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THE EVALUATION OF NUCLEAR DATA

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ABSTRACT

The authors consider a method of calculating a weighted average value, and the uncertainty in it, for a set of measurements of varying accuracy. Attention is drawn to the possibility of allowing for unknown systematic errors or underestimated uncertainties in individual measurements when evaluating the true value of the quantity of interest. A programme is described and its operation illustrated by various examples. The work should be regarded as an attempt to recommend a unified approach to the process of evaluating experimental nuclear data.

The main purpose of any quantitative experiment is to determine the true value of some quantity that is being measured. To obtain an absolutely accurate value of the quantity by experiment is clearly impossible, although approximations are getting much closer to real values as a result of developments in experimental technology and improvements in measuring methods.

A simple comparison shows, however, that the experimental results quoted by different authors generally differ not only within the limits of the quoted statistical uncertainty, but also because some of the measurements - if not all - contain systematic errors. As a rule, the authors of experimental studies do not quote the systematic errors.

The evaluation of nuclear (and not only nuclear) data can be defined as obtaining, from the experimental results of different authors, the most accurate and reliable value of the measured quantity and determining the uncertainty in this value. This process should include the following stages:

- Analysis of the measuring method;
- Analysis of errors;

- Determination of the reliability of the measurements;
- Allocation of statistical weights to the individual measurements;
- Derivation of an evaluated value and its uncertainty.

Unfortunately there is at present no unified approach to the evaluation of experimental results. This applies not so much to the actual evaluation method as to the method of determining the uncertainty in the evaluation; consequently there are large differences in the levels of significance that can be attributed to different evaluations and the value of the results is accordingly reduced.

The present work should be regarded as an attempt to recommend a unified approach to the process of evaluating experimental data.

1. The average value and its uncertainty

Let us suppose that we have a series of measurements of some quantity X*/, given in the following form:

$$\begin{array}{l} x_1, x_2, \ldots, x_n \\ \sigma_1, \sigma_2, \ldots, \sigma_n \end{array} \tag{1}$$

Two approaches are possible to the series in expression (1). It can be regarded simply as a series of measurements of different accuracy with statistical weights p_i given by the formula

$$p_i = \frac{\sigma^2}{\sigma_i^2} \tag{2}$$

where σ is the uncertainty in the unit weight. The weighted average value and its uncertainty will then be [3]:

$$\bar{x} = \frac{1}{p}\sum_i p_i x_i , \tag{3}$$

$$\sigma'_{\bar{x}} = \frac{\sigma'}{\sqrt{p}} , \tag{4}$$

*/ Methods of calculating average values have been explained in detail in courses on mathematical statistics and the theory of errors [1-3].

where

$$p = \sum_i p_i \qquad (5)$$

and

$$\sigma' = \sqrt{\frac{1}{n-1} \sum_i p_i (x_i - \bar{x})^2} \qquad (6)$$

Here, $\sigma'_{\bar{x}}$ is the average uncertainty in the weighted average value from expression (3), and σ' is the average uncertainty in the unit weight obtained from expression (2).

Alternatively, we can assume that, for the quantity X, n series of measurements have been carried out and that we know only the average values for each series and the average uncertainties. If the average value of each series is regarded as the result of some particular measurement, we obtain a series similar to that in expression (1). It can be shown [4] that in this case $\bar{x}$ is again determined by formula (3) and that the uncertainty in the weighted average value is

$$\sigma_{\bar{x}} = \frac{\sigma}{\sqrt{p}} \qquad (7)$$

Here σ, having the significance of an average uncertainty in the unit weight, is determined as in expression (2) with an accuracy to within a constant factor and can be taken as equal to one.

It is customary to assume for a series as in expression (1) that the uncertainty obtained from formula (7) is a quantity reflecting the internal consistency of the data in that series and taking account only of the uncertainties in the values of x_i. The uncertainty obtained from formula (4), which takes account both of the uncertainties in the x_i values and of the deviations of x_i from $\bar{x}$, reflects the external consistency of the data in the series.

Thus the uncertainty based on internal consistency ($\sigma_{\bar{x}}$) is essentially a hypothesis concerning the uncertainty in the weighted average value of the series in expression (1), while the uncertainty based on external consistency ($\sigma'_{\bar{x}}$) is the answer to this hypothesis.

2. Criterion for comparison of the quantities $\sigma_{\bar{x}}$ and $\sigma'_{\bar{x}}$

As a criterion for the consistency of data in the series in expression (1), Birge [4] suggested using the ratio between the uncertainty calculated on the basis of external consistency (σ_{ext}) and the uncertainty calculated on the basis of internal consistency (σ_{int}) (Eqs (4) and (7) respectively).

If the measured x_i are distributed according to their individual uncertainties σ_i, then σ_{ext} must be equal to σ_{int} and the Birge criterion

$$R = \frac{\sigma_{ext}}{\sigma_{int}} \tag{8}$$

must be equal to 1, accurate to within the statistical deviations.

If on the other hand R is very much greater than 1, the data in the series in expression (1) are not consistent and it is highly likely that some values of σ_i are too low or that some of the data contain systematic errors. If R is less than 1, then all data are consistent and some (or all) values of σ_i are too high.

