

PROGRAM DESCRIPTION I

Program Title Non-Linear Curve Fit Using Simplex Function MinimizationContributor's Name Kenneth ButterfieldAddress 2020 23rd Street, Apt. CCity Los Alamos State/Country New Mexico Zip Code 87544

This program is used to fit a set of experimental data to an arbitrary user supplied function. The function used can be nonlinear, and have up to three free parameters (variables). The program will prompt the user for all required data. The experimental data is stored in (x,y) pairs. Initial values (guesses), and step sizes for the free parameters are also required. The better the initial guess the quicker the program will reach a good fit.

The method used performs a least squared error fit of the theoretical curve to the experimental data. This is accomplished using the simplex function minimization of Nelder and Mead (ref 1). The function that is minimized is the square root of the sum of the errors at each data point. The simplex method is used because it is relatively fast at converging toward a minimum even when the initial guess for the free parameters is not very good. Many other data fitting methods can have problems finding the region of the minimum unless they are started close to the minimum. The main requirement for the simplex method is the storage of an $N+1$ by $N+1$ array to store the simplex, where N is the number of free parameters.

Necessary Accessories At least two extra memory modules (with program separation).Operating Limits and Warnings The more memory, the better.Reference(s) "A Simplex Method for Function Minimization"J.A. Nelder and R. MeadComput. J. vol. 7, 308 (1965)

This program has been verified only with respect to the numerical example given in Program Description II. User accepts and uses this program material AT HIS OWN RISK, in reliance solely upon his own inspection of the program material and without reliance upon any representation or description concerning the program material.

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PROGRAM DESCRIPTION I

This program requires a large amount of memory for data and program storage. A large part of the memory is used to support generality. Both the number of data points, and the size of the simplex can vary in size. In fact, one third of the program does nothing more than initialize the data structure, and prompt for input. These sections of the program could be loaded and ran separately from the main program loop to allow more memory space for data storage.

Another resource the program uses freely is time. One pass through the main loop may take several seconds. In order to calculate the sum of the squared errors, the theoretical function must be evaluated at each of the data points. This must be done an average of two or three times per pass. For a function with three free parameters it may take 150-200 evaluations to reach a minimum.

Note: For many problems the program will reach the region of the minimum quickly (20 iterations), and then take many more iterations to zero in on the final result. Therefore the program is written to display the latest calculated value for the RMS error. The user can monitor this value to determine how the program is doing. ~~If it is fluctuating rapidly from large to small values, the program is searching for the region of a minimum.~~ Once such a region is found the value displayed will more or less continually decrease until the required error is reached. It is possible, however, to have theoretical functions that are either very slow in converging, or that can 'fool' the program into finding a 'local' minimum. For example of such functions see reference one. The user should be aware that the program can find spurious results. There is no guarantee that the best minimum has been found. One method of checking the results is to start the program with a different set of initial values for the free parameters. Approximately the same final values should be found for a 'good' minimum. Another good check is to plot the experimental and theoretical data on the same graph.

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DATA STRUCTURE

A simplex is a set of $N+1$ points in an N dimensional space. For example, one free parameter has a simplex composed of two points. Each point is a value of the free parameter and the value of the RMS error for that parameter.

$$p_i = \begin{bmatrix} V_i \\ P_i \end{bmatrix} \quad \begin{array}{l} \text{RMS error} \\ \text{parameter value} \end{array}$$

the simplex for one free parameter is

$$s = \begin{bmatrix} p_0 \\ p_1 \end{bmatrix} = \begin{bmatrix} V_0 & P_0 \\ V_1 & P_1 \end{bmatrix}$$

The geometric representation for this simplex is a line segment.

For two free parameters there will be three points, and the geometric representation is a triangle.

