KfK 4077
EUR 9616e
August 1986

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ISSN 0303-4003

Abstract

The DoD-method for measurement data evaluation allows meaningful estimation of variances or standard deviations without the necessity to reject outlier values. It has been developed at KfK in particular for evaluating analytical data. The basic elements used for statistical treatment are all D = (N-1)*N/2 absolute differences that can be formed between N measurement values.
For $N \leq 10$ it is shown that the D absolute differences can be divided into (N-1) subgroups, each of them consisting of N/2 stochastically independent elements. Furthermore, a relationship is given between the estimates for the standard deviations of the subgroups and the estimate for the standard deviation of the total group of absolute differences. Numerical examples are presented.

Betrachtungen zum DoD-Verfahren
zur Auswertung von Meßdaten

Zusammenfassung

Das am KfK entwickelte DoD-Verfahren zur Auswertung analytischer Meßdaten ermöglicht die sinnvolle Schätzung von Varianzen bzw. Standardabweichungen ohne den Ausschluß von Ausreißerwerten. Es verwendet als statistische Grundelemente alle D = (N-1)*N/2 absoluten Differenzen, die zwischen N Meßwerten gebildet werden können.
Für $N \leq 10$ wird gezeigt, daß sich die Menge der D absoluten Differenzen in (N-1) Teilmengen zerlegen läßt, von denen jede aus N/2 stochastisch unabhängigen Elementen besteht. Außerdem wird eine Ungleichung für den Zusammenhang der Schätzwerte der Standardabweichungen dieser Teilmengen vom Schätzwert der Standardabweichungen der Gesamtmenge angegeben. Die Aussagen werden an Zahlenbeispielen illustriert.

Study on the DoD-Method
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W. Beyrich[a)]

1. Introduction

During the last years, the DoD-Method[b)] was proposed as an empirical approach of measurement data evaluation in particular in the field of interlaboratory exercises /1,2,3/. With this method, the absolute differences of the results of repetitive measurements are used as the basis for statistical data treatment. It allows to derive meaningful estimates of standard deviations without the necessity to reject extreme values by the application of statistical outlier criteria. This latter procedure is unsatisfactory, since different criteria lead to different results and since wrong decisions may be made if data are suppressed by purely statistical reasons /4/.

If $y_1, y_2 \dots y_N$ are measurement results obtained on samples of the same material, the method consists in the calculation of all $\frac{N}{2}(N-1)$ absolute differences $d_{ij} = |y_i - y_j|$ (i<j) and their cumulative plotting. As an example, the DoD-evaluation of Pu-concentration determinations of a diluted reprocessing input solution by 27 laboratories is shown in Fig. 1[c)].

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a) Delegate of the Commission of the European Communities.

b) 'DoD'stands for Distribution of Differences.

c) Example taken from /5/.