It can be shown [3] that the Birge criterion is very closely related to the χ^2 distribution:

$$R^2 = \frac{\chi^2_{n-1}}{n-1} \; . \tag{9}$$

Expression (9) is basic to any consideration of the consistency of fundamental data that are being subjected to a process of refinement. In the evaluation of nuclear data, however, when one has to subject a very large number of different data arrays to this process, it is convenient to replace the criterion in expression (9) by the relation

$$\frac{|\sigma^2_{int} - \sigma^2_{ext}|}{\sigma^2_{int}} \leqslant k\sqrt{\frac{2}{n-1}} \; , \tag{10}$$

for purposes of determining data consistency. Expression (10) follows from the fact that the mathematical expectation for the ratio $\sigma^2_{ext}/\sigma^2_{int}$ is one, while its dispersion is $\frac{2}{n-1}$; the coefficient k is an index of the level of significance of the assumed relation [5].

In Fig. 1 we have plotted $\chi^2_{n-1}/n-1$ and $1+k\sqrt{\frac{2}{n-1}}$ versus n. It can be seen that for k = 2 the divergence between the two functions is insignificant (for n = 30 it is no more than 3%). For the other values of k (1 and 3) the discrepancy becomes very important. For k = 2, therefore, we can regard expressions (9) and (10) as practically equivalent. The value k = 2 corresponds to a 95% level of significance for fulfillment of expression (10) in the case of a normal distribution and a 70–95% level of significance (depending on n) when a Student distribution is applied.

As a criterion for the existence of a systematic error or an over-estimated uncertainty σ_i we can thus take the expression

$$\frac{|\sigma_{\bar{x}}^2 - \sigma_{\bar{x}}'^2|}{\sigma_{\bar{x}}^2} \cdot \left(\sqrt{\frac{2}{n-1}}\right)^{-1} = k \qquad (11)$$

When k > 2, we may be confident that processing of the series in expression (1) revealed the presence of systematic errors in some of the x_i data, or that some of the σ_i values were underestimated by the authors.

If $k \leq 2$, the data included in the evaluation process are consistent and can be processed.

3. Calculating the average value and its uncertainty

From what we have said above, the whole process of obtaining an average value for the data in a series like that in expression (1) amounts to the following operations:

(1) From formula (2) the statistical weights of the individual measurements are calculated ($\sigma = 1$);

(2) The values of $\bar{x}$ are calculated from expressions (3) and (5), $\sigma_{\bar{x}}$ from expression (7) and $\sigma'_{\bar{x}}$ from expression (6);

(3) If $\sigma_{\bar{x}} > \sigma'_{\bar{x}}$, the final result is obtained in the form:

$$x_0 = \bar{x} \pm \frac{1}{2}(\sigma_{\bar{x}} + \sigma'_{\bar{x}}); \qquad (12)$$

(4) If $\sigma_{\bar{x}} < \sigma'_{\bar{x}}$ and $k \leq 2$ (expression (11)), the final result is obtained in the form:

$$x_0 = \bar{x} \pm \sigma'_{\bar{x}} \tag{13}$$

(5) If $\sigma_{\bar{x}} < \sigma'_{\bar{x}}$ and $k > 2$ (expression (11)), the values of σ_i are renormalized to make $k \leq 2$, new values of $\bar{x}'$ and of the external error $\sigma''_{\bar{x}}$ are calculated, and the final value is obtained in the form:

$$x_0 = \bar{x}' \pm \sigma''_{\bar{x}} \tag{14}$$

The process of renormalizing σ_i for $k > 2$ is described in detail below.

(6) If for any of the values of x_i in the series no uncertainty is quoted, an unweighted average value is calculated:

$$\bar{x}^0 = \frac{\sum_i x_i}{n} \tag{15}$$

along with uncertainty:

$$\sigma^0_{\bar{x}} = \sqrt{\frac{\sum_i (x_i - \bar{x}^0)^2}{n(n-1)}} \tag{16}$$

and the final result takes the form:

$$x_0 = \bar{x}^0 \pm \sigma^0_{\bar{x}} \tag{17}$$

4. Description of the programme for calculating average values (PREAVV)

The programme is written in the FORTRAN-1010B language and consists of a MAIN segment, in which the actual calculation is carried out, and two sub-programmes (STROKA and VVNEF). Figure 2 shows a block diagram of the PREAVV programme for calculating unweighted and weighted averages and their uncertainties.

With the call of the dual programme PREAVV, the message "N OF RESULTS" is printed on the output unit and the STROKA sub-programme activates the data input device and introduces the line information. The VVNEF sub-programme inserts (without format) the number of results being averaged, followed by the actual values and their uncertainties.

After input of the data a print-out control is performed. Should any of the averaged results have zero error, the unweighted average and its uncertainty are calculated from formulae (15) and (16). The $\bar{x}^{o}$ and $\sigma^{o}_{\bar{x}}$ values found are then printed out on the output device with the message

UNWEIGHTED AVERAGE

X=

S=

If all the data being inserted have non-zero error, the weighted average value and its uncertainty (see section 3) are calculated.

The preliminary weighted average and its uncertainty are printed after the messages

P.AV.= P.ER.=

On the same line after the messages

INT.= EXT.=

the internal and external uncertainties of the preliminary weighted average value are printed.

Next, the preliminary value of k (see formula (11)) is found and printed after the message

P.K.=

If $k \leq 2$, the final value is printed:

K=

The preliminary value of the weighted average is rounded off to the sign corresponding to the order of the uncertainty. The final result is printed out under the heading:

* WEIGHTED AVERAGE *

X=

S=

If $k > 2$, the k_i values are scrutinized to find which results contain a systematic error or an underestimated σ_i value. The k_i values are determined from expression (11) for the (n - 1)th result, whereby each of the n results is rejected in turn. For results whose rejection gives $k_i \leq 2$ for the remaining n - 1 values, the existence of a systematic error is also assumed and printed out after the message:

SYST. ERROR OF VALUE n.XXX DX= .

