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A NOTE ON LEAST-SQUARES FITTING OF ATOMIC-BEAM RESONANCE CURVES

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March 26, 1957

ABSTRACT

A routine is described for fitting bell-shaped curves to data points by use of the IBM 650 computer.

A NOTE ON LEAST-SQUARES FITTING OF ATOMIC-BEAM RESONANCE CURVES

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An objective criterion is desirable for assigning a "best" resonance frequency to the data for counting rate vs frequency obtained from radioactive atomic-beam experiments.

Under idealized conditions – which are not met in practice – the line shape theoretically has the form $(1 + x^2)^{-1}$, where x is the departure from resonance suitably normalized. This suggests the fitting of a "best" curve of this form by a procedure which, if possible, weights the points near the maximum of the curve more heavily than the tails and thus minimizes the effect of departures from the theoretical shape. Reducing the weight assigned to the tails of the curve also minimizes the effect of uncertainties in the background to be subtracted from the counting rates.

A curve of this sort can be obtained by taking the reciprocals of the counting rates, assigning uncertainties in the obvious way, $\boxed{\sigma(1/y) = \sigma(y)/y^2}$, and fitting a weighted least-squares parabola by the usual formulas.

The coefficients of the parabola $cx^2 + bx + a$ are the solution of

$$a \Sigma y^4/\sigma^2 + b \Sigma xy^4/\sigma^2 + c \Sigma x^2y^4/\sigma^2 = \Sigma y^3/\sigma^2,$$

$$a \Sigma xy^4/\sigma^2 + b \Sigma x^2y^4/\sigma^2 + c \Sigma x^3y^4/\sigma^2 = \Sigma xy^3/\sigma^2, \qquad (1)$$

$$a \Sigma x^2y^4/\sigma^2 + b \Sigma x^3y^4/\sigma^2 + c \Sigma x^4y^4/\sigma^2 = \Sigma x^2y^3/\sigma^2$$

($y \pm \sigma$ is the counting rate at frequency x),

which yield $a = A/\Delta$, etc., in the usual solution by determinants.

Then the parameters of the bell-shaped curve are given by:

$$\text{position:} \quad x_{max} = -B/2C ,$$

$$\text{half width at half max:} \quad w = \left(\frac{A}{C} - x_{max}^2\right)^{1/2} ,$$

$$\text{height:} \quad y_{max} = \Delta/cw^2 .$$

We also wish to know the uncertainty of x_{max} in terms of the statistical uncertainties of the input data. In terms of the reciprocal data points $z \pm \eta = \frac{1}{y} \pm \frac{\sigma}{y^2}$, Eqs. (1) read

$$a \Sigma 1/\eta^2 + b \Sigma x/\eta^2 + c \Sigma x^2/\eta^2 = \Sigma z/\eta^2 ,$$

$$a \Sigma x/\eta^2 + b \Sigma x^2/\eta^2 + c \Sigma x^3/\eta^2 = \Sigma zx/\eta^2 ,$$

$$a \Sigma x^2/\eta^2 + b \Sigma x^3/\eta^2 + c \Sigma x^4/\eta^2 = \Sigma zx^2/\eta^2 .$$

The standard deviation of x_{max} is

$$\sigma^2(x) = \Sigma \eta^2 \left[\frac{\partial}{\partial z} \left(\frac{B}{2C}\right)\right]^2 .$$

By straightforward manipulation this can be reduced to

$$\sigma^2(x) = \frac{\Delta}{4C^4} \Big[C^2(\text{minor of bb element of } \Delta) - 2BC(\text{minor of bc element of } \Delta) + B^2(\text{minor of cc element of } \Delta)\Big] .$$

A routine has been written for the IBM 650 computer which computes x_{max}, w^2, y_{max}, and $\sigma^2(x)$ from suitably normalized input data. Details of its operation are attached.

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

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Routine for $1/(1 + x^2)$ on IBM 650 Computer

1. Locations:
   a. routine lies in range 000-0399;
   b. routine starts at 0001;
   c. 0400-0459 used for input data;
   d. 0700-0716 used for temporary storage and output data;
   e. the locations in (d) could be moved into the 000-0399 range without much trouble, if drum space gets short.

2. Card deck:
   a. Memory clear;
   b. Long load and punch routine;
   c. This routine;
   d. Data deck.

3. Data deck:
   a. Location card: 00000 9 0400 (-) in the first field (minus in col. 10);
   b. Data cards: 00000 n xxxx (-) in first field (n = no. of words; xxxx arbitrary) then data in order $x_1 y_1 \sigma_1 x_2 y_2 \sigma_2$ - - - - $x_n y_n \sigma_n$(prob. no.) -- i.e. problem no. in place of $x_n + 1$ on last card only.
   c. Transfer card: 00000 0 0001 in first field;
   d. Repeat (a), (b), (c) for each problem.