For three free parameters the simplex is

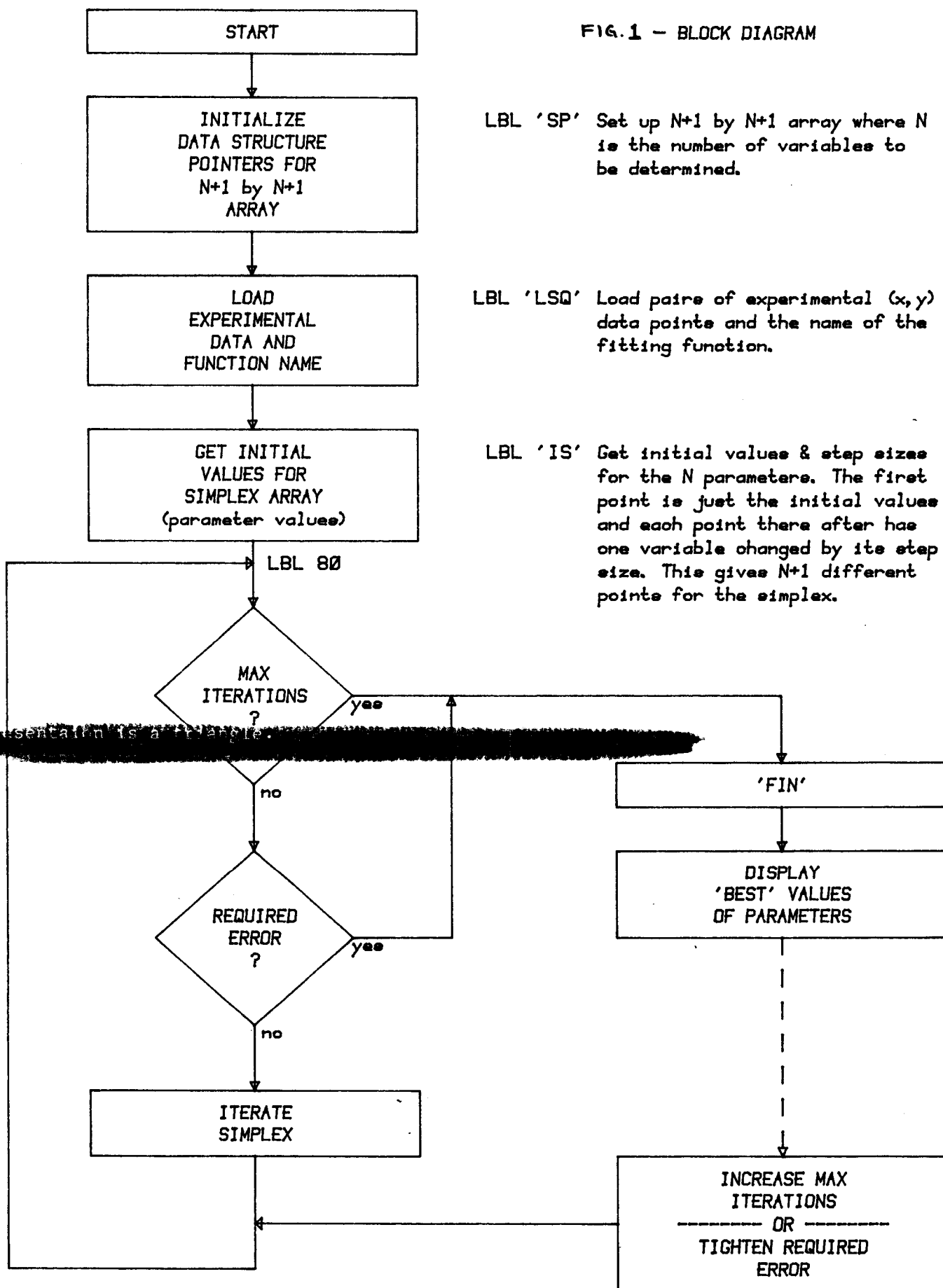
$$s = \begin{bmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{bmatrix} = \begin{bmatrix} V_0 & P_{01} & P_{02} & P_{03} \\ V_1 & P_{11} & P_{12} & P_{13} \\ V_2 & P_{21} & P_{22} & P_{23} \\ V_3 & P_{31} & P_{32} & P_{33} \end{bmatrix}$$

Graphically, this is a tetrahedron in a three dimensional space.

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FIG. 1 - BLOCK DIAGRAM



PROGRAM FLOW

A block diagram for the overall program flow is given in figure one. The first step in the program is to define the data pointers used in addressing the (N+1) by (N+1) simplex, and the (x,y) data pairs of the experimental data array. This is done in the routine 'SP' (Set Pointers). The program will prompt for N, the number of free parameters. This value is used to determine the size of the simplex. 'SP' then calculates the various pointers, offsets, and constants needed by the main program. This data resides in the first 25 data registers.

The next step is to input the experimental data (routine 'LSQ'). the program will prompt for the number of data points and for each of the x and y values of the data. The present value stored will be displayed as part of the prompt. If this value is correct, pressing R/S will keep the value without having to re-enter anything. This feature makes it possible to restart 'SIMP' either to check the data or to change selected values.

The last initialization is done in routine 'IS' (Initialize Simplex). The program prompts for the initial values and the step sizes of the free parameters. This information is used to form the initial simplex and each point in the simplex is evaluated.

For three parameters, the initial simplex has the form

$$s = \begin{bmatrix} V0 & IV1 & IV2 & IV3 \\ V1 & IV1+SS1 & IV2 & IV3 \\ V2 & IV1 & IV2+SS2 & IV3 \\ V3 & IV1 & IV2 & IV3+SS3 \end{bmatrix}$$

The main loop of the program starts at 'LBL 80'. An expanded flow chart for the main loop is given in figure two. The main goal of the algorithm is to use the present points in the simplex to find a direction to move. A point is calculated along this direction. The point is evaluated and copied into the simplex if it is better then the worst value presently in the simplex.

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For example, in two dimensions a simplex is a triangle. The program will determine the high and low points (PH, PL), and form a new point P* by reflecting PH across the center of mass (PBAR) of the remaining points. Another point P** will be calculated in this same direction. Its position will depend upon the success of P*. If P* is lower than PH, P** will be further along, otherwise P** will be stepped closer in. Which ever of P* or P** is the lowest will be compared to PH, and if it is an improvement copied into the simplex. Should it turn out that neither P* nor P** is better than PH, the whole simplex is contracted toward PL. The main advantage of this method is that the largest possible step in an intelligent direction is taken. Thus the method moves rapidly toward better function values. The shape of the simplex adapts itself to the local terrain, enlarging while searching for the region of the minimum, and elongating when entering narrow valleys.