These results are memorized. Next, since the true value of the systematic error is not known, the experimental uncertainty σ_i of the results is increased in steps of 0.1 σ_i and after each increment the weighted average, internal and external uncertainty and k are calculated until k is less than 2. As soon as k becomes less than 2, the message

ERROR OF VALUE n. MUST BE

is printed out, followed by the corrected uncertainty of the i-th result. After this the system prints the final value of k, the rounded-off value of the weighted average found from results with corrected uncertainties, and the uncertainty in the average value.

If, in the analysis k does not become less than 2, it is assumed that the accuracy of all the results is overestimated, and the process of renormalizing the uncertainty is applied to all the data.

5. Examples of the operation of the programme for calculating the weighted average value and its uncertainty

Tritium half-life

Table I shows eight experimental measurements of tritium half-life, together with their uncertainties. The preliminary weighted average, its uncertainty and k are shown in columns 4-6. Processing indicates the possibility of a systematic error in the fourth measurement ($\Delta x_4 = 0.084$). In order for the value of k to become less than 2, σ_4 must be adjusted to 0.036. All the results will then be consistent and the final values of $\bar{x}$ and $\sigma_{\bar{x}}$ are given in the last two columns. In the process of renormalizing σ_4 82 step increments were applied. The variation of k as a function of the number of increments is shown in Fig. 3.

920-keV gamma transition accompanying beta decay of molybdenum-99

Table II shows eleven experimental measurements of the 920-keV gamma line accompanying the beta decay of molybdenum-99. In this case, the programme assumes the existence of systematic errors in the first and second measurements ($\Delta x_1 = 0.35$, $\Delta x_2 = 1.6$). Three step increments in the values of σ_1 and σ_2 give us the final results shown in the last two columns of the table.

Speed of light

The possibilities of the programme are well demonstrated by the processing of experimental measurements of the speed of light.

From Taylor and co-workers [6], who give a recommended value $C = 299792.50 \pm 0.10$, we took 28 values of the speed of light and from these selected 8 values conforming to the condition $\sigma_j \leq 36$ min. These two data arrays were processed. The results are given in Table III. The second line of the table gives the weighted average values of C, their uncertainties, and the coefficient k for the original experimental data arrays. The most accurate value in each array 299792.55 ± 0.05, was then replaced by 299793.00 ± 0.05, and the programme - after indicating that this figure contained a systematic shift (0.44 and 0.43 for arrays of 8 and 29 values respectively) - gave the preliminary weighted average value of C, its uncertainty, and the coefficient k. These figures are given in the third line of the table. Next, the programme started to increase the quoted uncertainty to make $k \leq 2$. The results are given in the last line of the table.

Comparison of the figures in the second and third columns of the table shows also that including in the processing operation only the most accurate data, a procedure sometimes recommended, leads to a slight shift in the weighted average value as a result of the greater weight of such data (in our example, 1/3 S). We therefore consider that it is better to include all the known experimental data in the processing operation.

The above results obtained in processing experimental measurements of the speed of light are shown graphically in Figs 4 and 5. Along the abscissa are plotted the light speeds with their uncertainties, and along the ordinate $h_i = 1/\sigma_i^2$ (the h_i summed). Each figure shows the initial distribution of the light speeds and their uncertainties, the distribution obtained through the shift introduced to the most accurate value, and finally the distribution obtained after the programme has selected a new value for the uncertainty in the shifted value.

REFERENCES

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[5] SCHEFFE, H., The Analysis of Variance, New York, 1959.

[6] TAYLOR, B.N., PARKER, W.H., LANGENBERG, D.N., The fundamental constants and quantum electrodynamics, Academic Press, New York-London, 1969.

Table I

Half-life of tritium. Determination of the weighted average value and its uncertainty

№	x_i	σ_i	P.AV.	P.ER.	P.K	σ_i^k	K	$\bar{x}$	$\sigma_{\bar{x}}$
I	I2,I	0,5				-			
2	I2,46	0,I0				-			
3	I2,4I	0,20				-			
4	I2,262	0,004	I2,329	0,0I2	95	0,036	I,9	I2,346	0,003
5	I2,58	0,I8				-			
6	I2,346	0,002				-			
7	I2,25	0,03				-			
8	I2,43	0,04				-			

Table II

920-keV gamma transition accompanying beta decay of molybdenum-99. Determination of the weighted average value and its uncertainty

№	x_i	σ_i	P.AV.	P.ER.	P.K	σ_i^K	K	$\bar{x}$	$\sigma_{\bar{x}}$
I	920,47	0,II				0,I4			
2	922,36	0,66				0,85			
3	920,83	0,I0				-			
4	922,58	0,8I				-			
5	920,76	0,II				-			
6	922,29	0,78	920,72	0,089	2,8	-	I,7	920,75	0,085
7	920,64	0,63				-			
8	920,53	0,5I				-			
9	920,5	I,0				-			
I0	920,I9	0,68				-			
II	920,70	0,67				-			

Table III

Processing of measurements of the speed of light
(C = 2997 XX.XX)

Number of results averaged	8	29
$(X \pm S)'$	92,55 ± 0,03	92,56 ± 0,03
K'	I,I	I,5
$(X \pm S)''$	92,68 ± 0,08	92,68 ± 0,05
K''	I6	8,9
$(X \pm S)'''$	92,56 ± 0,04	92,57 ± 0,04
K'''	I,9	I,9

FIGURE CAPTIONS

Fig. 1. The dependence of $\chi^2_{n-1}/n-1$ and $1 + k\sqrt{\frac{2}{n-1}}$ on n for different levels of significance:

1. $\alpha = 0.3$, $k = 1$
2. $\alpha = 0.05$, $k = 2$
3. $\alpha = 0.01$, $k = 3$

Fig. 2. Block diagram of the programme for calculating average values and their uncertainties

Fig. 3. Dependence of k_ℓ ($\ell = 0, 1, \dots$) on the number of steps ℓ when increasing the uncertainty of the i-th value

$$\sigma_i^\ell = \sigma_i + 0{,}1 \cdot \ell \cdot \sigma_i$$

(tritium half-life)

Fig. 4. Distribution of 8 values of the speed of light

- Original distribution;
- Distribution with systematic error;
- After programme processing of the "spoiled" distribution.

