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## AN ABBREVIATION OF THE METHOD OF LEAST SQUARES

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Many physical and chemical data can be summarized by equations of the type

$$y = a + bx + cx^2 + gx^3$$

but the labor of accurate reduction by the method of least squares is too frequently discouraging or even prohibitive.

In the special case in which the successive values of  $x$  are in arithmetic progression, the calculation of the parameters of the power series can be much abbreviated. If an arbitrary origin is set in the middle of the range of observations, then for every positive value of  $x$  there will be a corresponding negative value of equal absolute magnitude and the sums of the odd powers of  $x$  will all be zero. The equation given above would then be altered to

$$y = A + BX + CX^2 + GX^3$$

in which the capital letters indicate that the equation has been referred to the arbitrary origin and  $X = x - h$ .

Baily (1) has shown that further abbreviation of the calculations can be made by extracting certain constant values which recur in the solution of the normal equations, such as those shown below for a third-order power series:

$$A = \frac{\sum y \sum X^4 - \sum X^2 y \sum X^2}{\sum X^4 \sum X^0 - (\sum X^2)^2}$$

$$B = \frac{\sum X y \sum X^6 - \sum X^3 y \sum X^4}{\sum X^6 \sum X^2 - (\sum X^4)^2}$$

$$C = \frac{\Sigma X^2 y \Sigma X^0 - \Sigma y \Sigma X^2}{\Sigma X^4 \Sigma X^0 - (\Sigma X^2)^2}$$

$$G = \frac{\Sigma X^3 y \Sigma X^2 - \Sigma X y \Sigma X^4}{\Sigma X^6 \Sigma X^2 - (\Sigma X^4)^2}$$

In these formulae the factors in  $y$  must be derived from the observations, but those involving  $X$  alone, including the denominators, are independent of the data. Baily (1) has tabulated the functions in  $X$ .

Use of the tables of Baily requires the determination of a quotient of the difference of two products. We have found that the calculation can be reduced to the difference of two products by the following consideration:

$$A = \frac{\Sigma y \Sigma X^4 - \Sigma X^2 y \Sigma X^2}{\Sigma X^4 \Sigma X^0 - (\Sigma X^2)^2}$$

$$= \frac{\Sigma y \Sigma X^4}{\Sigma X^4 \Sigma X^0 - (\Sigma X^2)^2} - \frac{\Sigma X^2 y \Sigma X^2}{\Sigma X^4 \Sigma X^0 - (\Sigma X^2)^2}$$

$$= k_3 \Sigma y - k_4 \Sigma X^2 y$$

in which

$$k_3 = \frac{\Sigma X^4}{\Sigma X^4 \Sigma X^0 - (\Sigma X^2)^2}$$

and

$$k_4 = \frac{\Sigma X^2}{\Sigma X^4 \Sigma X^0 - (\Sigma X^2)^2}$$

Similarly, the values of such functions in  $X$  necessary for the derivation of equations of order lower or higher than the third can be obtained. We have calculated the values of  $k_n$  necessary for the reduction of data to first-, second-, or third-degree equations through those required for fifty-one observations, as given in tables 1 and 2.

In table 3 are shown the products and differences of products used in the derivation of equations from data. The factors  $\Sigma y$ ,  $\Sigma X y$ ,  $\Sigma X^2 y$ , and  $\Sigma X^3 y$ , as needed for the degree of the equation chosen, are calculated from the data arranged with the midpoint as the origin. The factors  $k_1$  to  $k_5$ , inclusive, are taken from table 1 if the number of observations is odd; from table 2, if even.

If the number of observations is even, the midpoint of the data is taken halfway between the two middle items, and half an interval is used as the unit.