TWO DIMENSIONAL SIMPLEX =>

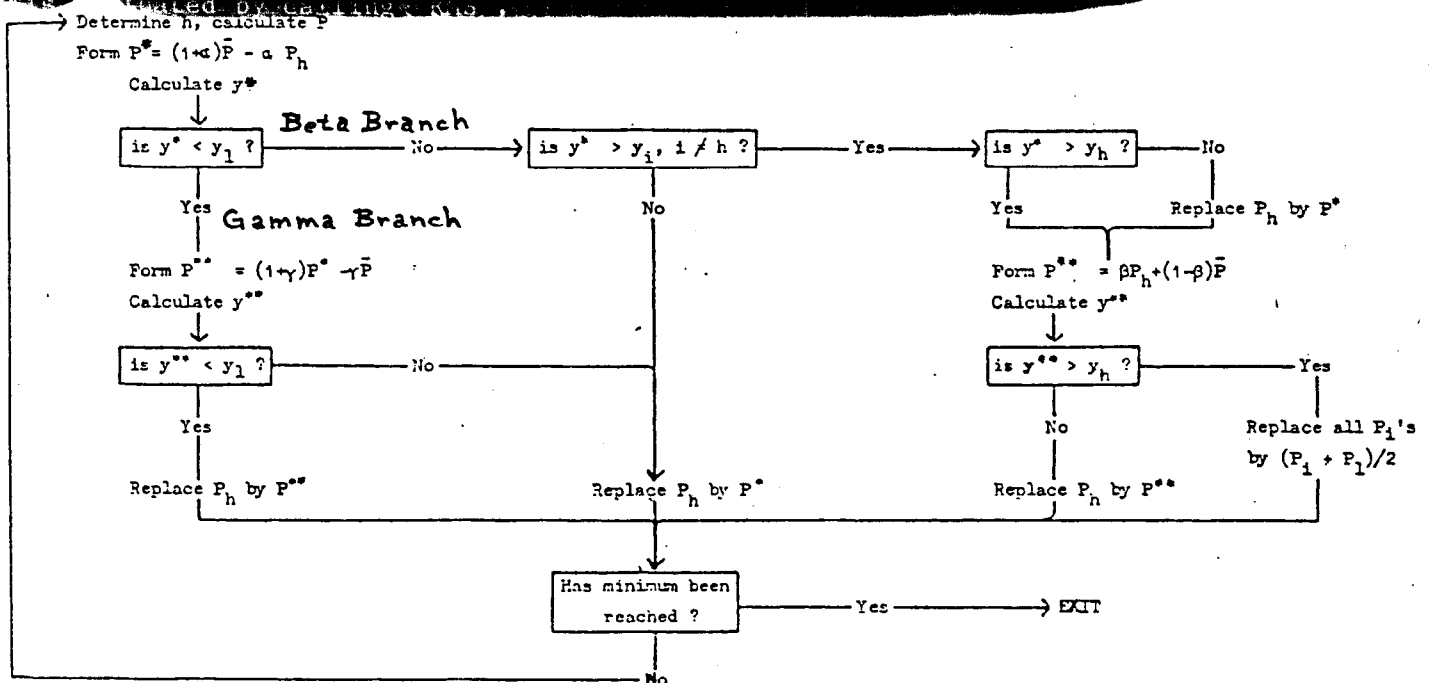
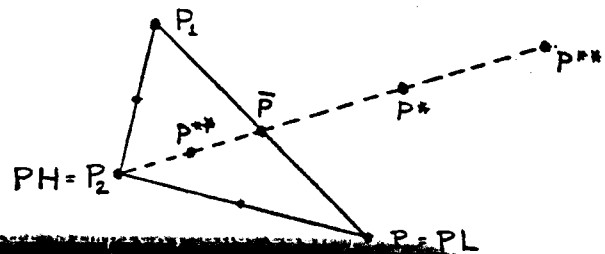


Fig. 2 - Flow Diagram, Main Loop

01333C PROGRAM DESCRIPTION II

Page 7 of 18

Sample Problem (Sketch if Desired)

Fit $F(x)$ to the data given.