4. Input data form:
   a. x in form 000000x.xxx mc $0 \leqslant x \leqslant 4$. Origin should be chosen to make peak come near x = 2; $1 \leqslant x_{max} \leqslant 3$ should be o.k.
   b. y in form 000 000 00 yy.cpm $30 \leqslant y_{max} \leqslant 100$ (actual requirement is not quite this strict).
   c. σ in form 000 000 00$\sigma\sigma$.cpm $10 \leqslant \sigma \leqslant 100$ (actual requirement is not quite this strict).
   d. y and σ will usually need to be scaled to fit the ranges above. Note the scale factors used.
   e. Problem number is simply copied to output, but 3 rt.-hand digits only are pertinent to another routine.

5. Output card form:
   a. 1st word, 00000 7 0700.
   b. 2nd word, x_{max} = x.xxx xxx xxx mc.
   c. 3rd word, w^2 = w.www wwwwww mc^2. w = the half width at half max.
   d. 4th word, y_{max} = yyy.yyyyyyy cpm.
   e. 5th word, $\sigma^2 = \sigma\sigma.\sigma\sigma\sigma\sigma\sigma\sigma\sigma\sigma\sigma$ mc^2; σ = std. dev. of x_{max} -- to get actual value it must be multiplied by the scale factor for y and divided by the scale factor for σ.
   f. 6th word, problem number.

6. If trouble develops, transfer to 0356. This will punch partial results and go on to next problem.

7. Rigid requirements on input data are $\sigma < 100$, $y^3/\sigma^2 < 10^6$ and $y^3 < 10^8$. Trouble may also occur if all the y^3/σ^2's are too small.

The actual program follows.

IBM 650 PROGRAM SHEET

PROBLEM: $(1+x^2)^{-1}$

INSTR NO.	LOCATION OF INSTRUCTION	OPERATION ABBRV.	OPERATION CODE	ADDRESS DATA	ADDRESS INSTRUCTION	REMARKS
	0001	RAL	65	0250	8002	
	[8002	STU	21	0714	0167]	
	0167	SL	16	0005	0010	
	0010	AU	10	8002	0019	clear 700 - 714
	0019	SU	11	0172	0027	
	0027	BRNZU	44	0081	0182	
	0081	RAL	65	8002	8002	
	0250		21	0714	0167	
	0005		00	0001	0000	constants
	0172		21	0699	0167	
	0182	RAU	60	0185	0026	
	0026	STU	21	0013	0066	
	0066	AU	10	0069	0024	set ~~[illegible]~~ data locations
	0024	STU	21	0015	0369	
	0369	AU	10	0069	0074	
	0074	STU	21	0017	0013	
	0185		60	0400	0014	constants
	0069		00	0001	0002	
	[0013	RAU	60	0400	0014]	
	0014	STD	24	0067	0015	
	[0015	RAU	60	0401	0016]	
	0016	STD	24	0169	~~[illegible]~~	0017
	[0017	RAU	60	0402	0018]	
	0018	BRNZU	44	0123	0275	
	0123	MULT	19	8003	0031	
	0031	SLT	35	0006	0098	
	0098	STL	20	0053	0056	
	0056	RAU	60	0169	0325	
	0325	MULT	19	8003	0333	
	0333	RAU	60	8002	0292	
	0292	MULT	19	0169	0075	
	0075	SLT	35	0002	0184	
	0184	RAU	60	8002	0343	
	0343	DIVRU	64	0053	0058	
	0058	SRD	31	0002	0117	
	0117	STL	20	0053	0106	
	0106	LD	69	0359	0062	
	0062	STD	24	0003	0156	
	0156	LD	69	0321	0124	
	0124	STD	24	0071	0174	
	0174	LD	69	0183	0036	
	0036	STD	24	0076	0079	
	0079	STL	20	0084	0050	
	0050	AU	10	0003	8003	
	[8003	AL	15	0706	0039]	
	0039	AU	10	0042	8003	