Equations derived by use of tables 3 and 1 or 2 generally should be transformed with respect to the independent variable to either the point

TABLE I  
Value of  $k_n$ . Odd number of observations

$N$	$k_1$	$k_2$	$k_3$	$k_4$	$k_5$	$k_6$	$k_7$	$k_8$	$k_9$	$k_{10}$
3	3333 3333 (8)	5000 0000 (8)	1000 0000 (7)	1000 0000 (7)	1500 0000 (7)	9027 7778 (8)	2361 1111 (8)	6944 4444 (9)		
5	2000 0000	1000 0000	4857 1429 (8)	1428 5714 (8)	7142 8571 (9)	2625 6614	3240 7407 (9)	4629 6296 (10)		
7	1428 5714	3571 4286 (9)	3333 3333	4761 9048 (9)	1190 4762	1143 3782	8277 2166 (10)	7014 5903 (11)		
9	1111 1111	1666 6667	2554 1126	2164 5022	3246 7532 (10)	6037 9435 (9)	2881 3779	1618 7516		
11	9090 9091 (9)	9090 9091 (10)	2074 5921	1165 5012	1165 5012					
13	7692 3077	5494 5655	1748 2517	6993 0070 (10)	4995 0050 (11)	3584 6098	1214 0637	4856 2549 (12)		
15	6666 6667	3571 4286	1511 3122	4524 8869	2424 0465	2304 5899	5830 6799 (11)	1745 7125		
17	5882 3529	2450 9803	1331 2693	3095 9752	1289 9897	1570 2041	3081 6420	7166 6093 (13)		
19	5263 1579	1754 3860	1189 7391	2211 4109	7371 3696 (12)	1118 3168	1752 5617	3257 5497		
21	4761 9048	1298 7013	1075 5149	1634 5211	4457 7848	8248 5070 (10)	1056 2015	1605 1694		
23	4347 8261	9881 4229 (11)	9813 6646 (9)	1242 2360	2823 2637	6259 0791	6672 0719 (12)	8445 6606 (14)		
25	4000 0000	7692 3077	9024 1546	9661 8357 (11)	1858 0453	4862 3545	4382 3395	4692 0837		
27	3703 7037	6105 0061	8352 4904	7662 8352	1263 1047	3852 7423	2974 5396	2728 9299		
29	3448 2759	4926 1084	7774 0700	6179 7058	8828 1512 (13)	3104 7316	2076 4076	1650 5625		
31	3225 8065	4032 2581	7270 7048	5056 1230	6320 1537	2538 6983	1485 0296	1032 7049		
33	3030 3030	3342 2460	6828 6552	4189 3590	4620 6166	2102 4471	1084 7991	6655 2091 (15)		
35	2857 1420	2801 1204	6437 3464	3510 0035	3441 1799	1760 7811	8073 4407 (13)	4402 0942		
37	2702 7027	2370 7918	6088 5061	2970 0030	2605 2658	1489 7522	6108 7522	2979 8791		
39	2564 1026	2024 2015	5775 5692	2535 3684	2001 6066	1271 0408	4691 0081	2059 2661		
41	2439 0244	1742 1603	5493 2589	2181 5961	1558 2829	1093 4097	3650 4910	1449 7581		
43	2225 5814	1510 1178	5237 2849	1890 7166	1227 7380	9474 1490 (11)	2875 1015	1037 9428		
45	2222 2222	1317 5231	5004 1234	1649 3485	9778 7461 (14)	8263 1159	2289 2827	7545 3288 (16)		
47	2127 6596	1156 3367	4790 8525	1447 3875	7866 2362	7250 1033	1841 0171	5561 9852		
49	2040 8163	1020 4082	4595 0295	1277 1066	6385 5329	6396 2170	1494 1103	4152 6134		
51	1960 7843	9049 7738 (12)	4414 5960	1132 5285	5227 0545	5671 3855	1222 7830	3136 9497		