$$F(x) = A \exp(-Bx) + C$$

Initial values:

$$A = 7.0$$

$$B = 0.7$$

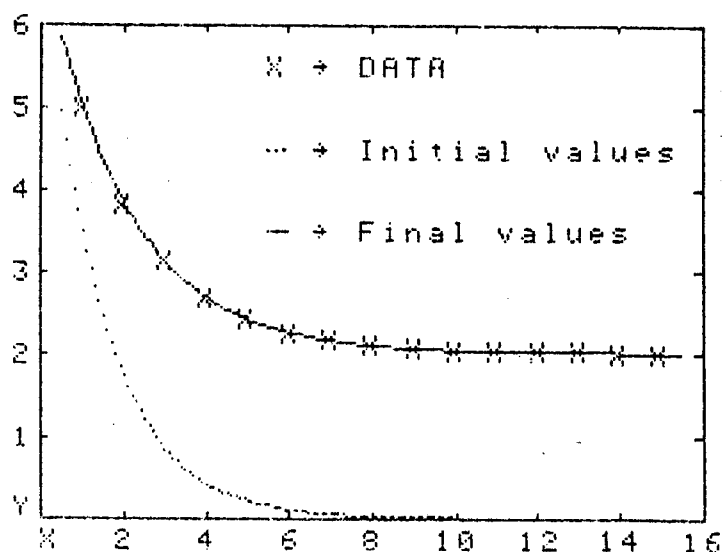
$$C = 0.0$$

Final values:

$$A = 4.91$$

$$B = 0.493$$

$$C = 2.00$$



SAMPLE PROBLEM

Fit the data listed below to the expression $A \exp(-Bx) + C$. This expression is non-linear, and can not be linearized by taking logarithms. The data could have come from an experiment, with an unknown background level. The program was run on a [REDACTED]

X	Y
1	5
2	3.82
3	3.14
4	2.67
5	2.41
6	2.25
7	2.15
8	2.09
9	2.05
10	2.03
11	2.02
12	2.01
13	2.01
14	2.0
15	2.0

Initial values were

$$\text{val1} = 7 \text{ step} = .1 = A$$

$$\text{val2} = .7 \text{ step} = .1 = B$$

$$\text{val3} = 0 \text{ step} = 3. = C$$

Final values were

$$\text{val1} = 4.91$$

$$\text{val2} = .493$$

$$\text{val3} = 2.00$$

Time to run was 55 minutes

It took 113 evaluations.

PROGRAM DESCRIPTION II

Step One Enter function into calculator.

on input x register contains value to evaluate

on output x register contains function value

REG 01 = val1 = A

REG 02 = val2 = B

REG 03 = val3 = C

LBL 'EX

RCL 02

CHS

*

E↑X

RCL 01

+

RTN

Step Two Run program (calculator display is underlined)

display input comments

<u>N?</u>	3 R/S	number of free parameters
<u>NAME?</u>	EX R/S	name of function to fit to
<u>DATA N</u>	15 R/S	number of data points
<u>FRR</u>	.001 R/S	required error (difference in value $v_h - v_l$)
<u>MAX EVAL</u>	100 R/S	maximum tries at fitting data before stopping
<u>X1::0.00</u>	1 R/S	data entry
<u>Y1::0.00</u>	5 R/S	
<u>X2::0.00</u>	2 R/S	
<u>Y2::0.00</u>	3.82 R/S	
<u>X3::0.00</u>	3 R/S	
<u>Y3::0.00</u>	3.14 R/S	
<u>X4::0.00</u>	4 R/S	
<u>Y4::0.00</u>	2.67 R/S	
<u>X5::0.00</u>	5 R/S	
<u>Y5::0.00</u>	2.41 R/S	

PROGRAM DESCRIPTION II

<u>X6::0.00</u>	6 R/S
<u>Y6::0.00</u>	2.25 R/S
<u>X7::0.00</u>	7 R/S
<u>Y7::0.00</u>	2.15 R/S
<u>X8::0.00</u>	8 R/S
<u>Y8::0.00</u>	2.09 R/S
<u>X9::0.00</u>	9 R/S
<u>Y9::0.00</u>	2.05 R/S
<u>X10::0.00</u>	10 R/S
<u>Y10::0.00</u>	2.03 R/S
<u>X11::0.00</u>	11 R/S
<u>Y11::0.00</u>	2.02 R/S
<u>X12::0.00</u>	12 R/S
<u>Y12::0.00</u>	2.01 R/S
<u>X13::0.00</u>	13 R/S
<u>Y13::0.00</u>	2.01 R/S
<u>X14::0.00</u>	14 R/S
<u>Y14::0.00</u>	2.00 R/S
<u>X15::0.00</u>	15 R/S

VAL1  initial guesses for free parameters

STEP .1 R/S

VAL2 .7 R/S

STEP .1 R/S

VAL3 0 R/S

STEP 3 R/S

*** END OF INPUT ***

If data editing is wanted stop input before entering the free parameters and restart the program. This time, the values for the data points are the values entered earlier. If the value is correct R/S will re-enter that value. If a change is needed, enter the new value and then R/S. This is a good way to verify data and doesn't add very much complexity to the program.

PROGRAM DESCRIPTION II

Step Three Improvement of result

After displaying 100 values representing the value of the RMS error at each iteration the program beeps and displays 'DONE'. It should be noted that flag 2 is set indicating that the maximum number of iterations has been reached.

Entering R/S will allow viewing the best point to data.

<u>DONE</u>	R/S	
<u>P0...:02947</u>	R/S	RMS error of fit at this point
<u>P1...:4.90975</u>	R/S	val1 = A
<u>P2...:49163</u>	R/S	val2 = B
<u>P3...:1.99480</u>	R/S	val3 = C
<u>MAX=200</u>		the last R/S forced an improvement
		Since the program had counted out,
		more evaluations were allowed.
		The program is again searching
		for the minimum RMS error.