IBM 650 PROGRAM SHEET

PROBLEM: _____

INSTR NO.	LOCATION OF INSTRUCTION	OPERATION ABBRV.	OPERATION CODE	ADDRESS DATA	ADDRESS INSTRUCTION	REMARKS
	[8003	STL	20	0706	[illegible]	0040]
	[illegible]					
	0040	SU	11	0043	0048	
	0048	STU	21	0003	0118	
	0118	SU	11	0071	0076	
	[0076	BRNZU	44	0330	0238]	accumulate
	0330	RAU	60	0084	0289	
	0289	MULT	19	0067	0272	$\Sigma x^p y^8/\sigma^2$
	0272	SRD	31	0003	0079	
	0238	RAU	60	0053	0108	
	0108	MULT	19	0169	0125	
	0125	SRD	31	0002	0234	
	0234	LD	69	0071	0224	
	0224	STD	24	0071	0274	
	0274	LD	69	0233	0036	
	0359		15	0706	0039	
	0321		15	0709	0039	
	0183		44	0330	0238	
	0042		05	0000	0001	constants
	0043		04	9999	0001	
	0371		15	0714	0039	
	0233		44	0330	0131	
	0131	RAU.	60	0013	0068	return to next data point
	0068	AU	10	0021	0026	
	0021		00	0003	0000	constant
	0275	LD	69	0067	0051	store problem # for punching
	0051	STD	24	0704	0007	
	0007	RAU	60	0708	0365	
	0365	LD	69	8002	0204	
	0204	SCT	36	0000	0155	
	0155	STIA	23	0311	0278	
	0278	RAU	60	0113	0328	
	0328	LD	69	8002	0393	
	0393	STIA	23	0337	0342	
	0342	RAL	65	0311	0378	set shift commands and shift.
	0378	SL	16	0329	0392	
	0392	BRMIN	46	0295	0317	
	0295	AL	15	8001	0265	
	0317	RAL	65	8001	0265	
	0265	SLT	35	0004	0078	
	0078	LD	69	0324	[illegible]	0319
0319	[illegible]	STDA	22	0324	0227	
	0227	LD	69	0277	0121	
	0121	STDA	22	0277	0180	

IBM 650 PROGRAM SHEET

PROBLEM: _____

INSTR NO.	LOCATION OF INSTRUCTION	OPERATION ABBRV.	OPERATION CODE	ADDRESS DATA	ADDRESS INSTRUCTION	REMARKS
	0180	LD	69	0196	0091	
	0091	STDA	22	0196	0049	
	0049	LD	69	0248	0243	
	0243	STDA	22	0248	0101	
	0101	RAU	60	0254	0374	
	0374	STU	21	0229	0126	
	0126	SU	11	0029	0034	
	~~0034~~	~~BRNZU~~	~~44~~	~~0324~~	~~0135~~	
	[0324	SLT	35	—	0189]	
	0034	STU	21	0189	0229	
	[0229	RAU	60	0706	0380]	
	0380	BRNZU	44	0324	0135	
	[0324	SLT	35	—	0189]	
	[0189	STU	21	0706	0209]	
	0209	RAU	60	0229	0032	
	0032	AU	10	0005	0110	
	0110	STU	21	0229	0126	
	0324		35	0000	0189	
	0277		35	0000	0252	
	0196		35	0000	0171	constants
	0248		35	0000	0073	
	0254		60	0706	0380	
	0029		39	0000	0171	
	0135	LD	69	0710	0113	
	0113	STD	24	0166	0219	
	0219	LD	69	0711	0127	
	0127	STD	24	0080	0033	
	0033	LD	69	0280	0134	
	0134	STD	24	0087	0090	
	0090	RAU	60	0080	0235	compute determinant
	0235	MULT	19	0708	0163	
	0163	STU	21	0065	0168	C and set shift
	0168	STL	20	0023	0176	
	0176	RSU	61	0712	0373	
	0373	MULT	19	0707	0012	
	0012	AU	10	0065	0020	
	0020	AL	15	0023	0142	
	0142	STU	21	0065	0218	
	0218	RAU	60	8002	0128	
	0128	MULT	19	0709	0129	
	0129	STU	21	0023	0226	
	0226	RAU	60	0065	0220	
	0220	MULT	19	0709	0329	
	0329	AL	15	0023	0192	
	0192	STU	21	0045	0148	
	0148	STL	20	0103	0206	
	0206	RAU	60	0712	0375	
	0375	MULT	19	0706	0061	