TABLE 2  
Value of  $k_n$ . Even number of observations

$N$	$k_1$	$k_2$	$k_3$	$k_4$	$k_5$	$k_6$	$k_7$	$k_8$
4	2500 0000 (8)	5000 0000 (9)	6406 2500 (8)	7812 5000 (9)	1562 5000 (9)	6336 8056 (8)	7118 0556 (9)	8680 5556 (10)
6	1666 6667	1428 5714	3945 3125	1953 1250	1674 1071 (10)	1126 7499	4870 7562 (10)	2411 2654 (11)
8	1250 0000	5952 3810 (10)	2890 6250	7812 5000 (10)	3720 2381 (11)	4196 3534 (9)	9732 7441 (11)	2630 4714 (12)
10	1000 0000	3030 3030	2289 0625	3906 2500	1183 7121	2040 1329	2964 3389	5058 5988 (13)
12	8333 3333 (9)	1748 2517	1897 3214	2232 1429	4682 8172 (12)	1149 4485	1146 6157	1348 9597
14	7142 8571	1098 9011	1621 0938	1395 0893	2146 2912	7125 6741 (10)	5186 5517 (12)	4463 4695 (14)
16	6250 0000	7352 9412 (11)	1415 5506	9900 5952 (11)	1094 1877	4725 9999	2622 0143	1722 7426
18	5555 5556	5159 9587	1256 5104	6510 4167	6046 8266 (13)	3296 7149	1440 7871	7465 2181 (15)
20	5000 0000	3759 3985	1129 7349	4734 8485	3560 0365	2391 7243	8448 3844 (13)	3540 8149
22	4545 4545	2823 2637	1026 2784	3551 1364	2205 6748	1790 5616	5218 8071	1805 8156
24	4166 6667	2173 9130	9402 3164 (9)	2731 6434	1425 2052	1375 4794	3364 5791	9775 0702 (16)
26	3846 1538	1709 4017	8675 3091	2146 2912	9539 0720 (14)	1079 5940	2248 0302	5561 6779
28	3571 4286	1368 3634	8052 8846	1717 0330	6578 6704	8629 5508 (11)	1548 2276	3301 1249
30	3333 3333	1112 3471	7513 9509	1395 0893	4655 4704	7006 8080	1094 4042	2031 9424
32	3125 0000	9164 2229 (12)	7042 7390	1148 8971	3369 1996	5767 1532	7913 1009 (14)	1290 8811
34	2941 1765	7639 4194	6627 2213	9574 1423 (12)	2486 7902	4803 7846	5836 2361	8431 4304 (17)
36	2777 7778	6435 0064	6258 0624	8062 4358	1867 7458	4043 7597	4380 6481	5643 7105
38	2631 5789	5471 0581	5927 9058	6853 0703	1424 7547	3436 0952	3339 8722	3861 1239
40	2500 0000	4690 4315	5630 8741	5874 0602	1102 0751	2944 4203	2582 2837	2693 8074
42	2380 9524	4051 5355	5362 2160	5073 0520	8632 5332 (15)	2542 3116	2021 9092	1912 8753
44	2272 7273	3523 6081	5118 0477	4411 3495	6839 3016	2210 2564	1601 3580	1380 2431
46	2173 9130	3083 5646	4895 1643	3859 9309	5475 0792	1933 6316	1281 5606	1010 5351
48	2083 3333	2713 8515	4690 8968	3396 7392	4424 7580	1701 3314	1035 4426	7497 7742 (18)
50	2000 0000	2400 9604	4503 0048	3004 8077	3607 2121	1504 8177	8439 3512 (15)	5631 4922

of origin of the data or other origin such as zero. This translation of the axis requires the substitution of  $x = X + h$ . For ready reference the functions necessary for the transformation of the parameters in terms of  $X$  to those in  $x$  are given in table 4. The value of  $h$  may be obtained from the number of observations,  $N$ , and the initial observation,  $x_i$ . Equations for obtaining  $h$  are appended to table 4. For odd observations  $x_i$  is expressed in the original units, but for even observations in half-units.

In the calculation of equations to fit even numbers of observations the unit is half an interval. Therefore the unit of the original data must be restored by multiplying the parameters  $a$ ,  $b$ ,  $c$ , and  $g$  by 1, 2, 4, and 8,

TABLE 3  
*Functions for derivation of parameters for origin at midpoint of observations*

DEGREE OF EQUATION	PARAMETERS			
	A	B	C	G
1	$k_1 \Sigma y$	$k_2 \Sigma Xy$		
2	$k_3 \Sigma y - k_4 \Sigma X^2 y$	$k_5 \Sigma Xy$	$k_6 \Sigma X^2 y - k_7 \Sigma y$	
3	$k_8 \Sigma y - k_9 \Sigma X^2 y$	$k_{10} \Sigma Xy - k_{11} \Sigma X^2 y$	$k_{12} \Sigma X^2 y - k_{13} \Sigma y$	$k_{14} \Sigma X^3 y - k_{15} \Sigma Xy$

