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On the smoothing of empirical spectra

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1. Introduction

The spectral distribution of particles emitted in a nuclear reaction is usually measured by means of an analysis of the corresponding pulse heights. The spectrum available for study then consists of a set of numbers which indicate the contents of the kicksorter channels. As a result of the random nature of nuclear reactions, these numbers are always more or less disturbed by statistical fluctuations.

The problem of "smoothing" or "filtering" empirical data therefore arises naturally whenever a quantitative analysis of the spectrum is required, as will be the case for a precise location of the peaks (calibration) or for area determinations (intensity).

The shape of such a spectrum is in general too complicated to be described analytically, although attempts with multiple superpositions of "standard spectra" (with adjustable parameters for location and intensity) have been made repeatedly. But even if this approach is chosen, and perhaps especially in this case, the previous reduction of statistical scatter is often a necessity.

Under these circumstances, a fairly obvious attempt to obtain a smoothed spectrum is to make a "local" least-squares adjustment, and this technique has been described in detail by Savitzky and Golay [1], a paper which is still quoted as the basic reference and apparently much used by nuclear chemists. The approach has been known long before, however, and as an example for an earlier reference [2] might be quoted.

In the first part of the present report, we shall give a short summary of the underlying theory although this is just a simple application for the well-known general least-squares technique. However, it will give us the opportunity to correct some of the more disturbing misprints found in [1]. Today the main interest in [1] lies obviously in its extensive tabulation of the factors by which the original data have to be multiplied (for details see later). It may be somewhat surprising, therefore, that quite a large percentage of the listed coefficients have turned out to be erroneous when the tedious numerical values were recalculated.

Finally, some remarks on the quality of this type of adjustment will be added as far as the influence on the moments is concerned, and the eventual usefulness of weights is also briefly discussed.

2. Sketch of the least-squares approach

The empirical data are supposed to be available in the form of pairs (x_i, y_i), where x_i is the channel number and y_i its content (equally spaced observations). As the index i runs from 1 to, say 512 or more (depending on the type of analyzer used), the "true" shape of the spectrum in a limited region of $n = 2m + 1$ channels (i.e. the central one and m neighbours on each side) may be reasonably supposed to be smooth enough to be represented by a polynomial of order p (see Fig. 1)

$$f_p(x_i) = A_{p,o} + A_{p,1} \cdot x_i + A_{p,2} \cdot x_i^2 + \ldots + A_{p,p} \cdot x_i^p$$

$$= \sum_{k=o}^{p} A_{p,k} \cdot x_i^k , \qquad (1)$$

where $p < 2m$.

(The case $p = 2m$ corresponds to a problem of interpolation, whereas $p > 2m$ has no solution).

The first derivative of (1) with respect to x is obviously

$$f'_p(x_i) = \sum_{k=1}^{p} k \cdot A_{p,k} \cdot x_i^{k-1} . \qquad (2)$$

In particular, we observe that for $x_i = 0$, which will later be chosen as the "central" point to be adjusted, the "smoothed" value is simply given by

$$f_p(o) = A_{p,o} , \quad \text{for any } p , \qquad (1')$$

because it lies on the polynomial (1). Likewise, the adjusted first derivative is

$$f'_p(o) = A_{p,1} . \qquad (2')$$

Similar formulae exist for the higher derivatives, but they are omitted here as only the first derivative is needed for the exact peak location.

The best fit of the polynomial $f_p(x_i)$ to the n measured values (x_i, y_i) by the method of least squares leads to the conditions

$$\frac{\partial}{\partial A_{p,k}} \sum_{i=1}^{n} \left\{ y_i - f_p(x_i) \right\}^2 = 0, \qquad k = 0, 1, \ldots, p .$$

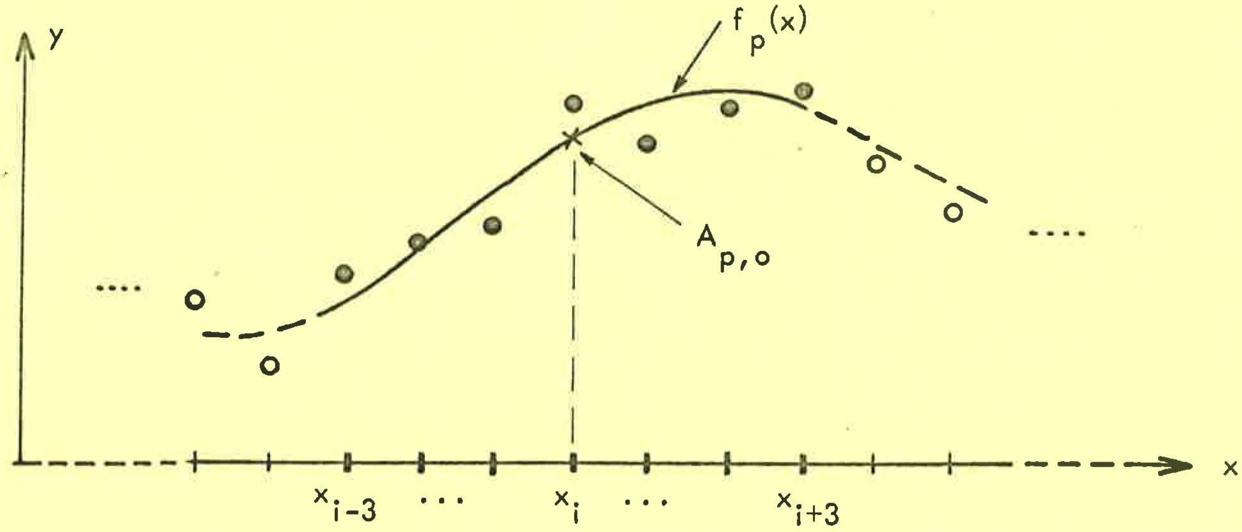

Fig. 1 - Schematic plot for the local fit of a polynomial $f_p(x)$ to the measurements around x_i (for m = 3). $A_{p,o}$ is the smoothed value at the mid-point x_i.