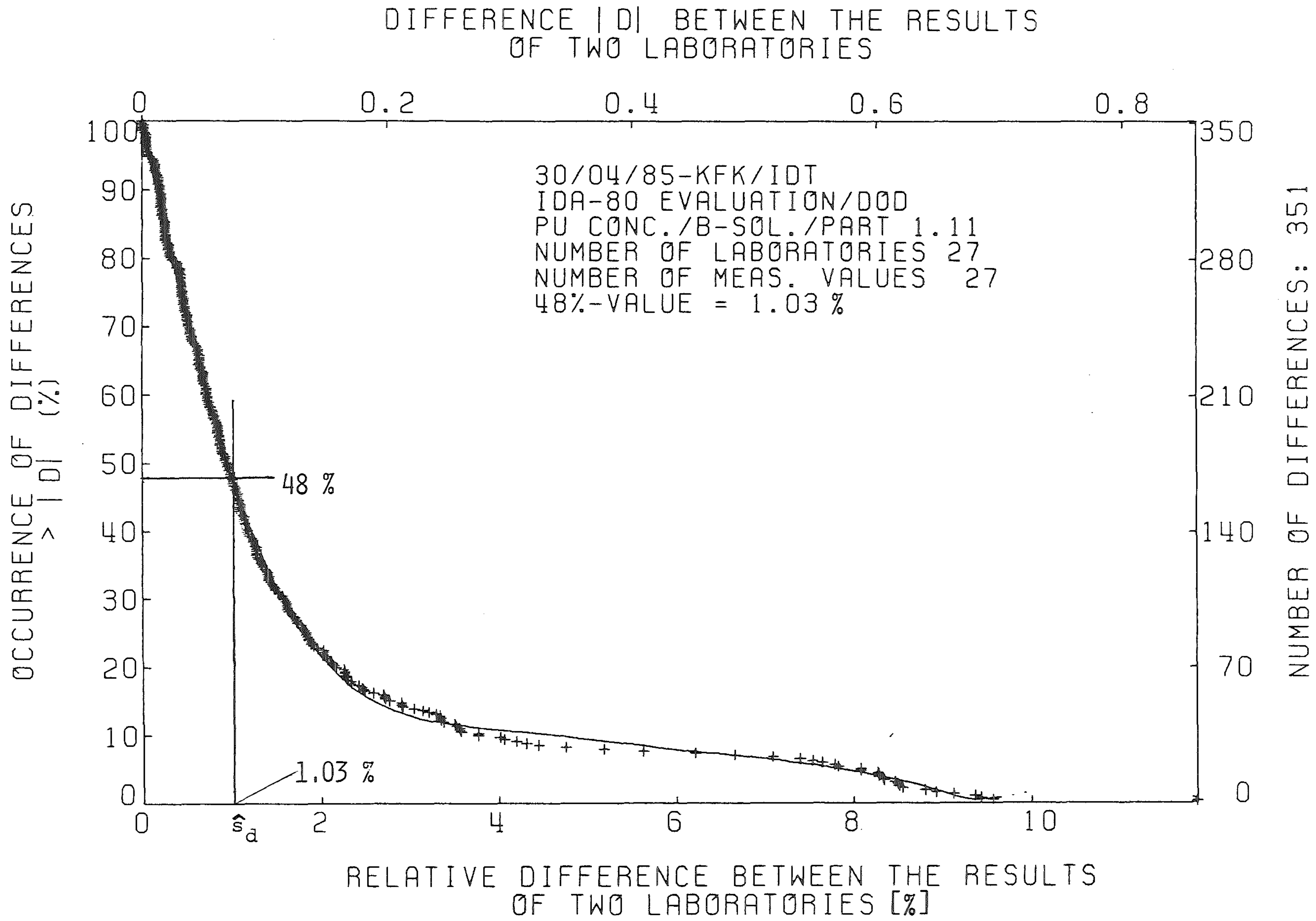

Fig. 1: Example of a Measurement Data Evaluation by the DoD-Method

(The computer graph was prepared at the Institut für Datenverarbeitung in der Technik, IDT/KfK.)

2. Estimation of the Standard Deviation

Under the assumptions that the measurement values $y_1, y_2 \dots y_N$ are normally distributed and that only N/2 independent absolute differences $|y_1-y_2|$, $|y_3-y_4| \dots |y_{N-1}-y_N|$ are used, it can be shown that - in a presentation like Fig. 1 - the abscissa value of the DoD-curve which corresponds to the ordinate value of about 48 % is an estimate of the standard deviation of the basic group of measurement data $y_1, y_2 \dots y_N$. There is $s_y \approx 1.17\ s_d$ if s_y and s_d are the expectation values for the standard deviations of the measurement values y_i and the independent absolute differences $|y_i-y_j|$, respectively /6/. However, for the case of using all $\frac{N}{2}(N-1)$ interdependent differences as it is preferably done in practice, these relations could not be confirmed so far /7/.