TABLE 4  
*Formulae for transformation of equations*

DEGREE OF EQUATION	PARAMETERS FOR $x = X + h$			
	a	b	c	g
1	$A - Bh$	$B$		
2	$A - Bh + Ch^2$	$B - 2Ch$	$C$	
3	$A - Bh + Ch^2 - Gh^3$	$B - 2Ch + 3Gh^2$	$C - 3Gh$	$G$

For odd observations  $h = \frac{N-1}{2} + x_i$ , with  $x_i$  in the original units.

For even observations  $h = N - 1 + x_i$ , with  $x_i$  in half-units.

respectively. If, in addition, it is desired to alter the original measure of the independent variable,  $a$ ,  $b$ ,  $c$ , and  $g$  are to be multiplied by  $m^0$ ,  $m^1$ ,  $m^2$ , and  $m^3$ , in which  $m$  is the ratio of the desired unit to the original measure.

Frequently a series of experiments yields sets of parallel data, namely, with an equal number of observations for which a special set of factors can be derived by combining the values of table 1 or 2 with tables 3 and 4, with the inclusion of  $m$  so that the desired equation is obtained directly. Such a combination yields little if any advantage over the procedure of derivation and transformation in the case of third-order equations. But

for first- and second-degree expressions such procedures can lead to economies if many sets of data are to be reduced.

USE OF TABLES 1 AND 2

The values of  $k_n$  in tables 1 and 2 as required for the equation are to be multiplied by  $10^{-r}$ , in which  $r$  is appended in parentheses to  $k_n$  given to

TABLE 5  
*Derivation of an equation for an odd number of observations*

RAT WEIGHT		SUM	DIFFERENCE	T
<i>grams</i>	<i>grams</i>	<i>grams</i>	<i>grams</i>	
58.6	11.6	70.2	47.0	21
57.6	12.7	70.3	44.9	20
57.1	13.3	70.4	43.8	19
54.8	14.1	68.9	40.7	18
54.2	15.6	69.8	38.6	17
53.8	16.1	69.9	37.7	16
51.4	17.0	68.4	34.4	15
50.4	18.0	68.4	32.4	14
50.0	18.8	68.8	31.2	13
47.8	20.0	67.8	27.8	12
46.7	21.9	68.6	24.8	11
46.4	22.0	68.4	24.4	10
45.3	22.9	68.2	22.4	9
42.8	24.0	66.8	18.8	8
42.3	24.4	66.7	17.9	7
40.0	25.6	65.6	14.4	6
39.1	27.6	66.7	11.5	5
39.0	28.5	67.5	10.5	4
37.0	29.5	66.5	7.5	3
35.5	32.0	67.5	3.5	2
35.0	32.5	67.5	2.5	1
984.8	448.1	1432.9	536.7	
481.1	33.0	33.0	448.1	
1465.9	481.1	1465.9	984.8	

$$\Sigma W = 1465.9; \Sigma WT = 7630.0; \Sigma WT^2 = 229,323.0; \Sigma WT^3 = 2,092,861.6$$

$$(1) W = 33.41 + 1.212T + 0.004388T_1^2 - 0.0002143T_1^3$$

$$(2) W = 5.913 + 0.2218t + 0.02561t^2 - 0.0002143t^3$$

$$(3) W = 5.913 + 0.6654d + 0.2305d^2 - 0.005786d^3$$

eight places. The exponent  $r$  is shown only for the first entry of a series of  $k_n$  for which  $r$  is the same, subsequent values taking the same  $r$ .

EXAMPLES OF CALCULATIONS

In tables 5 and 6 are shown the data of the weight of a suckling rat taken at 8-hr. intervals from the fourth to the eighteenth day. Table 6

contains one more weight (60.9 g. at 18 days, 8 hr.) than table 5; thus the differences in the treatment of almost identical data are illustrated in the cases of odd and even observations.