After 13 more evaluations the program again stops. This time flag 2 is not

~~the results, press R/S.~~ To view the results, press R/S.

<u>DONE</u>	R/S	
<u>P0...:02943</u>	R/S	this has not changed much
<u>P1...:4.91623</u>	R/S	
<u>P2...:4925</u>	R/S	
<u>P3...:1.99484</u>		

At this point if R/S is entered the program will divide the required error by 100 and continue searching. Since it appears that we have a good minimum it is time to stop. The total time to solve the problem was 55 minutes.

Calculator Requirements

This problem required 200 registers to run. There were 50 registers for the simplex, $2 \times 15 = 30$ registers for the data, and 120 registers for the program. For machines without this much memory the routines 'SP', 'LSQ', and 'IS' can be loaded into memory separately from 'SIMP'. Run each routine (in the above order), and then load 'SIMP' into the same memory space. The first few lines of 'SIMP' will need to be modified to remove the calls to the missing routines.

Program Modifications

There are several possible modifications that may improve the program in certain problems. For the sample problem the x data values were consecutive integers and didn't really need to be stored. For other problems a different type of fit may be required, such as a chi squared minimization. In another type of problem the minimum value of an analytic function may be needed. To facilitate changes of these natures I have listed the routines and registers available.

Routines

LSQ	LSQ defines the data storage structure
RMS	RMS uses the data stored by LSQ and calls the user function. It also calculates the sum of the squared errors.

Registers

24	'rms' contains name of function to minimize
25	'user name' contains name of function to fit to
5,6,7	available for counters, ect
9	start of data offset
10	data counter, used to initialize loops
21	required error
22	maximum allowed iterations
0,1,2,3	point evaluated by 'RMS'. 0 is used to return the value.

<u>STEP</u>	<u>INSTRUCTIONS</u>
-------------	---------------------

1	
---	--

	Adjust the number of data registers to allow for storage of the simplex, and the experimental data. See the registers and status section to determine this size.
--	--

2	
---	--

	Enter the program from cards, or by the light wand.
--	---

3	
---	--

	Enter the function to be used in the data fit. This function should get its argument from the x register, and return its value in the x register. The values for the free parameters should be obtained from registers 1, 2, and 3 (see sample problem)
--	---

4	
---	--

	Run the program. It will prompt for all required data (see sample problem).
--	---

5	
---	--

	When the program stops it will display the RMS error, and the free parameters one at a time. At this point the option exists to try to improve the result. This is done by simply continuing the program (see sample problem).
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STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS	STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
1	LBL 'SIMP'			50	RCL 20		
2	XEQ 'SP'		SET POINTERS	51	.5		
3	XEQ 'LSQ'		LOAD	52	ENTER		
			EXPERIMENTAL	53	XEQ 23		P** =
			DATA	54	RCL IND 17		.5*(PBAR+PH)
4	XEQ 'IS'		INITIALIZE	55	RCL 00		
5	LBL 80		SIMPLEX	56	X>Y?		V**>VH?
6	FS? 02		MAIN LOOP	57	GTO 26		SHRINK SIMPLEX
			MAXIMUM #	58	LBL 85		PH=P** AND LOOP
			ITERATIONS?	59	0		
7	XEQ 'FIN'		DISPLAY RESULTS	60	RCL 17		
8	XEQ 20		GET HI,LO	61	XEQ 25		COPY P** TO PH
			POINTS	62	GTO 80		LOOP TO MAIN
9	FS?C 01						LOOP
10	XEQ 30		DISPLAY CURRENT	63	LBL 84		PH=P* AND LOOP
			VALUES	64	XEQ 83		
11	XEQ 21		CALC CURRENT	65	GTO 80		
			ERROR	66	LBL 83		PH=P* AND
12	RCL 21		GET REQUIRED				RETURN
			ERROR	67	RCL 18		POINTER TO P*
13	X>Y?		END CHECK	68	RCL 17		POINTER TO PH
14	XEQ 'FIN'			69	XEQ 25		COPY P* TO PH
15	XEQ 22		FIND PBAR	70	RTN		
16	RCL 17		FIND P*	71	LBL 81		GAMMA BRANCH
17	RCL 20		P*=2PBAR-PH	72	RCL 17		P**=3*PBAR-2*PH
18	-1			73	RCL 20		
19	ENTER			74	-2		
20	2			75	ENTER		
21	XEQ 23		DO CALC.	76	3		
22	0			77	XEQ 23		
23	RCL 18			78	RCL 00		
24	XEQ 25						
25	RCL IND 18			81	GTO 85		PH=P**
26	RCL IND 16			82	GTO 84		PH=P*
27	X>Y?		VL>V*?	83	LBL 08		FORM POINTER
28	GTO 81		GAMMA BRANCH	84	INT		
29	RCL 11		(V* < V1?) I < > H	85	RCL 12		J INIT 1
30	STO 05			86	*		
31	LBL 82			87	RCL 13		J INIT 2
32	RCL 05			88	+		
33	INT			89	RTN		
34	RCL 17			90	LBL 25		COPY POINTX =
35	INT						POINTY
36	X=Y?		I=H?	91	XEQ 08		
37	GTO 79		THEN SKIP	92	STO 05		TO POINTER
38	RCL IND 18		ELSE	93	RDN		
39	RCL IND 05			94	XEQ 08		
40	X>Y?		VI>V*?	95	STO 06		FROM POINTER
41	GTO 84		REPLACE PH BY	96	LBL 99		COPY LOOP
			P* AND LOOP	97	RCL IND 06		
42	LBL 79			98	STO IND 05		
43	ISG 05		CHECK ALL	99	ISG 05		
			POINTS	100	RDN		
44	GTO 82			101	ISG 06		
45	RCL IND 18		BETA BRANCH	102	GTO 99		LOOP BACK
46	RCL IND 17			103	RTN		
47	X>Y?		VH>V*?	104	LBL 23		NEW POINT
48	XEQ 83		PH=P*	105	STO 14		INPUT PARAMS=
49	RCL 17			106	RDN		X=A