Fig. 5. Distribution of 29 values of the speed of light

- Original distribution;
- Distribution with systematic error;
- After programme processing of the "spoiled" distribution.

A N N E X

The Annex illustrates the print-out results of processed measurements of the gamma line accompanying the beta decay of molybdenum-99 (920 keV). Two types of print-out are shown:

- With intermediate values of k_ℓ, $\bar{x}$ and $\sigma_{\bar{x}}$;
- With only the final values of k, $\bar{x}$ and $\sigma_{\bar{x}}$.

N OF RESULTS= 11

CONTROL

```
 1, +0,920470E+03 +0,11E+00
 2, +0,922360E+03 +0,66E+00
 3, +0,920830E+03 +0,10E+00
 4, +0,922580E+03 +0,81E+00
 5, +0,920760E+03 +0,11E+00
 6, +0,922290E+03 +0,78E+00
 7, +0,920640E+03 +0,63E+00
 8, +0,920530E+03 +0,51E+00
 9, +0,920530E+03 +0,10E+01
10, +0,920190E+03 +0,68E+00
11, +0,920700E+03 +0,67E+00

                     P,AV,=+0,920721E+03   P,ER,=+0,89E-01   INT=+0,59E-01   EXT=+0,89E-01
                                  P,K=+0,28E+01
```

ANALISYS FOR K

```
 1,+0,920825E+03   +0,92E-01   AKN=+0,15E+01                     INT=+0,70E-01   EXT=+0,92E-01
SYST, ERROR OF VALUE   1,+0,920469E+03    DX=+0,35E+00
 2,+0,920708E+03   +0,81E-01   AKN=+0,17E+01                     INT=+0,59E-01   EXT=+0,81E-01
SYST, ERROR OF VALUE   2,+0,922359E+03    DX=-0,16E+01
 3,+0,920662E+03   +0,11E+00   AKN=+0,28E+01                     INT=+0,74E-01   EXT=+0,11E+00
 4,+0,920711E+03   +0,83E-01   AKN=+0,20E+01                     INT=+0,59E-01   EXT=+0,83E-01
 5,+0,920706E+03   +0,11E+00   AKN=+0,32E+01                     INT=+0,70E-01   EXT=+0,11E+00
 6,+0,920712E+03   +0,86E-01   AKN=+0,22E+01                     INT=+0,59E-01   EXT=+0,86E-01
 7,+0,920722E+03   +0,95E-01   AKN=+0,32E+01                     INT=+0,59E-01   EXT=+0,95E-01
 8,+0,920724E+03   +0,95E-01   AKN=+0,32E+01                     INT=+0,59E-01   EXT=+0,95E-01
 9,+0,920722E+03   +0,94E-01   AKN=+0,32E+01                     INT=+0,59E-01   EXT=+0,94E-01
10,+0,920725E+03   +0,93E-01   AKN=+0,31E+01                     INT=+0,59E-01   EXT=+0,93E-01
11,+0,920721E+03   +0,95E-01   AKN=+0,32E+01                     INT=+0,59E-01   EXT=+0,95E-01

                     P,AV,=+0,920732E+03   P,ER,=+0,88E-01   INT=+0,61E-01   EXT=+0,88E-01
                                  P,K=+0,24E+01
```

```
P.AV.=+0.920742E+03    P.ER.=+0.86E-01    INT=+0.62E-01    EXT=+0.86E-01

           P.K=+0.20E+01

P.AV.=+0.920749E+03    P.ER.=+0.85E-01    INT=+0.63E-01    EXT=+0.85E-01

           P.K=+0.17E+01
ERROR OF VALUE   1.MUST BE +0.14E+00
ERROR OF VALUE   2.MUST BE +0.85E+00
      K=+0.17E+01

                                                   *WEIGHTED AVERAGE*
                                                   X=+0.920750E+03
                                                   S=+0.85E-01

IF CONTINUE,TYPE 1,ELSE-1
```

N OF RESULTS= 11

CONTROL

```
 1, +0,920470E+03 +0,11E+00
 2, +0,922360E+03 +0,66E+00
 3, +0,920830E+03 +0,10E+00
 4, +0,922580E+03 +0,81E+00
 5, +0,920760E+03 +0,11E+00
 6, +0,922290E+03 +0,78E+00
 7, +0,920640E+03 +0,63E+00
 8, +0,920530E+03 +0,51E+00
 9, +0,920530E+03 +0,10E+01
10, +0,920190E+03 +0,68E+00
11, +0,920700E+03 +0,67E+00

            P,AV,=+0,920721E+03   P,ER,=+0,89E-01   INT=+0,59E-01   EXT=+0,89E-01
                          P,K=+0,28E+01
```