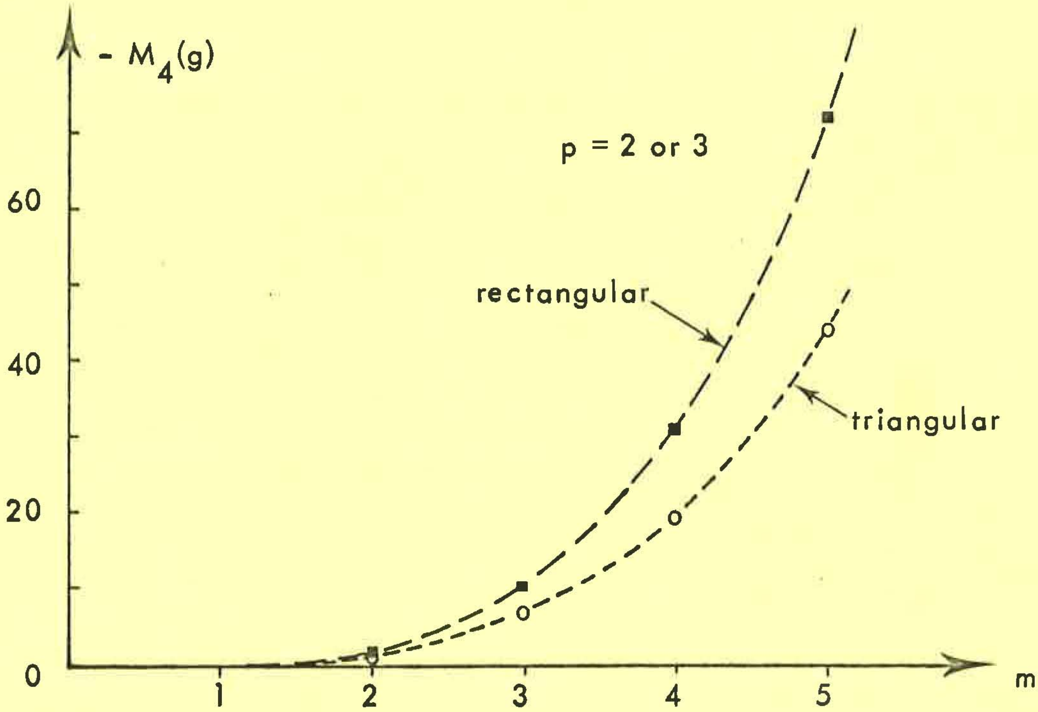

Fig. 2 - Graphical plot of the first non-vanishing moment M_4 of the convolution function g_i (for rectangular and triangular weights, see text)

If the n channels are located symmetrically around a central channel x_i, this corresponds to the p+1 equations

$$\sum_{j=-m}^{m} \left\{ y_{i+j} - f_p(x_{i+j}) \right\} x_{i+j}^k = 0 , \tag{3}$$

since $\frac{\partial}{\partial A_{p,k}} f_p(x) = x^k$.

These are the well-known normal equations which, when written in full, are

$$\left.\begin{array}{l} A_{p,o}\, n + A_{p,1}[x] + A_{p,2}[x^2] + \ldots + A_{p,p}[x^p] = [y] \\ A_{p,o}[x] + A_{p,1}[x^2] + A_{p,2}[x^3] + \ldots + A_{p,p}[x^{p+1}] = [xy] \\ A_{p,o}[x^2] + A_{p,1}[x^3] + A_{p,2}[x^4] + \ldots + A_{p,p}[x^{p+2}] = [x^2y] \\ \quad \ldots \\ A_{p,o}[x^p] + A_{p,1}[x^{p+1}] + A_{p,2}[x^{p+2}] + \ldots + A_{p,p}[x^{2p}] = [x^py] \end{array}\right\} \tag{4}$$

where for instance

$$[x^2y] \equiv \sum_{j=-m}^{m} x_{i+j}^2 \cdot y_{i+j} .$$

With the abbreviations

$$S_r \equiv [x^r] \quad \text{and} \quad F_r \equiv [x^r \cdot y] , \tag{5}$$

this can also be expressed in shorter form as

$$\sum_{k=o}^{p} S_{r+k} \cdot A_{p,k} = F_r , \qquad r = 0, 1, \ldots, p, \tag{6}$$

which corresponds (apart from a misprint) to equation Vb in [1] .

The abscissa x_i stands for the channel number and is therefore a (positive) integer. As we can always take the central channel x_i as the origin, the quantity x_{i+j} may now be identified with j. Then

$$S_r = \sum_{j=-m}^{m} j^r = \begin{cases} 2\sum_{j=1}^{m} j^r & \text{for } r \text{ even } (\neq 0) \\ 0 & \text{" } r \text{ odd} , \end{cases} \tag{7}$$

whereas $S_o = 2m + 1$.

This, in turn, results in a splitting of the system of normal equations (6) into two separate groups which are

$$\sum_{k=o}^{Q} S_{2(k+r)} \cdot A_{p,2k} = F_{2r} \tag{8a}$$

and

$$\sum_{k=o}^{Q} S_{2(k+r)+1} \cdot A_{p,2k+1} = F_{2r+1} \ , \tag{8b}$$

with r ranging in both cases from 0 to $Q \equiv \left[\left[\frac{p+1}{2}\right]\right]$, where $[[y]]$ stands as usual for the largest integer below y. Accordingly, all the "even" coefficients $A_{p,o}$, $A_{p,2}$, $A_{p,4}$, ... appear only in the system (8a), whereas the "odd" coefficients $A_{p,1}$, $A_{p,3}$, $A_{p,5}$, ... are restricted to the set of equations (8b).

It is a peculiarity of the system (8) that, as a result of (7), augmenting p by one unit adds only one new equation to either (8a) or (8b), while the other set remains unchanged. Therefore

$$A_{p,k} = A_{p+1,k} \ , \tag{9}$$

provided that k and p have the same parity (i.e. are both even or both odd). In this case, also the corresponding coefficients α (or β) and the normalizations N (see later for the definitions) are obviously the same.

The determination of the coefficients $A_{p,k}$ is straightforward. Thus for <u>p = 3</u>, for example, we get from (8a)

$$A_{3,o} \cdot S_o + A_{3,2} \cdot S_2 = F_o$$

$$A_{3,o} \cdot S_2 + A_{3,2} \cdot S_4 = F_2 \ ,$$

hence

$$A_{3,o} = \frac{S_4 F_o - S_2 F_2}{S_o S_4 - S_2^2} \ , \tag{10}$$

and likewise from (8b)

$$A_{3,1} \cdot S_2 + A_{3,3} \cdot S_4 = F_1$$

$$A_{3,1} \cdot S_4 + A_{3,3} \cdot S_6 = F_3 \ ,$$

hence

$$A_{3,1} = \frac{S_6 F_1 - S_4 F_3}{S_2 S_6 - S_4^2} \ . \tag{11}$$

The quantities S_r depend also on m, as is evident from their definition (5). A short table of their numerical values is given in Table A1 of the Appendix. It is sufficient for determining $A_{p,o}$ and $A_{p,1}$ for polynomials of degree p = 2 to 5 and up to n = 11 points. These explicit results of very elementary, but quite tedious calculations are only given to allow easy checking of those coefficients α or β (see later) which have been found to be erroneous in the more extended tabulation in [1].