IBM 650 PROGRAM SHEET

PROBLEM: _____

INSTR NO.	LOCATION OF INSTRUCTION	OPERATION ABBRV.	OPERATION CODE	ADDRESS DATA	ADDRESS INSTRUCTION		REMARKS
	0061	STU	21	0065	0268		
	0268	STL	20	0023	0276		
	0276	RSU	61	0166	0372		
	0372	MULT	19	0108	0063		
	0063	AU	10	0065	0070		
	0070	AL	15	0023	0242		
	0242	STU	21	0065	0318		
	0318	RAU	60	0002	0178		
	0178	MULT	19	0710	0179		
	0179	STU	21	0023	0326		
	0326	RAU	60	0065	0270		
	0270	MULT	19	0710	0379		
	0379	AL	15	0023	0092		
	0092	AU	10	0045	0100		
	0100	AL	15	0103	0160		
	0160	STU	21	0045	0198		
	0198	STL	20	0103	0256		
	0256	RAU	60	0166	0173		
	0173	MULT	19	0707	0112		
	0112	STU	21	0065	0368		
	0368	STL	20	0023	0376		
	0376	RSU	61	0080	0285		
	0285	MULT	19	0106	0011		
	0011	AU	10	0065	0120		
	0120	AL	15	0023	0143		
	0143	STU	21	0065	0269		
	0269	RAU	60	0002	0228		
	0228	MULT	19	0711	0130		
	0130	STU	21	0023	0177		
	0177	RAU	60	0065	0320		
	0320	MULT	19	0711	0231		
	0231	AL	15	0023	0013		
	0013	AU	10	0045	0150		
	0150	AL	15	0103	0087		
	[0087	SLT	35	0005	0145]		
	0145	SCT	36	0000	0110		
	0110	LD	69	0037	0188		
	0188	STIA	23	0037	0190		
	0190	SRT	30	0001	0240		
	0240	STU	21	0095	0298		
	0298	RAL	65	0037	0293		
	0293	SLT	35	0004	0207		
	0207	LD	69	0151	0246		
	0246	STDA	22	0151	0054		
	0054	LD	69	0104	0011		
	0011	STDA	22	0104	0057		
	0057	LD	69	0211	0336		
	0336	STDA	22	0211	0214		
	0214	LD	69	0011	0239		
	0239	STDA	22	0011	0017		

IBM 650 PROGRAM SHEET

PROBLEM: _____

INSTR NO.	LOCATION OF INSTRUCTION	OPERATION ABBRV.	OPERATION CODE	ADDRESS DATA	ADDRESS INSTRUCTION	REMARKS
	0280		35	0005	0145	
	0037		00	0000	0000	
	0151		35	0000	0300	constants
	0104		35	0000	0052	
	0211		35	0000	0157	
	0044		35	0000	0137	
	0097	LD	69	0344	0047	
	0047	STD	24	0087	0153	
	0153	LD	69	0706	0059	
	0059	STD	24	0710	0213	
	0213	LD	69	0707	0111	
	0111	STD	24	0080	0083	compute determinant B
	0083	LD	69	0708	0161	
	0161	STD	24	0707	0210	
	0210	LD	69	0711	0088	
	0088	STD	24	0706	0109	
	0109	LD	69	0713	0138	
	0138	STD	24	0708	0090	
	[0087	SLT	35	0004	0151]	
	[0151	SLT	35	—	0300]	
	0300	STU	21	0205	0008	
	0344	[illegible]	35	0004	0151	constant
	0008	LD	69	0394	0147	
	0147	STD	24	0087	0290	
	0290	LD	69	0709	0089	
	0089	STD	24	0713	0216	
	0216	LD	69	0710	0139	
	0139	STD	24	0709	0162	
	0162	LD	69	0080	0193	
	0193	STD	24	0710	0263	compute determinant [illegible] A
	0263	LD	69	0707	0399	
	0399	STD	24	0711	0164	
	0164	LD	69	0706	0159	
	0159	STD	24	0080	0133	
	0133	LD	69	0712	0115	
	0115	STD	24	0707	0092	
	[0087	SLT	35	0004	0104]	
	[0104	SLT	35	—	0052]	
	0052	STU	21	0107	0310	
	0394		35	0004	0104	constant