ANALISYS FOR K

```
 1,+0,920825E+03   +0,92E-01   AKN=+0,15E+01      INT=+0,70E-01   EXT=+0,92E-01
SYST, ERROR OF VALUE   1,+0,920469E+03   DX=+0,35E+00
 2,+0,920708E+03   +0,81E-01   AKN=+0,17E+01      INT=+0,59E-01   EXT=+0,81E-01
SYST, ERROR OF VALUE   2,+0,922359E+03   DX=-0,16E+01
 3,+0,920662E+03   +0,11E+00   AKN=+0,28E+01      INT=+0,74E-01   EXT=+0,11E+00
 4,+0,920711E+03   +0,83E-01   AKN=+0,20E+01      INT=+0,59E-01   EXT=+0,83E-01
 5,+0,920706E+03   +0,11E+00   AKN=+0,32E+01      INT=+0,70E-01   EXT=+0,11E+00
 6,+0,920712E+03   +0,86E-01   AKN=+0,22E+01      INT=+0,59E-01   EXT=+0,86E-01
 7,+0,920722E+03   +0,95E-01   AKN=+0,32E+01      INT=+0,59E-01   EXT=+0,95E-01
 8,+0,920724E+03   +0,95E-01   AKN=+0,32E+01      INT=+0,59E-01   EXT=+0,95E-01
 9,+0,920722E+03   +0,94E-01   AKN=+0,32E+01      INT=+0,59E-01   EXT=+0,94E-01
10,+0,920725E+03   +0,93E-01   AKN=+0,31E+01      INT=+0,59E-01   EXT=+0,93E-01
11,+0,920721E+03   +0,95E-01   AKN=+0,32E+01      INT=+0,59E-01   EXT=+0,95E-01

            P,AV,=+0,920749E+03   P,ER,=+0,85E-01   INT=+0,63E-01   EXT=+0,85E-01
```

```
ERROR OF VALUE  1,  MUST BE +0,14E+00


ERROR OF VALUE  2,  MUST BE +0,85E+00
         K=+0,17E+01

                                              *WEIGHTED AVERAGE*
                                              X=+0,920750E+03
                                              S=+0,85E-01



IF CONTINUE,TYPE 1,ELSE-1

 GOOD-BYE!
```