□ 67 □ 97 □ 41C

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS	STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
107	STO 15		Y=B	165	STO IND 07	07	
108	RDN		Z=POINT1	166	ISG 07		
109	XEQ 08		T=POINT2	167	GTO 91		
110	STO 05			168	RCL 11		
111	RDN			169	STO 05		
112	XEQ 08			170	LBL 94		PBAR=AVG OF ALL
113	STO 06			171	RCL 20		POINTS EXCEPT
114	RCL 13		ON OUTPUT THE	172	STO 07		PH
115	STO 07		NEW POINT P	173	RCL 17		
116	LBL 98		P=A*P1+B*P2	174	INT		
117	RCL IND 05		WHERE P IS	175	RCL 05		
			STORED	176	INT		
118	RCL 14		IN REG 1,2,3	177	X=Y?		
119	*		AND THE VAL AT	178	GTO 93		
120	RCL IND 06		P IS IN REG 0	179	RCL 12		
121	RCL 15			180	*		
122	*			181	RCL 13		
123	+			182	+		
124	STO IND 07			183	STO 06		
125	ISG 07			184	LBL 92		ADD IN PI
126	RDN			185	RCL IND 06	06	
127	ISG 06			186	ST+ IND 07	07	
128	RDN			187	ISG 07		
129	ISG 05			188	RDN		
130	GTO 98			189	ISG 06		
131	XEQ IND 24		EVALATE P	190	GTO 92		
132	RTN			191	LBL 93		
133	LBL 20		FIND HI,LO	192	ISG 05		
			POINTS	193	GTO 94		DO NEXT POINT
134	RCL 11		FOR I=P1 TO PN	194	RCL 20		
135	STO 05			195	STO 07		
136	STO 16		SET PL=PH=PI	196	RCL 06	06	
137	STO 16			197	LBL 92		
138	ISG 05			198	ST/ IND 07	07	AND DIVIDE BY N
139	LBL 95		COMPARE LOOP	199	ISG 07		
140	RCL IND 05			200	GTO 90		
141	RCL IND 16			201	RTN		
142	X>Y?		VL>VI?	202	LBL 26		SHRINK SIMPLEX
143	XEQ 97		SET PL=PI	203	RCL 11		
144	RDN			204	STO 08		ALL POINTS
145	RCL IND 17			205	LBL 89		ARE AVG OF
146	X<=Y?		VH<=VI?	206	RCL 16		POINT AND PL
147	XEQ 96		SET PH=PI	207	INT		
148	ISG 05			208	RCL 08		
149	GTO 95		LOOP	209	INT		
150	RTN			210	X=Y?		CAN'T SHRINK PL
151	LBL 96		SET PH=PI	211	GTO 88		
152	RCL 05			212	.5		
153	STO 17			213	ENTER		
154	RTN			214	XEQ 23		
155	LBL 97		SET PL=PI	215	0		
156	RCL 05			216	RCL 08		
157	STO 16			217	XEQ 25		
158	RDN			218	LBL 88		
159	RTN			219	ISG 08		
160	LBL 22		CALCULATE PBAR	220	GTO 89		
161	RCL 20			221	GTO 80		GO TO MAIN LOOP
162	STO 07			222	LBL 21		ERROR
163	0						CALCULATION
164	LBL 91		PBAR SET TO 0	223	RCL IND 17		ERROR=VH-VL