If we continue our example, for instance with m = 4, and restrict ourselves to the evaluation of $A_{3,o}$, the quantities needed further are F_o and F_2, for which we get (with $x_i = 0$) from (5)

$$F_o = (-4)^o \cdot y_{i-4} + (-3)^o \cdot y_{i-3} + \dots + 4^o \cdot y_{i+4}$$

and

$$F_2 = (-4)^2 \cdot y_{i-4} + (-3)^2 \cdot y_{i-3} + \dots + 4^2 \cdot y_{i+4} ,$$

which may also be written as

$$F_o = y_i + D_1^+ + D_2^+ + D_3^+ + D_4^+$$

and

$$F_2 = D_1^+ + 2^2 \cdot D_2^+ + 3^2 \cdot D_3^+ + 4^2 \cdot D_4^+ ,$$

where $D_j^+ \equiv y_{i+j} + y_{i-j}$. (12)

Hence, the numerator in (10) is

$$S_4 F_o - S_2 F_2 = S_4 \cdot y_i + (S_4 - S_2) \cdot D_1^+ + (S_4 - 2^2 S_2) \cdot D_2^+ + (S_4 - 3^2 S_2) \cdot D_3^+ + (S_4 - 4^2 S_2) \cdot D_4^+$$

$$= 708 \, y_i + 648 \, D_1^+ + 468 \, D_2^+ + 168 \, D_3^+ - 252 \, D_4^+ ,$$

where the corresponding values for S_r have been taken from Table A1. Since the denominator of (10) is

$$S_o S_4 - S_2^2 = 2\,772 ,$$

dropping of the common factor 12 finally leads to

$$A_{3,o} = \frac{1}{231} (59 \, y_i + 54 \, D_1^+ + 39 \, D_2^+ + 14 \, D_3^+ - 21 \, D_4^+) .$$

By generalizing the explicit calculations made in this example it is easy to see that the coefficients F_r, originally defined by (5), can also be written as

$$F_r = \begin{cases} \sum_{j=1}^{m} j^r D_j^+ & \text{for r even (except 0)} \\ \sum_{j=1}^{m} j^r D_j^- & \text{" r odd ,} \end{cases} \tag{13}$$

whereas

$$F_o = y_i + \sum_{j=1}^{m} D_j^+ ,$$

with

$$D_j^{\pm} \equiv y_{i+j} \pm y_{i-j} . \tag{14}$$

It is practical to introduce the following abbreviations for certain combinations of the factors S_r which appear repeatedly in the evaluation of the coefficients $A_{p,k}$:

$$\begin{aligned} T_2 &= S_o S_4 - S_2^2 , & T_6 &= S_4 S_8 - S_6^2 , \\ T_4 &= S_2 S_6 - S_4^2 , & T_7 &= S_4 S_{10} - S_6 S_8 , \\ T_5 &= S_2 S_8 - S_4 S_6 , & T_8 &= S_6 S_{10} - S_8^2 . \end{aligned} \tag{15}$$

These coefficients are listed in Table A2 of the Appendix. With their help, the formulae for $A_{p,o}$ and $A_{p,1}$, as they result from the normal equations (8), can now be simplified to

- for p = 2 or 3:

$$A_{p,o} = \frac{S_4 F_o - S_2 F_2}{T_2} \tag{10'}$$

$$A_{p,1} = \frac{S_6 F_1 - S_4 F_3}{T_4} , \tag{11'}$$

- for p = 4 or 5:

$$A_{p,o} = \frac{T_6 F_o - T_5 F_2 + T_4 F_4}{T_6 S_o - T_5 S_2 + T_4 S_4} \tag{16}$$

$$A_{p,1} = \frac{T_8 F_1 - T_7 F_3 + T_6 F_5}{T_8 S_2 - T_7 S_4 + T_6 S_6} . \tag{17}$$

It is now easy to realize that, in the general case, the result for $A_{p,o}$ will always be of the form

$$A_{p,o} = \frac{1}{N_o} (\alpha_o y_i + \sum_{j=1}^{m} \alpha_j D_j^+) , \tag{18}$$

and for $A_{p,1}$ a similar reasoning leads to the expression

$$A_{p,1} = \frac{1}{N_1} \sum_{i=1}^{m} \beta_i D_i^- \ . \qquad (19)$$

The coefficients α_i and the normalization factors N_o (or the corresponding quantities β_i and N_1 for evaluating the derivatives) are given in Tables 1 and 2 for p up to 6 and m not exceeding 10. A more extended tabulation (up to m = 12) can be found in [1], but it should be used with caution.

Table 1 - Coefficients needed for evaluating the smoothed value $f_p(o) = A_{p,o}$ (with equal weights)

For p = 2 or 3:

m	N_o	α_o	α_1	α_2	α_3	α_4
2	35	17	12	-3		
3	21	7	6	3	-2	
4	231	59	54	39	14	-21
5	429	89	84	69	44	9
6	143	25	24	21	16	9
7	1 105	167	162	147	122	87
8	323	43	42	39	34	27
9	2 261	269	264	249	224	189
10	3 059	329	324	309	284	249

m	α_5	α_6	α_7	α_8	α_9	α_{10}
5	-36					
6	0	-11				
7	42	-13	-78			
8	18	7	-6	-21		
9	144	89	24	-51	-136	
10	204	149	84	9	-76	-171

Table 1 (cont'd)

For p = 4 or 5:

m	N_o	α_o	α_1	α_2	α_3	α_4
3	231	131	75	-30	5	
4	429	179	135	30	-55	15
5	429	143	120	60	-10	-45
6	2 431	677	600	390	110	-135*
7	46 189	11 063	10 125	7 500	3 755	-165
8	4 199	883	825	660	415	135
9	7 429	1 393	1 320	1 110	790	405
10	260 015	44 003	42 120	36 660	28 190	17 655

m	α_5	α_6	α_7	α_8	α_9	α_{10}
5	18					
6	-198	110				
7	-2 937	-2 860	2 145			
8	-117	-260	-195	195		
9	18	-290	-420	-255	340	
10	6 378	-3 940	-11 220	-13 005	-6 460	11 628

* Corrects the corresponding value given in [1].