The weights in the first column of table 5 are, reading from the bottom, the weights of the last twenty-one 8-hr. periods; those of the second

TABLE 6

*Derivation of an equation for an even number of observations*

RAT WEIGHT		SUM	DIFFERENCE	T
<i>grams</i>	<i>grams</i>	<i>grams</i>	<i>grams</i>	
60.9	11.6	72.5	49.3	43
58.6	12.7	71.3	45.9	41
57.6	13.3	70.9	44.3	39
57.1	14.1	71.2	43.0	37
54.8	15.6	70.4	39.2	35
54.2	16.1	70.3	38.1	33
53.8	17.0	70.8	36.8	31
51.4	18.0	69.4	33.4	29
50.4	18.8	69.2	31.6	27
50.0	20.0	70.0	30.0	25
47.8	21.9	69.7	25.9	23
46.7	22.0	68.7	24.7	21
46.4	22.9	69.3	23.5	19
45.3	24.0	69.3	21.3	17
42.8	24.4	67.2	18.4	15
42.3	25.6	67.9	16.7	13
40.0	27.6	67.6	12.4	11
39.1	28.5	67.6	10.6	9
39.0	29.5	68.5	9.5	7
37.0	32.0	69.0	5.0	5
35.5	32.5	68.0	3.0	3
35.0	33.0	68.0	2.0	1
1045.7	481.1	1526.8	564.6	
481.1			481.1	
1526.8			1045.7	

$$\Sigma W = 1,526.8; \Sigma WT = 16,412.8; \Sigma WT^2 = 1,000,842.0; \Sigma WT^3 = 18,877,307.2$$

$$(1) W = 33.99 + 0.6047T + 0.001098T^2 - 0.00002275T^3$$

$$(2) W = 5.247 + 0.1512t_1 + 0.005671t_1^2 - 0.00002275t_1^3$$

$$(2a) W = 5.247 + 0.3024t + 0.02268t^2 - 0.0001820t^3$$

$$(3) W = 5.247 + 0.9072d + 0.2041d^2 - 0.004914d^3$$

column, reading from the top, are of the first twenty-one periods. The weight at the midperiod was 33.0 g. In table 6, twenty-two weights appear in each column and no weight for a midperiod.

The third and fourth columns show, respectively, the sums and differences of the items of the first and second columns. A check on the

accuracy of these sums and differences is shown by the totals of the columns.

$\Sigma W$  is obtained by summing the weights of the forty-three observations of table 5 and of the forty-four observations of table 6.

$\Sigma WT$  is the sum of the products of the items of columns 4 and 5 of each table.

$\Sigma WT^2$  is the sum of the product of the items of column 3 and the square of the items in column 5.

$\Sigma WT^3$  is the sum of the product of the items of column 4 and the cube of the items in column 5.

The values of  $k_n$  were taken for  $N = 43$  in table 1 and  $N = 44$  in table 2 for the data of tables 5 and 6, respectively.

Equation 1 in each table represents the data referred to the midpoint origin in terms of 8-hr. intervals. Equation 2 in each table shows equation 1 translated to origin at birth of the suckling rat through the use of  $h = 33$  for table 5 and  $h = 67$  for table 6. Equation 2a of table 6 shows the restoration of the original unit of measurement by multiplication of the successive parameters by 1, 2, 4, and 8, respectively. For odd observations the value of  $x_i$  was 12, as the first weight was recorded on the 4th day,—namely, twelve 8-hr. periods from zero origin,—but  $x_i$  was 24 for even observations, as the 4th day was twenty-four 4-hr. periods removed from the time of birth. Equation 3 in table 5 shows the weight as a function of age in days obtained from equation 2 by multiplying the coefficients of  $t$ ,  $t^2$ , and  $t^3$  by  $m$ ,  $m^2$ , and  $m^3$ , respectively, in which  $m = d/t = 3$ . Equation 3 of table 6 was similarly derived from equation 2a. All calculations and transformations of equations in tables 5 and 6 were carried out to eight significant figures and then rounded to four.

The foregoing equations merely summarize the data and *are not to be regarded as expressions of the law of growth of suckling rats*. The equations are excellent interpolation formulae but fail in extrapolation, as can readily be seen by their difference at zero time.

#### REFERENCE

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