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STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS	STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
224	RCL IND 16			283	XEQ IND 25		TO DATA
225	-			284	ISG 07		
226	RTN			285	RCL IND 07		
227	LBL 40		DISPLAY ROUTINE	286	-		
228	FIX 0			287	X^2		
229	ARCL Y			288	ST+ 00		
230	'F: '			289	ISG 07		
231	FIX 5			290	GTO 41		
232	ARCL X			291	RCL 00		
233	RTN			292	SQRT		
234	LBL 'FIN'		DISPLAY FINAL	293	STO 00		
235	BEEP		RESULTS AND	294	ISG 22		
236	'DONE'		THEN ALLOW MORE	295	GTO 03		
237	PROMPT		ITERATIONS	296	SF 02		
238	LBL 30		TO IMPROVE	297	LBL 03		
239	RCL 16		RESULTS	298	CLA		
240	INT			299	RCL 22		DISPLAY VALUE
241	RCL 12			300	RCL 00		WHILE FORMING
242	*			301	XEQ 40		NEXT POINT
243	RCL 13			302	AVIEW		
244	STO 06			303	RTN		
245	+			304	LBL 'SP'		SET POINTERS
246	STO 05			305	.00001		
247	LBL 31			306	STO 14		
248	'P'			307	.001		
249	RCL 06			308	STO 13		
250	INT			309	STO 19		
251	RCL IND 05			310	1		
252	XEQ 40			311	+		
253	PROMPT			312	STO 12		JINIT 1
254	ISG 06			313	26		
255	ENTER						
256							
257	GTO 22			315	*		SET TO SIMPLEX
258	FS90		CHECK TYPE OF END	316	STO 11		
259	GTO 32			317	RCL 04		
260	100		IMPROVE BY	318	'N?'		GET NUMBER OF VARIABLES
261	ST/ 21		TIGHTNING	319	PROMPT		
262	'R.E. ='		REQUIRED	320	STO 04		
263	ARCL 21		ERROR	321	ST* 13		JINIT 2
264	AVIEW			322	1		
265	RTN			323	+		
266	LBL 32		IMPROVE BY	324	STO 15		
267	RCL 22		ALLOWING MORE	325	ST* 14		
268	INT		ITERATIONS	326	X^2		
269	RCL 19			327	STO 05		
270	*			328	1		
271	ST+ 22			329	-		
272	'MAX ='			330	RCL 19		
273	ARCL 22			331	*		
274	AVIEW			332	ST+ 11		
275	RTN			333	RCL 14		
276	LBL 'RMS'		FUNCTION	334	ST+ 11		
277	RCL 10		MINIMIZED	335	RCL 05		
278	STO 07		BY SIMPLEX	336	RCL 23		
279	0			337	+		
280	STO 00			338	STO 20		
281	LBL 41		FIND RMS ERROR	339	STO 18		
282	RCL IND 07		OF FIT	340	STO 09		
				341	RCL 15		

□ 67 □ 97 □ 41C

STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS	STEP/ LINE	KEY ENTRY	KEY CODE (67/97 only)	COMMENTS
342	ST+ 20			398	'FCN'		EVALUATION TO
343	ST+ 09			399	PROMPT		'FCN'
344	ST+ 09		DATA OFFSET	400	ASTO 25		
345	RCL 12			401	ROFF		
346	ST* 18		P* POINTER	402	'RMS'		
347	ST* 20		PBAR POINTER	403	ASTO 24		
348	RCL 13			404	'DATA N'		NUM. OF DATA
349	ST+ 18			405	PROMPT		POINTS
350	ST+ 20			406	STO 00		
351	RTN			407	.002		
352	LBL 'IS'		FORM INITIAL	408	*		
			SIMPLEX	409	STO 10		DATA INIT
353	RCL 13			410	RCL 09		
354	1			411	RCL 12		
355	+			412	*		
356	STO 06			413	ST+ 10		
357	LBL 61		INITIAL SIMP.	414	'ERR'		REQUIRED ERROR
358	RCL 06		IS FORMED	415	PROMPT		
359	INT		FROM INITIAL	416	STO 21		
360	RCL 11		VALUES AND	417	RCL 19		
361	+		STEP SIZES	418	ST- 10		
362	STO 05			419	ST* 00		
363	RCL 06		ONE SS. IS	420	'MAX EVAL'		MAX ALLOWED
364	RCL IND 05		ADDED TO IT'S	421	PROMPT		ITERATIONS OF
365	'VAL'		VALUE PER POINT	422	*		MAIN LOOP
366	XEQ 40		EXCEPT P1	423	STO 22		
367	PROMPT		WHICH HAS ONLY	424	1.1		
368	LBL 62		VALUES.	425	ST+ 00		
369	STO IND 05			426	RCL 10		
370	ISG 05			427	STO 05		
371	GTO 62			428	LBL 51		
372	RCL 15			429	'X'		GET X DATA
373	LBL 63			430	STO 05		
374	*			431	RCL IND 05		
375	RCL 06			432	XEQ 40		SHOW PRESENT
376	+			433	PROMPT		VALUE
377	RCL 06			434	STO IND 05		
378	+			435	ISG 05		
379	'STEP'		GET STEP SIZE I	436	'Y'		SAME FOR Y
380	PROMPT			437	RCL 00		DATA
381	ST+ IND Y		ADD TO PROPER	438	RCL IND 05		
382	ISG 06		POINT IN	439	XEQ 40		
			SIMPLEX	440	PROMPT		
383	GTO 61			441	STO IND 05		
384	RCL 11			442	ISG 00		
385	STO 00			443	ISG 05		
386	LBL 63		EVALUATE INTIAL	444	GTO 51		
387	RCL 08		SIMPLEX TO GET	445	RTN		
388	0		VALUES VI	446	END		
389	XEQ 25						
390	XEQ IND 24						
391	RCL 00						
392	STO IND 08						
393	ISG 08						
394	GTO 63						
395	RTN						
396	LBL 'LSQ'		LOAD				
			EXPERIMENTAL				
			DATA				
397	ADN		FOR LEAST				
			SQUARE				