Table 1 (cont'd)

For p = 6**

m	N_1	α_o	α_1	α_2	α_3	α_4
4	1 287	797	392	-196	56	-7
5	2 431	1 157	784	28	-308	161
6	46 189	18 063	14 000	4 550	-3 500	-3 605
7	12 597	4 199	3 500	1 750	-140	-1 085
8	96 577	28 109	24 500	15 050	3 500	-5 215
9	37 145	9 605	8 624	5 978	2 492	-679
10	334 305	77 821	71 344	53 508	28 812	3 801

m	α_5	α_6	α_7	α_8	α_9	α_{10}
5	-28					
6	3 388	-770				
7	-476	910	-260			
8	-6 916	-910	6 500	-2 275		
9	-2 380	-1 918	344	2 261	-952	
10	-14 364	-19 908	-11 016	7 021	18 088	-9 044

** These values are not tabulated in [1] .

Table 2 - Coefficients needed for evaluating the smoothed derivative $f'_p(o) = A_{p,1}$ (with equal weights)

For p = 2:

m	N_1	β_1	β_2	β_3	β_4
2	10	1	2		
3	28	1	2	3	
4	60	1	2	3	4
5	110	1	2	3	4
6	182	1	2	3	4
7	280	1	2	3	4
8	408	1	2	3	4
9	570	1	2	3	4
10	770	1	2	3	4

m	β_5	β_6	β_7	β_8	β_9	β_{10}
5	5					
6	5	6				
7	5	6	7			
8	5	6	7	8		
9	5	6	7	8	9	
10	5	6	7	8	9	10

Table 2 (cont'd)

For p = 3 or 4 :

m	N_1	β_1	β_2	β_3	β_4
2[x]	12	8	-1		
3	252	58	67	-22	
4	1 188	126*	193	142	-86
5	5 148	296	503	532	294
6	24 024	832	1 489	1 796	1 578
7	334 152	7 506	13 843	17 842	18 334
8	23 256	358	673	902	1 002
9	255 816	2 816	5 363	7 372*	8 574
10	3 634 092	29 592	56 881	79 564*	95 338

m	β_5	β_6	β_7	β_8	β_9	β_{10}
5	-300					
6	660	-1 133				
7	14 150	4 121	-12 922			
8	930	643	98	-748		
9	8 700	7 481	4 648	-68	-6 936	
10	101 900	96 947	78 176	43 284	-10 032	-84 075

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x The coefficients given in this line are only meaningful for an adjustment with the lower value of p.

* Corrects the corresponding value given in [1] .

for p = 4 or 5:

m	N_2	γ_0	γ_1	γ_2	γ_3	γ_4
3	132*	- 70*	- 19*	67*	- 13*	
4	1 716*	- 370*	- 211*	151*	371*	- 126*
5	1 716*	- 190*	- 136*	1*	146*	174*
6	58 344*	- 3 780*	- 3 016*	- 971*	1 614*	3 504*
7	1 108 536*	- 45 780*	- 38 859*	- 19 751*	6 579*	31 856*
8	100 776*	- 2 820*	- 2 489*	- 1 557*	- 207*	1 256*
9	1 961 256*	- 38 940*	- 35 288*	- 24 867*	- 9 282*	8 792*
10	980 628*	- 14 322*	- 13 224*	- 10 061*	- 5 226*	626*

m	γ_5	γ_6	γ_7	γ_8	γ_9	γ_{10}
5	- 90*					
6	2 970*	- 2 211*				
7	44 495*	29 601*	- 31 031*			
8	2 405*	2 691*	1 443*	- 2 132*		
9	25 610*	36 357*	35 148*	15 028*	- 32 028*	
10	6 578*	11 451*	13 804*	11 934*	3 876*	- 12 597*

* Corrects the corresponding value given in [1] .

3. A simple check

In view of the real danger of errors in the lengthy numerical calculations, any control for the coefficients α, β and N would be very welcome, even if this were only a necessary, but not a sufficient condition for the values to be correct.

As a matter of fact, such a control can be easily derived by assuming a particular distribution of the experimental measurements y_i. For

$$y_{i+j} = j^q , \quad \text{with } q \leqslant p , \tag{20}$$

the adjusted polynomial (1) will only consist of one term, thus

$$A_{p,j} = \delta_{j,q} . \tag{21}$$

Inserting (20) into (14) gives

$$D_j^+ = \begin{cases} 2\, j^q & \text{for } q \text{ even} \\ 0 & \text{" } q \text{ odd ,} \end{cases}$$

but

$$D_j^- = \begin{cases} 0 & \text{for } q \text{ even} \\ 2\, j^q & \text{" } q \text{ odd.} \end{cases}$$

By applying (21), we get therefore in particular

- for $q = 0$, from (18)

$$A_{p,o} = 1 = \frac{1}{N_o} (\alpha_o \cdot 0^o + 2 \sum_{j=1}^{m} \alpha_j \cdot j^o) ,$$

and hence for the normalization

$$N_o = \alpha_o + 2 \sum_{j=1}^{m} \alpha_j ; \tag{22}$$

- for $q = 1$, from (19)

$$A_{p,1} = 1 = \frac{1}{N_1} 2 \sum_{j=1}^{m} \beta_j \cdot j^1 ,$$

and hence for the normalization

$$N_1 = 2 \sum_{j=1}^{m} j \cdot \beta_j . \tag{23}$$

Similar checks obviously exist for the coefficients used in determining the higher derivatives of $f_p(x)$, which have not been treated here but can be found in [1]. We note, however, that what these authors call "Apq" would correspond to our $q! \cdot A_{p,q}$.

Further checks for $A_{p,o}$ will result from a discussion of the moments (section 5).

4. Smoothing and folding

The individual adjustment of a polynomial to each measured point (and its neighbours) for determining the "smoothed" value as well as the corresponding procedure for obtaining the derivative can also be considered from the point of view of the folding of two functions. As a matter of fact, the relation (18) may be written in the equivalent form

$$f_i \equiv f_p(x_i) = \sum_{j=-m}^{m} y_{i+j} \cdot g_j = \sum_{j=-m}^{m} y_{i-j} \cdot g_j \ , \tag{24}$$

if the discrete function g_j is identified with

$$g_j \equiv \alpha_{|j|}/N_o \ , \quad \text{for } |j| \leqslant m \ . \tag{25}$$

The values of g_j are seen to be essentially identical with our tabulated coefficients α_j. Therefore, such a set of values can be thought of as representing some kind of discrete weighing function with which the observed data have to be convoluted in order to obtain the smoothed values, or in the usual shorthand notation (see e.g. [3], p. 37 ff.)

$$f_i = y_i \circledast g_i = y_i * g_i \ . \tag{24a}$$

Similarly, the (smoothed) first derivative, according to (19), can now be written as

$$f'_i \equiv f'_p(x_i) = \sum_{j=-m}^{m} y_{i+j} \cdot h_j = -\sum_{j=-m}^{m} y_{i-j} \cdot h_j \ , \tag{26}$$

or $$f'_i = y_i \circledast h_i = -y_i * h_i \ , \tag{26a}$$

with

$$h_j \equiv \begin{cases} -\beta_{|j|}/N_1 & \text{for } j < 0 \\ 0 & \text{"} \quad j = 0 \\ \beta_j/N_1 & \text{"} \quad j > 0 \ . \end{cases} \tag{27}$$

The discrete function h_i plays a role similar to g_i above, but is antisymmetrical. We note, however, that neither g_i nor h_i can be taken as probability functions since they may assume negative values.

