ IY	
3446	2011	ISZ IY	
3447	2011	ISZ IY	
3450	2010	ISZ IX	
3451	2010	ISZ IX	
3452	2010	ISZ IX	
3453	2366	ISZ NEGN	
3454	5221	JMP BEGIN	/CONTINUE SUMMATION LOOP
3455	7200	CLA	
3456	1117	TAD N	/FLOAT N
3457	4777	CALL FLOAT	
3460	4407	FLPT	
3461	6114	FPUT G	
3462	5175	FGET SUMXX	/CALC S AND B
3463	3114	FMPY G	
3464	6156	FPUT TEM2	
3465	5164	FGET SUMX	
3466	3164	FMPY SUMX	
3467	2156	FSUB TEM2	
3470	6156	FPUT TEM2	/DENOMINATOR
3471	5172	FGET SUMXY	
3472	3114	FMPY G	
3473	6161	FPUT TEM3	
3474	5164	FGET SUMX	
3475	3167	FMPY SUMY	
3476	2161	FSUB TEM3	
3477	6111	FPUT ERROR	/NUMERATOR, TEMP STORAGE
3500	4156	FDIV TEM2	/SLOPE
3501	6100	FPUT S	
3502	5175	FGET SUMXX	
3503	3167	FMPY SUMY	
3504	6161	FPUT TEM3	
3505	5164	FGET SUMX	
3506	3172	FMPY SUMXY	
3507	2161	FSUB TEM3	
3510	4156	FDIV TEM2	
3511	6103	FPUT B	/INTERCEPT
3512	5153	FGET SUMYY	/CALCULATE R
3513	3114	FMPY G	
3514	6161	FPUT TEM3	
3515	5167	FGET SUMY	
3516	3167	FMPY SUMY	
3517	2161	FSUB TEM3	
3520	3156	FMPY TEM2	
3521	0002	FSQRT	

3522	6161		FPUT TEM3	
3523	5111		FGET ERROR	
3524	4161		FDIV TEM3	
3525	6106		FPUT R	
3526	0000		FEXT	
3527	7200		CLA	/SET UP REGISTERS
3530	1120		TAD LX	
3531	3010		DCA IX	
3532	1121		TAD LY	
3533	3011		DCA IY	
3534	1122		TAD LCALC	
3535	3012		DCA I CALC	
3536	1123		TAD LDIF	
3537	3013		DCA IDIF	
3540	1117		TAD N	
3541	7041		CIA	
3542	3776		DCA NEGN2	/INDEX
3543	4407		FLPT	
3544	5111		FGET ERROR	
3545	6161		FPUT TEM3	/NUMERATOR
3546	5361		FGET ZERO	
3547	6111		FPUT ERROR	
3550	6172		FPUT SUMXY	
3551	6167		FPUT SUMY	/ERROR SUMS
3552	0000		FEXT	
3553	4755		CALL CONT	
3554	5600		RETURN LSQ	
3555	3600	CONT,	3600	
3556	0000	ONE,	FLTG 1.0	
3557	3777			
3560	7774			
3561	0000	ZERO,	FLTG 0.0	
3562	0000			
3563	0000			
3564	7777	M1,	-1	
3565	7776	M2,	-2	
3566	0000	NEGN,	0	
		/PG 2 OF LEAST SQUARES PROGRAM		
3576	3666	*3600		
3577	4355			
3600	0000	LSQ2,	0	
3601	4407		FLPT	
3602	5164		FGET SUMX	
3603	4114		FDIV G	
3604	6164		FPUT SUMX	
3605	0000		FEXT	
3606	4407	LOOP,	FLPT	
3607	5410		FGET I IX	/CALC RMS ERROR
3610	3100		FMPY S	/AND ERROR IN SLOPE
3611	1103		FADD B	
3612	6412		FPUT I I CALC	
3613	2411		FSUB I IY	
3614	6413		FPUT I IDIF	
3615	3413		FMPY I IDIF	
3616	1111		FADD ERROR	

3617	6111	FPUT ERROR	/SUM (ERROR)**2
3620	5410	FGET I IX	
3621	2164	FSUB SUMX	
3622	3413	FMPY I IDIF	
3623	6156	FPUT TEM2	
3624	3156	FMPY TEM2	
3625	1172	FADD SUMXY	
3626	6172	FPUT SUMXY	/SUM (X-XAVE)*(ERROR)**2
3627	0000	FEXT	
3630	2010	ISZ IX	
3631	2010	ISZ IX	
3632	2010	ISZ IX	
3633	2011	ISZ IY	
3634	2011	ISZ IY	
3635	2011	ISZ IY	
3636	2012	ISZ ICALC	
3637	2012	ISZ ICALC	
3640	2012	ISZ ICALC	
3641	2013	ISZ IDIF	
3642	2013	ISZ IDIF	
3643	2013	ISZ IDIF	
3644	2266	ISZ NEGN2	
3645	5206	JMP LOOP	
3646	4407	FLPT	
3647	5111	FGET ERROR	
3650	4114	FDIV G	
3651	0002	FSQRT	
3652	6111	FPUT ERROR	/ERROR CALCULATED
3653	5172	FGET SUMXY	
3654	0002	FSQRT	
3655	3114	FMPY G	
3656	4161	FDIV TEM3	
3657	3263	FMPY HUNDRED	
3660	6156	FPUT TEM2	/% ERROR IN SLOPE
3661	0000	FEXT	
3662	5600	RETURN LSQ2	
3663	0007	HUNDRED, FLTG 100.0	
3664	3077		
3665	7776		
3666	0000	NEGN2, 0	

/SUBROUTINE TO FLOAT FIXED POINT NUMBERS
/NUMBER IS IN AC; RETURNED IN FL(AC)

*4355

4355	0000	FLOAT,	0	
4356	3045		DCA 45	/PUT NUMBER IN HIGH ORDER
4357	3046		DCA 46	/PUT ZERO IN LOW ORDER
4360	1366		TAD C13	/11(10) INTO
4361	3044	C,	DCA 44	/EXPONENT
4362	4407		JMS I 7	/CALL INTERPRETER
4363	7000		FNOR	/NORMALIZE
4364	0000		FEXT	/LEAVE INTERPRETER
4365	5755		JMP I FLOAT	
4366	0013	C13,	13	/11 DECIMAL

(Cf. Floating-Point System Programming Manual p 3-10)