REGISTERS, STATUS, FLAGS, ASSIGNMENTS

PROGRAM STORAGE

The program uses 120 registers when packed, and 123 registers when loaded by the light wand. This can be reduced by dividing the program into two parts. The first part initializes the data structure, and is then removed. Then the main program is loaded to find the fit. Additional program space is needed to store the theoretical function used in the least squares data fit.

DATA STORAGE

01

FLAG USED flag 02

set indicates maximum number of iterations
has been reached
clear indicates required error has been reached
flag is valid only at program end.

REGISTER	USE	STORAGE		
		ONE DIM	TWO DIM	THREE DIM
0				
2	param 2	temporary point		
3	param 3			
4	N	number of free params.		
5	I	temporary counters		
6	J			
7	K			
8	L			
9	Data offset	34	41	50
10	Data init			
11	Iinit	26.029	26.034	26.041
12	Jinit1	1.001	1.001	1.001
13	Jinit2	.001	.002	.003
14	temp A			
15	temp B			
16	PL pointer to 'best' point			
17	PH pointer to 'worst' point			
18	P* pointer	30.031	35.037	42.045
19	.001	.001	.001	.001
20	PBAR pointer	32.033	38.040	46.049
21	required error			
22	maximum iterations			
23	simplex offset	26	26	26
24	type of fit	RMS	RMS	RMS
25	function name			

REGISTERS, STATUS, FLAGS, ASSIGNMENTS

REGISTER USE

STORAGE

ONE DIM

TWO DIM

THREE DIM

SIMPLEX STORAGE

26	V0	V0	V0
	P0	P01	P01
	V1	P02	P02
	P1	V1	P03
	V*	P11	V1
	P*	P12	P11
	VBAR	V2	P12
33	PBAR	P21	P13
		P22	V2
		V*	P21
		P*1	P22
		P*2	P23
		VBAR	V3
		PBAR1	P31
40		PBAR2	P32
			P33
			V*
			P*1
			P*2
			VBAR
			PBAR1
			PBAR2
49			PBAR3

DATA POINTS

34 OR 41 OR 50

.	X1	X1	X1
.	Y1	Y1	Y1
.	X2	X2	X2
.	Y2	Y2	Y2
.	.	.	.
.	.	.	.
.	.	.	.
.	XM	XM	XM
.	YM	YM	YM

ROW 1 (1 : 3)



ROW 2 (3 : 7)



ROW 3 (7 : 11)



ROW 4 (11 : 15)



ROW 5 (16 : 23)



ROW 6 (23 : 29)



ROW 7 (30 : 38)



ROW 8 (38 : 44)



ROW 9 (44 : 50)



ROW 10 (51 : 57)



ROW 11 (58 : 63)



ROW 12 (64 : 69)



ROW 13 (69 : 76)



ROW 14 (77 : 82)



ROW 15 (83 : 92)



ROW 16 (93 : 99)



ROW 17 (100 : 108)



ROW 18 (109 : 116)



ROW 19 (117 : 125)	
ROW 20 (126 : 133)	
ROW 21 (133 : 140)	
ROW 22 (141 : 147)	
ROW 23 (148 : 155)	
ROW 24 (155 : 164)	
ROW 25 (164 : 171)	
ROW 26 (171 : 180)	
ROW 27 (181 : 189)	
ROW 28 (189 : 194)	
ROW 29 (195 : 202)	
ROW 30 (202 : 211)	
ROW 31 (211 : 218)	
ROW 32 (218 : 223)	
ROW 33 (224 : 230)	
ROW 34 (230 : 234)	
ROW 35 (235 : 241)	
ROW 36 (242 : 251)	

ROW 37 (252 : 258)



ROW 38 (258 : 262)



ROW 39 (262 : 269)



ROW 40 (270 : 276)



ROW 41 (276 : 282)



ROW 42 (282 : 289)



ROW 43 (290 : 297)



ROW 44 (298 : 304)



ROW 45 (304 : 307)



ROW 46 (308 : 317)



ROW 47 (318 : 326)



ROW 48 (327 : 336)



ROW 49 (336 : 344)



ROW 50 (344 : 352)



ROW 51 (352 : 359)



ROW 52 (360 : 366)



ROW 53 (367 : 374)



ROW 54 (375 : 381)



ROW 55 (382 : 389)



ROW 56 (389 : 396)



ROW 57 (396 : 400)



ROW 58 (400 : 404)



ROW 59 (404 : 412)



ROW 60 (413 : 418)



ROW 61 (419 : 422)



ROW 62 (423 : 429)



ROW 63 (430 : 436)



ROW 64 (437 : 443)



ROW 65 (444 : 446)