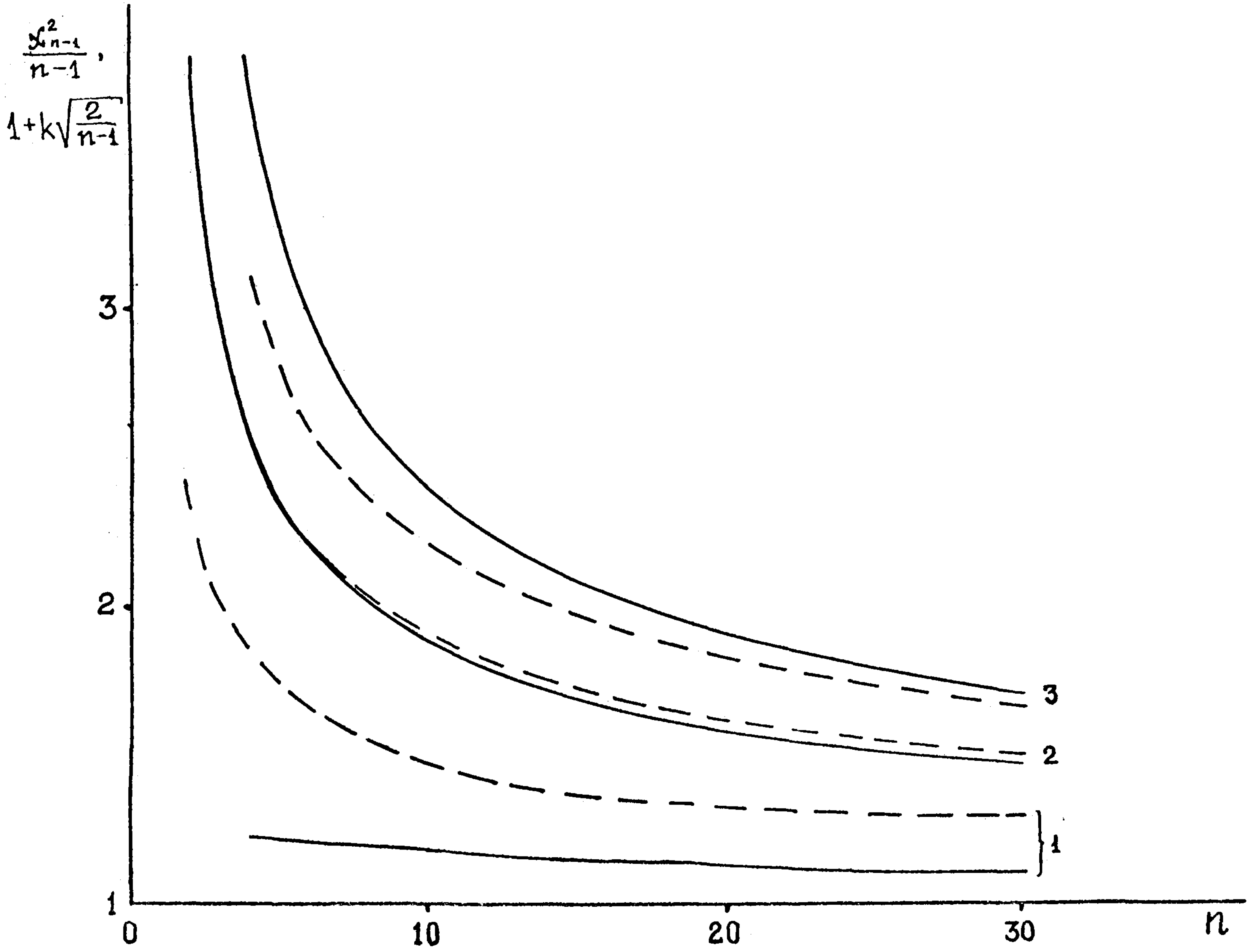
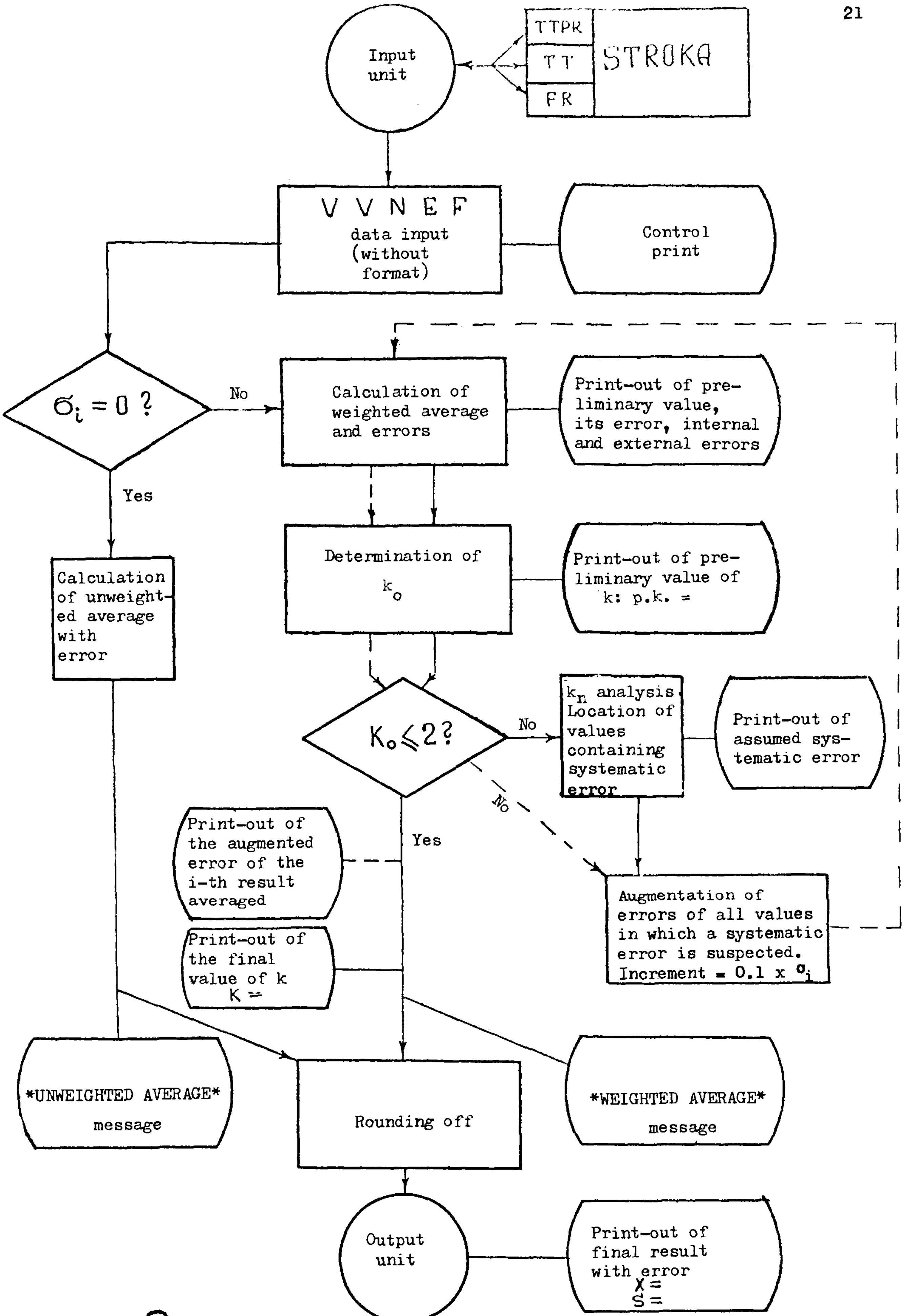


Fig. 1



Input unit
TTPR
TT
FR
STROKA
VVNEF data input (without format)
Control print
σi = 0 ?
No
Yes
Calculation of weighted average and errors
Print-out of preliminary value, its error, internal and external errors
Determination of ko
Print-out of preliminary value of k: p.k. =
Calculation of unweighted average with error
Ko≤2?
No
kn analysis. Location of values containing systematic error
Print-out of assumed systematic error
No
Yes
Print-out of the augmented error of the i-th result averaged
Augmentation of errors of all values in which a systematic error is suspected. Increment = 0.1 x σi
Print-out of the final value of k K =
UNWEIGHTED AVERAGE message
Rounding off
WEIGHTED AVERAGE message
Output unit
Print-out of final result with error X = S =