IBM 650 PROGRAM SHEET

PROBLEM: _____

INSTR NO.	LOCATION OF INSTRUCTION	OPERATION ABBRV.	OPERATION CODE	ADDRESS DATA	ADDRESS INSTRUCTION	REMARKS
	0310	LD	69	0257	0260	
	0260	STD	24	0257	0140	
	0140	LD	69	0113	0266	
	0266	STD	24	0709	0212	compute determinant Δ
	0212	LD	69	0166	0056	
	0056	STD	24	0710	0313	
	0313	LD	69	0000	0165	
	0165	STD	24	0711	0010	
	[0087	SLT	35	0004	0211]	
	[0211	SLT	35	—	0157	
	0157	STU	21	0312	0215	
	0257		35	0004	0211	constant
	0215	RSU	61	0205	0360	
	0360	SRT 30 ~~35~~		0001	0267	
	~~0267~~	~~DIVRU~~	~~64~~	~~0095~~	~~0217~~	compute x_{max}
	~~0217~~	~~STL~~	~~20~~	~~0025~~	~~0028~~	
	~~0028~~	~~R~~				
	0267	DIVRU	64	0095	0350	
	0350	DIVRU	64	0022	0363	
	0363	STL	20	0700	0203	
	0022		00	0000	0002	constant
	0203	RAU	60	0107	0315	
	0315	SRT 30 ~~35~~		0001	0322	
	0322	DIVRU	64	0095	0217	
	0217	STL	20	0025	~~0030~~ 0028	compute w^2
	0028	RSU	60	0700	0305	
	0305	MULT	19	8001	0221	
	0221	SLT	35	0001	0072	
	0072	AU	10	0025	0030	
	0030	STU	21	0701	0154	
	0154	RAU	60	0312	0175	
	0175	SRT	30	0002	0284	
	0284	DIVRU	64	0095	0327	
	0327	STL	20	0082	0085	compute y_{max}
	0085	RAU	60	8002	0245	
	0245	DIVRU	65	0701	0279	
	0279	STL	20	0702	0255	
	0255	RAU	60	0709	0316	
	0316	MULT	19	0711	0132	
	0132	STU	21	0041	0094	
	0094	STL	20	0149	~~0099~~ 0102	
	0102	RSU	61	0710	0366	
	0366	MULT	19	8001	0038	

IBM 650 PROGRAM SHEET

PROBLEM: _____

INSTR NO.	LOCATION OF INSTRUCTION	OPERATION ABBRV.	OPERATION CODE	ADDRESS DATA	ADDRESS INSTRUCTION	REMARKS
	0038	AU	10	0041	0046	
	0046	AL	15	0149	0277	
	[0277	SLT	35	—	0252]	
	0252	SLT	35	0001	0309	
	0309	RAU	60	8003	0370	
	0370	MULT	19	0700	0144	
	0144	STU	21	0009	0362	
	0362	RAU	60	0710	0367	compute σ_x^2.
	0367	MULT	19	0711	0348	
	0348	STU	21	0041	0144	
	0144	STL	20	0149	0152	
	0152	RSU	61	0709	0223	
	0223	MULT	19	0712	0002	
	0002	AU	10	0041	0096	
	0096	AL	15	0149	0196	
	[0196	SLT	35	—	0171]	
	~~0171~~	~~RAU~~				
	0171	RAU	60	8003	0006	
	0006	AU	10	0009	0064	
	0064	SLT	35	0001	0271	
	0271	MULT	19	0700	0259	
	0259	STU	21	0009	0264	
	0264	RAU	60	0709	0273	
	0273	MULT	19	0708	0314	
	0314	STU	21	0041	0244	
	0244	STL	20	0149	0202	
	0202	RSU	61	0711	0323	
	0323	MULT	19	8001	0116	
	0116	AU	10	0041	0146	
	0146	AL	15	0149	0248	
	[0248	SLT	35	—	0073]	
	0073	RAU	60	8003	0282	
	0282	MULT	19	0241	0122	
	0122	AU	10	0009	0114	
	0114	DIVRU	64	0095	0201	
	0201	RAU	60	8002	0377	
	0377	RAU	60	8003	0136	
	0136	MULT	19	0082	0044	
	[0044	SLT	35	—	0137]	
	0137	STU	21	0703	0356	
	0241		25	0000	0000	constant
	0356	RAL	65	0004	8002	
	[8002	STU	21	0459	0262]	
	0262	SL	16	0005	0060	clear data space
	0060	AU	10	8002	0119	
	0119	SU	11	0222	0077	
	0077	BRNZU	44	0181	0391	
	0181	RAL	65	8002	8002	

IBM 650 PROGRAM SHEET

PROBLEM: _____

INSTR NO.	LOCATION OF INSTRUCTION	OPERATION ABBRV.	OPERATION CODE	ADDRESS DATA	ADDRESS INSTRUCTION	REMARKS
	0004		21	0459	0262	constants
	0222		21	0349	0262	
	0391	RAL	65	0704	0398	
	0398	STU	21	0706	0232	
	0232	RAL	65	0035	0340	set entry and exit for punch routine
	0340	LD	69	1902	0055	
	0055	STIA	23	1902	0105	
	0105	RAL	65	0158	1971	
	0035		00	0000	1996	constants
	0158		07	0700	0706	