In the language of electrical network theory, the function g_i would be called a digital "filter". As its function in the smoothing process is obviously to reduce the "noise" caused by the statistical fluctuations, it should act as a low-pass filter because the noise has a "white" frequency spectrum. This means that, since the different channels are uncorrelated, its density extends with an approximately constant value from zero to high frequencies (limited by the reciprocal of the channel width).

However, this aspect of the smoothing problem will not be discussed here further as it has been treated repeatedly. Two examples of frequency spectra of such filters are given in [4].

Let us finally deduce (although by somewhat heuristic arguments, as will become more obvious later) an interesting, simple relation between the functions g_i and h_i. If the Laplace transform, defined by

$$\mathcal{L}\{y_i, s\} \equiv E(e^{-si}) \equiv \sum_{i=-\infty}^{\infty} y_i \cdot e^{-si} \equiv \tilde{y}(s) , \tag{28}$$

is applied to (24) and (26), we get

$$\mathcal{L}\{f_i\} = \tilde{y}(s) \cdot \tilde{g}(s) \tag{24'}$$

and

$$\mathcal{L}\{f_i'\} = -\tilde{y}(s) \cdot \tilde{h}(s) . \tag{26'}$$

However, since $\mathcal{L}\{f_i\} = \tilde{f}(s)$,

but $\mathcal{L}\{f_i'\} = s \cdot \tilde{f}(s)$,

we see by comparing (24') with (26') that

$$\tilde{h}(s) = -s \cdot \tilde{g}(s) ,$$

which corresponds for the original weighing functions to the relation

$$h_i = -g_i' . \tag{29}$$

The relation (29) could be used for checking the coefficients α_i and β_i, but in general this will first require some interpolation formula, as the function g_i is discrete and therefore cannot be differentiated directly. However, g_i' in (29) may be identified with the derivative of the corresponding interpolation polynomial of degree 2m.

Nevertheless, in some simple cases a direct comparison is still possible. Thus, for p = 2 and, say m = 5, we get the following values (normalization neglected):

i :	-5	-4	-3	-2	-1	0	1	2	3	4	5
$g_i \sim$	-36	9	44	69	84	89	84	69	44	9	-36
$(g_{i+1}-g_i)\sim$	45	35	25	15	5	-5	-15	-25	-35	-45	
$g_i' \sim$	(50)	40	30	20	10	0	-10	-20	-30	-40	(-50)
$h_i \sim$	-5	-4	-3	-2	-1	0	1	2	3	4	5 .

The values g_i have been taken from Table 1 (since $g_i \sim \alpha_i$). As the quantity $g_{i+1}-g_i$ is manifestly linear in i, the derivative g_i' at the values i can be guessed readily. A comparison with the β's from Table 2 then confirms the proportionality implied by (29).

5. Moments, distortions and controls

A relation between the moments of g_i and h_i can be obtained as follows. If $\tilde{g}(s)$ is the Laplace transform of g_i, then the moments of order k of the function g_i are known to be given by

$$M_k(g) \equiv E(i^k) = (-1)^k \cdot \tilde{g}^{(k)}\Big|_{s=o} , \qquad (30)$$

with $\tilde{g}^{(k)} \equiv \frac{d^k}{ds^k}\left[\tilde{g}(s)\right]$.

Since $\tilde{h}(s) = -s \cdot \tilde{g}(s)$, we get similarly for h_i

$$M_k(h) = (-1)^{k+1} \cdot (s \cdot \tilde{g})^{(k)}\Big|_{s=o} . \qquad (31)$$

But for the n-th derivative of a product of two functions A and B, Leibnitz's rule states that

$$(A \cdot B)^{(n)} = \sum_{i=0}^{n} \binom{n}{i} A^{(n-i)} \cdot B^{(i)} , \qquad (32)$$

with $A^{(o)} = A$, $B^{(o)} = B$.

In our case we therefore obtain

$$(s \cdot \tilde{g})^{(k)} = s \cdot \tilde{g}^{(k)} + k \cdot \tilde{g}^{(k-1)} \quad , \tag{33}$$

because $s^{(o)} = s$ and $s^{(1)} = 1$,

but $\quad s^{(2)} = \ldots = s^{(k)} = 0$.

This then yields for the moment of order k of h_i

$$M_k(h) = (-1)^{k+1} \cdot k \cdot \tilde{g}^{(k-1)}\Big|_{s=o} = k \cdot M_{k-1}(g) \quad . \tag{34}$$

In particular, for $k=1$ we therefore obtain

$$M_1(h) = M_o(g) = 1 \quad , \tag{35}$$

in accordance with (22) and (23).

As a result of the symmetry of the functions g_i and the antisymmetry of h_i, we have obviously for the moments ($k = 0, 1, 2, \ldots$)

$$\begin{aligned} M_{2k+1}(g) &= 0 \quad \text{for } k \text{ odd} \\ M_{2k}(h) &= 0 \quad \text{" } k \text{ even.} \end{aligned} \tag{36}$$

By looking at the relation (34), one might now feel tempted to conclude that all moments (for $k > 1$, say) of g_i and h_i vanish. However, this is certainly not possible, since the requirement for all moments $M_{2k}(g)$ to disappear corresponds to infinitely many equations, whereas the number of conditions which can be fulfilled by the $m+1$ values α_i is necessarily limited. The origin of this discrepancy lies in our previous (and perhaps somewhat hasty) identification of the sequence α_i with the interpolating polynomial g_i (and similarly for h_i). A closer look at the situation reveals that - in addition to (35) - only the following moments can be used for checking the coefficients α_i and β_i (when p does not exceed 5)

$$\begin{aligned} &- \underline{\text{for } \alpha_i}: \quad M_{2k}(g) = 0 \quad \text{for } 1 \leq k \leq \left[\left[\frac{p+1}{2}\right]\right] , \\ &\text{thus} \quad \sum_{i=1}^{m} i^2 \alpha_i = 0 \quad \text{for } p \geq 2 \\ &\text{and} \quad \sum_{i=1}^{m} i^4 \alpha_i = 0 \quad \text{" } p \geq 4 \; . \end{aligned} \tag{37}$$

- for β_i: $\mathcal{M}_{2k+1}(h) = 0$ for $1 \leqslant k \leqslant [[p/2]]$,

$$\text{thus} \quad \sum_{i=1}^{m} i^3 \beta_i = 0 \quad \text{for } p \geqslant 3 \tag{38}$$

$$\text{and} \quad \sum_{i=1}^{m} i^5 \beta_i = 0 \quad \text{" } p \geqslant 5 .$$

The smoothing of the original data is a process which inevitably introduces distortions, some of which are "wanted" whereas others will be considered as "unwanted". As a matter of fact, it is usually most difficult, if not impossible, to tell in advance how a favourable balance between these two possibilities can be achieved. As the judgment is usually based on visual inspection of the smoothed data, even the separation between the welcome and the undesirable effects is obviously subjective.