Recent studies now gave evidence that the total group of $\frac{N}{2}(N-1)$ absolute differences can be subdivided into (N-1) subgroups, each one consisting of $\frac{N}{2}$ stochastically independent elements. This is proved for all even numbers of $N \leq 10$[d)] and it can hardly be questioned that this is of general validity. (Probably it can be shown by mathematical induction.) Since the expectation value for the estimate of the standard deviation of each subgroup is the same - namely that of the basic data group $y_1, y_2 \dots y_N$ - the expectation value for the estimate of the standard deviation based on the total of the absolute differences of all (N-1) subgroups is obviously the same too. This shows, that the empirical approach of data treatment which uses all existing absolute differences of measurement data for the estimation of the standard deviation is meaningful[e)].

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d) See Appendix A.

e) At least for $N \leq 10$. (In the case of odd numbers for N, the last value is neglected.)

3. Relationship between the Different Estimates of the Standard Deviation

As far as the relationship is concerned between the values estimated for the standard deviation from the subgroups of (independent) differences and the estimate derived from the total group of (interdependent) differences, the following consideration can be made:

If $y_1, y_2 \ldots y_N$ denotes a group of measurement data determined on the same sample material, according to the DoD-method, all $D = \frac{N}{2}(N-1)$ absolute differences

$$d_{i,j} = \left| y_i - y_j \right| \tag{1}$$

with i<j are formed[f)]. These differences have the mean value

$$\bar{d} = \frac{1}{D} * \sum_{i,j=1}^{D} d_{ij} \quad ; \; i<j \tag{2}$$

and the standard deviation

$$\hat{s}_d = \sqrt{\frac{\sum_{i,j}^{D} (d_{i,j} - \bar{d})^2}{D-1}} \quad ; \; i<j \tag{3}$$

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f) It is assumed that N is an even number. If not, the last value is neglected.

As shown before, the total of the $D = \frac{N}{2}(N-1)$ differences $d_{i,j}$ can be subdivided in N-1 subgroups of $\frac{N}{2}$ independent differences each.

If $d_{k,l}$ denotes difference k of subgroup l ($k=1,2....\frac{N}{2}$; $l=1,2...(N-1)$), then mean and standard deviation of subgroup l are given by

$$\bar{d}_l = \frac{1}{N/2} \sum_{k=1}^{N/2} d_{k,l} \qquad (4)$$

and

$$\hat{s}_l = \sqrt{\frac{\sum_{k=1}^{N/2} (d_{k,l}-\bar{d}_l)^2}{\frac{N}{2} - 1}} \qquad (5)$$

Using these denotions of the subgroups, eq. 3 can be written as

$$\hat{s}_d = \sqrt{\frac{\sum_{l=1}^{N-1} \sum_{k=1}^{N/2} (d_{k,l}-\bar{d})^2}{\frac{N}{2}(N-1)-1}} \qquad (6)$$

or

$$\hat{s}_d^2 = \frac{\sum_{k=1}^{N/2} (d_{k,1}-\bar{d})^2}{\frac{N}{2}(N-1)-1} + \frac{\sum_{k=1}^{N/2} (d_{k,2}-\bar{d})^2}{\frac{N}{2}(N-1)-1} + \;.....$$

$$\ldots \quad \frac{\sum_{k=1}^{N/2} (d_{k,N-1}-\bar{d})^2}{\frac{N}{2}(N-1)-1} \qquad (7)$$

If the mean value $\bar{d}$ of all differences is always replaced by the mean value $\bar{d}_1$ of the related subgroup, each term is substituted by a smaller one. Therefore, and after extension of each fraction by $\frac{N}{2} - 1$, it follows

$$\hat{s}_d^2 \geq \frac{\frac{N}{2} - 1}{\frac{N}{2}(N-1)-1} (\hat{s}_1^2 + \hat{s}_2^2 + \ldots \hat{s}_{N-1}^2) \qquad (8)$$

or

$$\frac{\hat{s}_d^2}{\sum_{l=1}^{N-1} \hat{s}_l^2} \geq \frac{1}{N+1} \qquad (9)$$