Fig. 2

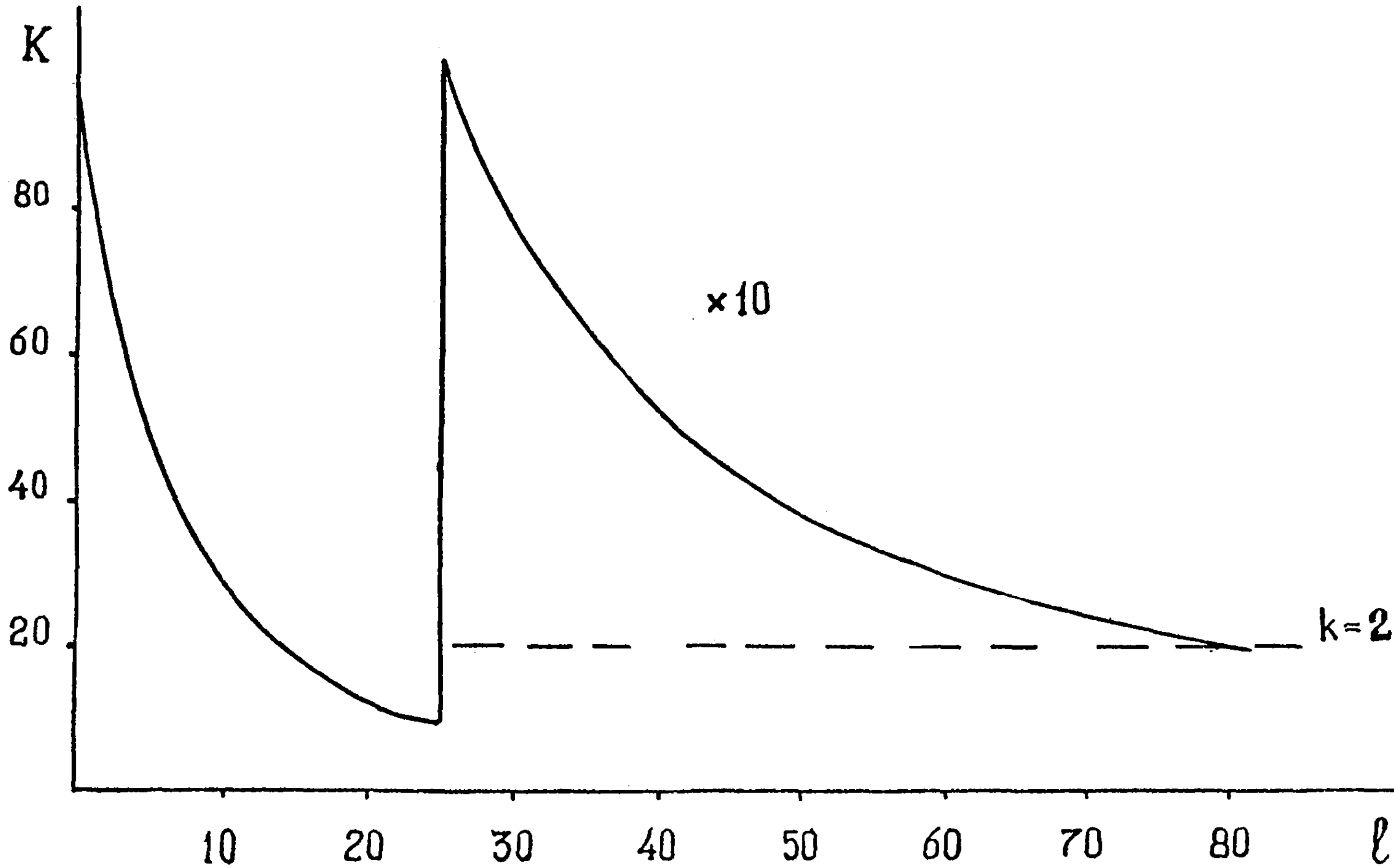


Fig. 3

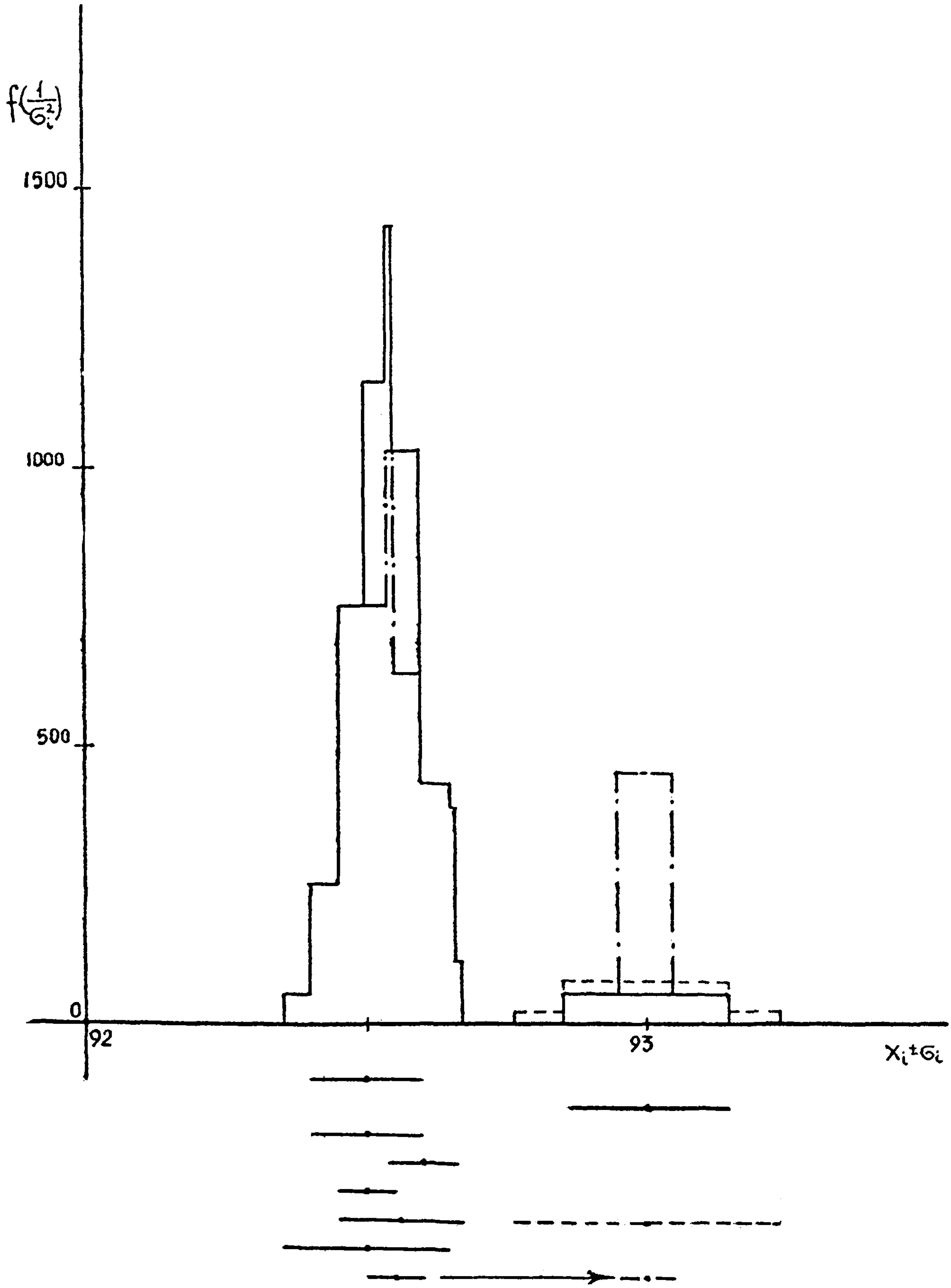


Fig. 4