Several attempts to improve this situation have been made. In particular, it would be desirable to have available a simple rule for choosing the degree p of the fitting polynomial and the number $n = 2m + 1$ of points to be selected. Thus, for $p = 3$ a special study has been made [5] where five different methods for choosing the best value of m and four criteria for testing the effectiveness of smoothing are discussed. However, no definite policy can be deduced from this, apart, of course, from the well-known and rather obvious rule that the amount of smoothing increases with m and decreases with p.

A more detailed insight into the mechanism of smoothing is provided by a look at the integral transforms of y_i and g_i . The high-frequency contributions of the experimental spectrum $\tilde{f}_i(\nu)$, with $\nu = s/(2\pi i)$, which are supposed to be due to noise, are best eliminated by choosing values of p and m for which the corresponding low-pass filter $\tilde{g}_i(\nu)$ rejects the unwanted high frequencies. However, care must be taken so as to not seriously distort the low-frequency contributions which are characteristic of the "signal", i.e. of the true spectrum shape. These questions have been discussed for example in [4] and [6] .

Another general approach which may be useful for a rough estimate of the distortions brought in by the fitting procedure can be based on the moments. The fact expressed by (24a), namely that the smoothed curve f_i can be considered as the result of folding the original measurements y_i with a certain weighing function g_i, leads readily to a simple relation between the corresponding moments.

The moments $\mathcal{M}_k(f)$ of the function $f_i = y_i * g_i$ can be expressed in terms of the moments $\mathcal{M}_i(y)$ and $\mathcal{M}_i(g)$ of the convolution factors by means of (see [3], p. 54)

$$\mathcal{M}_k(f) = \sum_{i=0}^{m} \binom{k}{i} \mathcal{M}_{k-i}(y) \cdot \mathcal{M}_i(g) \ . \tag{39}$$

Since according to (35) and (36)

$$M_o(g) = 1 \quad \text{and} \quad M_{2k+1}(g) = 0 ,$$

the relation (39) reduces to

$$M_k(f) = \binom{k}{o} M_k(y) \cdot M_o(g) + \sum_i \binom{k}{2i} M_{k-2i}(y) \cdot M_{2i}(g) ,$$

with $1 \leqslant i \leqslant \left[\left[\frac{k+1}{2}\right]\right]$.

When this is combined with (37) we arrive at

$$M_k(f) = M_k(y) + \sum_i \binom{k}{2i} M_{k-2i}(y) \cdot M_{2i}(g) , \tag{40}$$

with $\left[\left[\frac{p+3}{2}\right]\right] \leqslant i \leqslant \left[\left[\frac{k+1}{2}\right]\right]$.

Therefore

$$M_k(f) = M_k(y) \quad \text{if} \quad k \leqslant \begin{cases} p+1 & \text{for } p \text{ even} \\ p & \text{" } p \text{ odd} \end{cases} , \tag{41}$$

i.e. these moments of the original curve are not influenced by the fitting procedure. The first change occurs for the moment of order

$$k' = 2 \left[\left[\frac{p+3}{2}\right]\right]$$

and amounts, according to (40), to

$$M_{k'}(f) - M_{k'}(y) = \binom{k'}{k'} M_o(y) \cdot M_{k'}(g) = M_{k'}(g) . \tag{42}$$

It is a fairly obvious condition for any acceptable fitting procedure to change neither the total number of observed events nor the position or the "width" of a spectral line. This corresponds to demanding that

$$M_o(g) = 1 \quad \text{and} \quad M_1(g) = M_2(g) = 0 .$$

A look at (35), (36) and (37) shows that this is always the case provided that $p \geqslant 2$. As for the moments of higher order, the situation is less clear. If we demand as little change as possible for them too, the best choice would be a high p (practically limited by the tables available for the corresponding coefficients α_i and β_i) and the lowest compatible value of m, which is $m = \left[\left[\frac{p+3}{2}\right]\right]$. On the other hand, this will clearly also diminish the smoothing effect so that in reality a compromise has to be made. The limiting case $g_i = \delta_{i,o}$ is of no practical interest as it corresponds to a pure interpolation, where always $f_p(x_i) = y_i$, thus giving no smoothing at all.

A plot of some numerical results for the first non-vanishing moment of the weighing function g_j is given in Fig. 2. It can be seen that its absolute value increases with m, indicating thereby a stronger distortion.

6. Additional remarks

If the process of smoothing were iterated a large number of times, the resulting set of adjusted values would tend towards a least-squares polynomial of degree p for the entire range of the measured values. This would obviously only be the case if "off-center" formulae had been used for the m values at the beginning and at the end of the interval, as it is customary in the related field of interpolation (see e.g. [7]). For the sake of simplicity, however, it will be preferred in most practical applications to renounce this refinement and to use, for instance, the original border values instead of the adjusted ones.

In any case, this limiting behaviour obviously restricts the usefulness of such repeated convolutions. Whereas a polynomial fit of degree p may be reasonable for $n = 2m+1$ points, this procedure will become doubtful for a much more extended range. Furthermore, we arrive at the (somewhat embarrassing) conclusion that the limiting polynomial (of degree p) obtained by repeating the convolution with n points each time is not independent of n (or m). This is a direct consequence of the fact that for a given p

$$g_i^{(m_1)} * g_i^{(m_2)} \not\equiv g_i^{(m_1+m_2)} . \qquad (43)$$

Indeed, a simple example with, say $m_1 = m_2 = 2$ and $p = 2$ or 3, already shows that the coefficients for $m_1+m_2 = 4$, when determined by a self-convolution of $g_i^{(2)}$, i.e. with $m = 2$, do not agree with the values listed in Table 1 for $m = 4$.
Putting for brevity