For the special case $\hat{s}_1 = \hat{s}_2 \ldots = \hat{s}_{N-1}$

$$\frac{\hat{s}_d^2}{\hat{s}_1^2} \geq \frac{N-1}{N+1} \qquad (10)$$

is obtained with

$$\hat{s}_d \approx \hat{s}_1 \qquad (11)$$

for large values of N[g)].

g) In all numerical applications carried out so far, also the relationship

$$\frac{\hat{s}_d^2}{\sum_{l=1}^{N-1} \hat{s}_l^2} \leq \frac{1}{N-1}$$

was found. However, yet no proof can be given for its general validity.

4. Numerical example

Analysing the same sample material, 10 laboratories obtained the following results[h)]

y_1	= 0.6006	y_6	= 0.5965
y_2	= 0.5966	y_7	= 0.6058
y_3	= 0.6071	y_8	= 0.5939
y_4	= 0.5984	y_9	= 0.5954
y_5	= 0.6002	y_{10}	= 0.5966

According to Par.4 of the Appendix, the following absolute values of differences are obtained:

Subgroup: I		II		III	
y_1-y_2	= 0.0040	y_1-y_3	= 0.0065	y_1-y_4	= 0.0022
y_3-y_4	= 0.0087	y_2-y_4	= 0.0018	y_2-y_5	= 0.0036
y_5-y_6	= 0.0037	y_5-y_7	= 0.0056	y_3-y_6	= 0.0106
y_7-y_8	= 0.0119	y_6-y_9	= 0.0011	y_7-y_{10}	= 0.0092
y_9-y_{10}	= 0.0012	y_8-y_{10}	= 0.0027	y_8-y_9	= 0.0015

IV		V		VI	
y_1-y_5	= 0.0004	y_1-y_6	= 0.0041	y_1-y_7	= 0.0052
y_2-y_9	= 0.0012	y_2-y_7	= 0.0092	y_2-y_6	= 0.0001
y_3-y_7	= 0.0013	y_3-y_8	= 0.0132	y_3-y_9	= 0.0117
y_4-y_8	= 0.0045	y_4-y_9	= 0.0030	y_4-y_{10}	= 0.0018
y_6-y_{10}	= 0.0001	y_5-y_{10}	= 0.0036	y_5-y_8	= 0.0063

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h) This concerns plutonium concentration determinations of an undiluted reprocessing input solution using the 'in-situ'-spike technique. See /8/, Evaluation Sheet 75-1, 'Subgroup II'.

VII		VIII		IX	
y_1-y_8	= 0.0067	y_1-y_9	= 0.0052	y_1-y_{10}	= 0.0040
y_2-y_{10}	= 0.0000	y_2-y_8	= 0.0027	y_2-y_3	= 0.0105
y_3-y_5	= 0.0069	y_3-y_{10}	= 0.0105	y_4-y_7	= 0.0074
y_4-y_6	= 0.0019	y_4-y_5	= 0.0018	y_5-y_9	= 0.0048
y_7-y_9	= 0.0104	y_6-y_7	= 0.0093	y_6-y_8	= 0.0026

In Tab. 1 the estimated standard deviations of the subgroups (calculated according to eq. 5) are compiled, the squares of these values and their sum. Furthermore, the mean of the standard deviations of the subgroups is given. At the bottom, the corresponding data are presented as calculated for the group of all measurement values according to eq.3: The standard deviation $\hat{s}_d$ estimated on the basis of all D = N/2(N-1) = 45 differences lies within the values estimated on the basis of the 9 subgroups, each one consisting of independent differences, and the relationship of eq. 9

$$\frac{\hat{s}_d^2}{\sum_{l=1}^{N-1} \hat{s}_l^2} \geq \frac{1}{N+1}$$

is fulfilled with

$$\frac{0.00001378}{0.00012712} = 0.108 \geq \frac{1}{11} = 0.091 \quad .$$

The standard deviation $\hat{s}_d$ estimated from all absolute differences deviates - at least in this example - by only 2 % from $\bar{\hat{s}}_l$, the mean value for the estimates of the standard deviations of the subgroups.