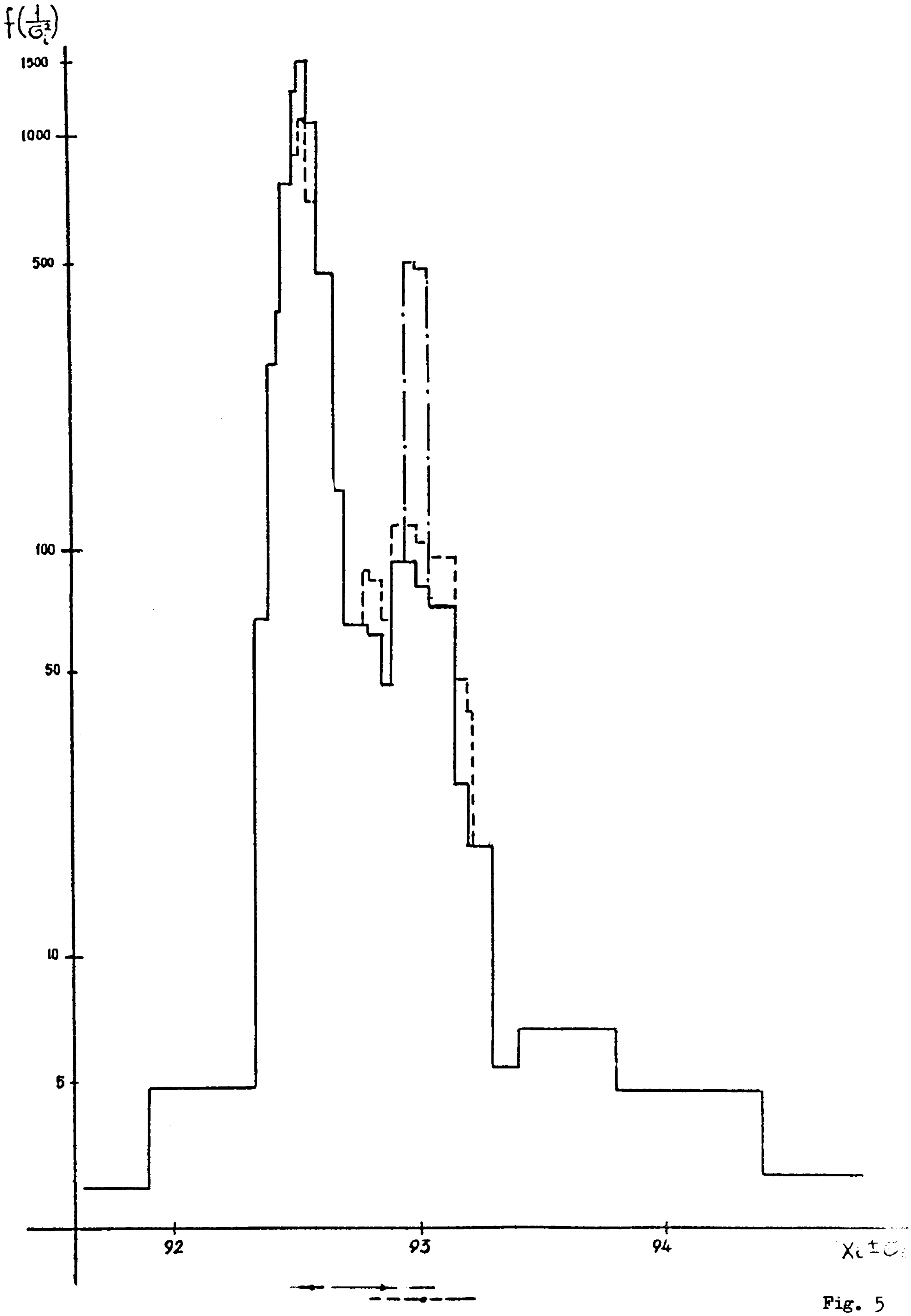


Fig. 5

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