$$g_i^{(m_{1,2}=2)} = g_i \quad \text{and} \quad g_i^{(m_1+m_2=4)} = G_i ,$$

equation (20) tells us to form

$$G_i = \sum_{k=-2}^{2} g_{i+k} \cdot g_k ,$$

which results in

$$G_o = g_{-2}\, g_{-2} + g_{-1}\, g_{-1} + g_o\, g_o + g_1\, g_1 + g_2\, g_2 ,$$

$$G_1 = g_{-1}\, g_{-2} + g_o\, g_{-1} + g_1\, g_o + g_2\, g_1$$

$$G_2 = g_o\, g_{-2} + g_1\, g_{-1} + g_2\, g_o$$

$$G_3 = g_1\, g_{-2} + g_2\, g_{-1}$$

$$G_4 = g_2\, g_{-2} ,$$

or with (21) and the numerical values from Table 1 (for m=2 and p=2 or 3):

whereas for m=4

$35^2 \cdot G_o = 595$,	$\alpha_o = 59$
$35^2 \cdot G_1 = 336$	$\alpha_1 = 54$
$35^2 \cdot G_2 = 42$	$\alpha_2 = 39$
$35^2 \cdot G_3 = -72$	$\alpha_3 = 14$
$35^2 \cdot G_4 = 9$	$\alpha_4 = -21$.

As the resulting weighing function G_i is clearly quite different from the values g_i obtained directly for m=4, it follows that an adjustment with a higher value of m cannot simply be replaced by the combined effect of simpler fits such that $m = \sum_i m_i$.

Finally, we should mention that the polynomial fits treated in this report could also have been described in a rather different form. Just as in the theory of interpolation, where (apart from minor variants) there exist two basic approaches which are either based on the values measured at the different points (Lagrangian form) or on the differences (of various order) between adjacent points (Newtonian form), the fitting of a polynomial can be likewise achieved by these two methods.

Although in general - as a detailed comparison would confirm - the form chosen above, in which the adjusted result is expressed explicitly in terms of the ordinates involved, turns out to be more practical, there are some special cases, where the difference-formalism turns out to be simpler. In particular, this is true when $m = \left[\left[\frac{p+3}{2}\right]\right]$. A single difference is then all we need and no coefficients have to be tabulated. We confine ourselves to mentioning the corresponding formulae which are

- for p = 2 or 3 and m = 2:
$$A_{p,o} = y_i - \frac{3}{35} \Delta^4 y_{i-2} \tag{44}$$

- for p = 4 or 5 and m = 3:
$$A_{p,o} = y_i + \frac{5}{231} \Delta^6 y_{i-3} \ , \tag{45}$$

where the (forward) differences are defined as usual recursively by

$$\Delta y_i \equiv y_{i+1} - y_i$$

and

$$\Delta^k y_i \equiv \Delta(\Delta^{k-1} y_i) = \Delta^{k-1} y_{i+1} - \Delta^{k-1} y_i \ . \tag{46}$$

The relation of these formulae with the approach given above can be readily established by use of the identity

$$\Delta^k y_i = \sum_{j=0}^{k} \binom{k}{j} (-1)^j \cdot y_{i+k-j} \quad . \tag{47}$$

Starting from the originally measured values y_i, the corrections can thus be easily determined for instance on a computer by forming numerically the successive differences, where the last alone has to be retained. Again, the differences for the first and the last m values y_i will not be available for determining the corrected values $A_{p,o}$ by this algorithm. As suggested before, the simplest way is then to replace them by the original values.

For other conditions than those given in (44) and (45), more than one difference as well as new coefficients are involved so that the advantage of simplicity is lost.

7. Triangular weights

In establishing the normal equations (4), it has been tacitly assumed that the 2m+1 experimental values y_i used for the adjustment have equal weight. Although this is not strictly true in general, it can be argued that the local fitting involves only a few neighbouring channels the contents of which are usually not very different from each other. In reality, a more stringent reason for adopting the simplification was that otherwise no formalism with general coefficients α_i (or likewise β_i) could have been elaborated.

On the other hand, weights which are associated not with y_i, but with g_i, seem perfectly acceptable. We therefore first have to ask whether they could be of any interest in the smoothing. We think that this might be the case for the following reason. The sole purpose of adjusting a polynomial is to obtain an improved value at its mid-point (and eventually the derivatives). Therefore, the polynomial is only a mathematical vehicle and has no physical meaning in itself. The choice of its characteristic parameters p and m is usually difficult to justify and somewhat arbitrary, as has been seen above. By choosing the least-squares criterion (3), deviations of the measured points from the polynomial towards the end of the interval are taken into account exactly in the same way as those occurring in the middle, although finally only the behaviour at the center is used for determining $A_{p,o}$ and $A_{p,1}$. It does not seem unreasonable, therefore, to expect an improved fit in the region of actual interest if the various points are weighted according to their distance from the center.

Unfortunately, we must admit that no objective criterion for determining such weights has been found so far. This might be used as an argument for rejecting the very idea of introducing weights; on the other hand, it could also mean that a subjective element has to be tolerated, at least for the moment, as is also the case in judging the quality of the fit.

For the sake of simplicity (in particular in view of the numerical calculations), we suggest tentatively the following weights

$$w_i = m + 1 - |j| , \qquad \text{for } |j| \leqslant m , \tag{48}$$

where the fit is supposed to extend over 2m+1 experimental points y_{i+j} which are situated symmetrically around the central channel x_i. When (48) is plotted graphically, its points form a discrete triangle and we therefore call them triangular weights. They are all integers and not normalized to unity, but this is of no consequence. The case treated previously "without" weights can now be described more correctly as involving equal or "rectangular" weights

$$w_i = 1 , \qquad \text{for } |j| \leqslant m ,$$

which, however, do not appear explicitly in the calculations.

If the idea of weights is accepted, the formalism outlined in section 2 has to be modified accordingly, the changes being modest.

If we now define, by generalizing (5), the corresponding quantities (marked with dashes on the left) by

$$'S_r \equiv \left[w\, x^r \right] \quad \text{and} \quad 'F_r \equiv \left[w\, x^r\, y \right] , \tag{49}$$

the normal equations (6) now read

$$\sum_{k=0}^{p} {'S_{r+k}} \cdot {'A_{p,k}} = {'F_r} . \tag{50}$$

The calculations needed to arrive at explicit formulae for $'A_{p,k}$ are exactly the same as before (all quantities are dashed now) and will not be repeated. When all this is done numerically - we confine ourselves to determining $'A_{p,o}$ for p = 2 or 3, for illustration -, one arrives at the values for $'S_r$ and $'T_r$ given in the Tables A3 of the Appendix. By inserting these quantities into a formula which corresponds to (10'), we finally arrive at the values for the coefficients $'\alpha_i$ and $'N_o$ given in Table 3. They allow in much the same way as before to obtain the smoothed value for the central point x_i by forming in analogy to (18)

$$'A_{p,o} = \frac{1}{'N_o} \left('\alpha_o\, y_i + \sum_{j=1}^{m} {'\alpha_j}\, D_j^+ \right). \tag{51}$$

Extended numerical checks have shown that adjustments performed with the weighted coefficients $'\alpha_i$ lead to results which show less distortion of the original data than do the corresponding coefficients α_i based on rectangular weights.