Table 1: Numerical example

Subgroup 1	$\hat{s}_1$	$\hat{s}_1^2$
I	0.004312	0.00001860
II	0.002382	0.00000567
III	0.004188	0.00001754
IV	0.001754	0.00000308
V	0.004431	0.00001963
VI	0.004496	0.00002022
VII	0.004186	0.00001753
VIII	0.003881	0.00001507
IX	0.003127	0.00000978
	$\bar{\hat{s}}_1$ = 0.003640	Σ = 0.00012712
	$\hat{s}_d$	$\hat{s}_d^2$
All values	0.003712	0.00001378

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Appendix

Proofs on the Possibility to Subdivide the Total of Differences into Groups of Independent Ones

If y_1, y_2 ... y_i ... y_N is a group of data, D = $\frac{N}{2}(N-1)$ differences of the type (y_i-y_j) with i<j can be formed. Since each value y_i is part of N-1 differences, there exists a considerable intercorrelation. However, as shown below, for all even values y≤N≤10, the total D of the differences can be subdivided into (N-1) groups of N/2 independent differences each.

1. N=4; D=6

Subgroup:	I	II	III
	y_1-y_2	y_1-y_3	y_1-y_4
	y_3-y_4	y_2-y_4	y_2-y_3

2. N=6; D=15

Subgroup:	I	II	III
	y_1-y_2	y_1-y_3	y_1-y_4
	y_3-y_4	y_2-y_5	y_2-y_6
	y_5-y_6	y_4-y_6	y_3-y_5

IV	V
y_1-y_5	y_1-y_6
y_2-y_4	y_2-y_3
y_3-y_6	y_4-y_5

3. N=8; D=28

Subgroup: I	II	III	IV
Y_1-Y_2	Y_1-Y_3	Y_1-Y_4	Y_1-Y_5
Y_3-Y_4	Y_2-Y_4	Y_2-Y_7	Y_2-Y_6
Y_5-Y_6	Y_5-Y_7	Y_3-Y_6	Y_3-Y_7
Y_7-Y_8	Y_6-Y_8	Y_5-Y_8	Y_4-Y_8

V	VI	VII
Y_1-Y_6	Y_1-Y_7	Y_1-Y_8
Y_2-Y_8	Y_2-Y_5	Y_2-Y_3
Y_3-Y_5	Y_3-Y_8	Y_4-Y_5
Y_4-Y_7	Y_4-Y_6	Y_6-Y_7

4. N=10; D=45

Subgroup: I	II	III	IV
Y_1-Y_2	Y_1-Y_3	Y_1-Y_4	Y_1-Y_5
Y_3-Y_4	Y_2-Y_4	Y_2-Y_5	Y_2-Y_9
Y_5-Y_6	Y_5-Y_7	Y_3-Y_6	Y_3-Y_7
Y_7-Y_8	Y_6-Y_9	Y_7-Y_{10}	Y_4-Y_8
Y_9-Y_{10}	Y_8-Y_{10}	Y_8-Y_9	Y_6-Y_{10}

V	VI	VII	VIII	IX
Y_1-Y_6	Y_1-Y_7	Y_1-Y_8	Y_1-Y_9	Y_1-Y_{10}
Y_2-Y_7	Y_2-Y_6	Y_2-Y_{10}	Y_2-Y_8	Y_2-Y_3
Y_3-Y_8	Y_3-Y_9	Y_3-Y_5	Y_3-Y_{10}	Y_4-Y_7
Y_4-Y_9	Y_4-Y_{10}	Y_4-Y_6	Y_4-Y_5	Y_5-Y_9
Y_5-Y_{10}	Y_5-Y_8	Y_7-Y_9	Y_6-Y_7	Y_6-Y_8