Table 3 – Coefficients needed for evaluating the smoothed value $'f_p(o) = 'A_{p,o}$ (with triangular weights)

For p = 2 or 3:

m	$'N_o$	$'\alpha_o$	$'\alpha_1$	$'\alpha_2$	$'\alpha_3$	$'\alpha_4$	$'\alpha_5$
2	15	9	4	-1			
3	132	58	36	9	-8		
4	675	235	168	81	4	-33	
5	717	207	160	98	36	-11	-28

This behaviour is also confirmed by a comparison of the respective moments (see Fig. 2). All the relations given in section 5 hold also for the moments of the convoluting functions which are based on triangular weights. Examples of actual fits are given in Fig. 3 and 4.

Notes added in proof

1. A new reading of the relevant chapters in [7] – they had originally been studied several years ago for a different purpose – reveals that two explicit formulae for obtaining α_i/N_o are actually stated there on page 301. In our notation they can be written in the form

– for p = 2 or 3:

$$\overline{N}_o \equiv C_m \cdot N_o = \frac{3}{(4m^2-1)\,(2m+3)}$$
$$\overline{\alpha}_i \equiv C_m \cdot \alpha_i = 3m^2+3m-1 - 5i^2 , \tag{52}$$

– for p = 4 or 5:

$$\overline{N}_o \equiv C'_m \cdot N_o = \frac{15}{4\,(4m^2-1)\,(4m^2-9)\,(2m+5)}$$
$$\overline{\alpha}_i \equiv C'_m \cdot \alpha_i = 15m^4+30m^3-35m^2-50m+12 - 35(2m^2+2m-3)i^2 + 63\,i^4 . \tag{53}$$

The quantities C_m and C'_m are the largest common factors between $\overline{N}_o$ and $\overline{\alpha}_i$ for a given value of m. They drop when the ratios

$$g_i = \alpha_{|i|}/N_o = \overline{\alpha}_{|i|}/\overline{N}_o$$

are formed. Actually, we did not check the various tedious summations needed

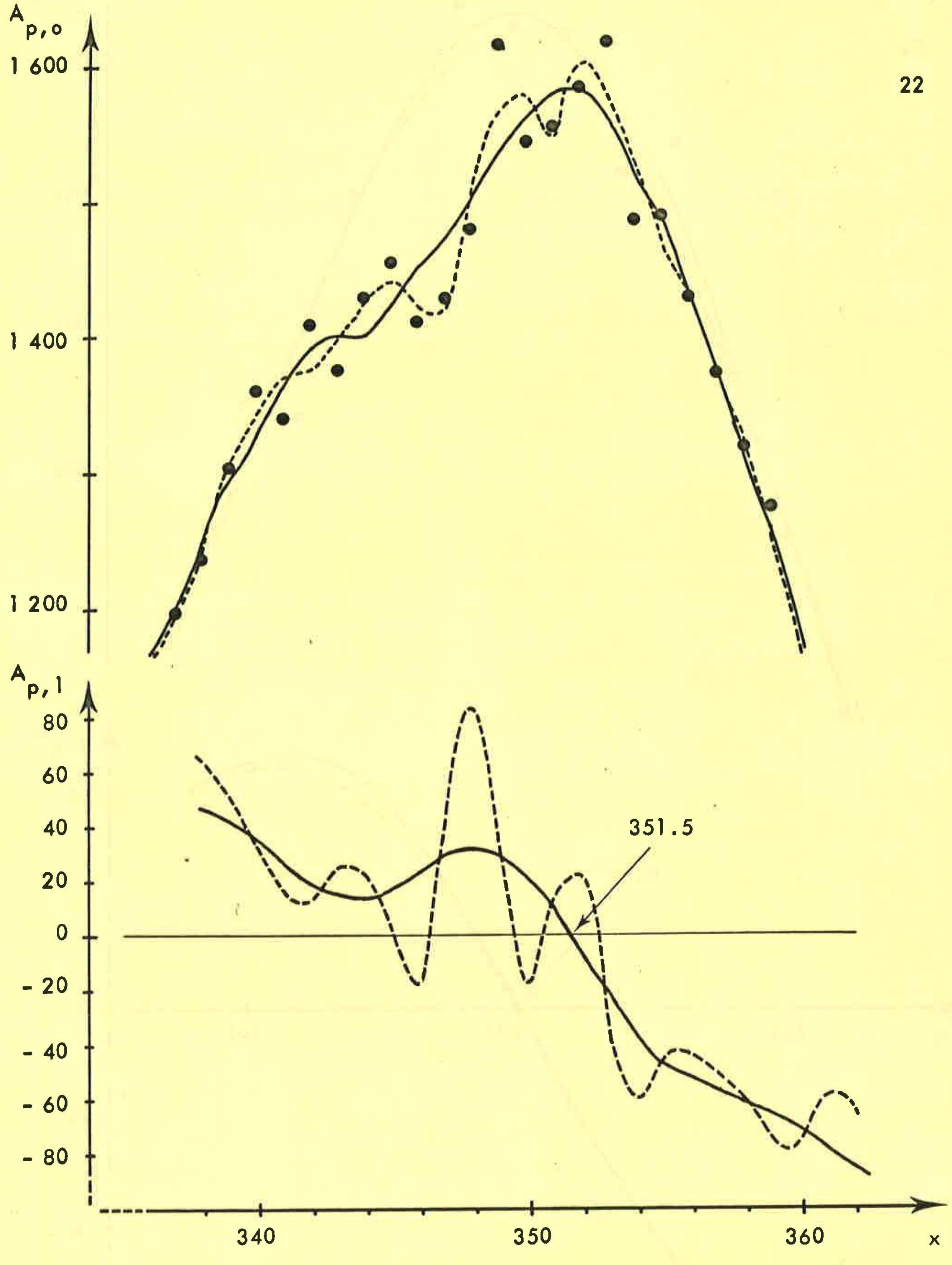

Fig. 3 - Polynomial fits to a peak of the response spectrum of a ^{3}He-counter to 565 keV neutrons

• experimental points

----- fit with p = 3 and m = 2

——— " " p = 3 " m = 5

In the first fit noise has not been sufficiently reduced