

Standard Errors of the Residues in a Least-Squares Analysis

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The covariance matrix between input and output data of a least-squares analysis is computed and hence the standard error of a residue may be evaluated. This leads directly to a means of evaluating the consistency of the data more precisely than is usually the case. This result is applied to the 1955 analysis of DuMond and Cohen.

IN a least-squares adjustment of data such as those bearing on the fundamental atomic constants,^{1,2} it is important to be able to assign standard deviations to the differences between the least-squares adjusted output data and the input data from which they are obtained. Unless this is done, it is not possible to make a well-defined decision on the significance of those differences. Thus, for example, in DC55² the input value of the wavelength conversion factor $\lambda_o/\lambda_s = \Lambda$ was 1.002020 ± 30 ppm (parts per million) while the least-squares output value was $\Lambda = 1.002039 \pm 14$ ppm, and the question arises whether the difference of 19 ppm indicates a significant and important discrepancy or whether it is indicative only of the statistical variation to be expected. It is certainly incorrect to calculate the standard deviation of the difference without considering the correlation which exists between input and output data.

We consider a set of observational equations, written in matrix form³ as

$$\mathbf{Ax} = \mathbf{C}.$$

To this system of linear equations must be assigned a weight matrix $\boldsymbol{\pi}$. The least-squares solution is $\mathbf{x}^* = \mathbf{P}^{-1}\mathbf{k}$, where $\mathbf{P} = \mathbf{A}^+\boldsymbol{\pi}\mathbf{A}$ and $\mathbf{k} = \mathbf{A}^+\boldsymbol{\pi}\mathbf{C}$. The vector \mathbf{x}^* is the adjusted value of the vector \mathbf{x} ; from this we can compute the adjusted values of the numerical input data:

$$\mathbf{C}^* = \mathbf{AP}^{-1}\mathbf{k} = \mathbf{A}[\mathbf{A}^+\boldsymbol{\pi}\mathbf{A}]^{-1}\mathbf{A}^+\boldsymbol{\pi}\mathbf{C}.$$

The covariance matrix which expresses the correlations between an input numeric c_i and an output numeric c_j^* can now be computed, and it turns out to be the same as the covariance matrix between data themselves, $\mathbf{AP}^{-1}\mathbf{A}^+$. (Recall that the covariance between input data is expressed by the matrix $\boldsymbol{\pi}^{-1}$.)

The standard deviation of the difference, $c_i^* - c_i$, between an input datum and its adjusted output value is given by $[\sigma_i^2 - \sigma_i^{*2}]^{1/2}$, where σ_i is the standard deviation of the input datum and σ_i^* , that of the output value. This surprisingly simple result justifies the description of the adjusted value as being compounded from two terms—the direct input datum itself plus a

single quantity which represents the effect of all the other data. This effective value is statistically independent of the input datum even though observational correlations exist in the actual inputs. The variance of the difference $c_i^* - c_i$ is then just the variance of this effective value. The DC55 least-squares adjusted value of Λ referred to above is then made up of the direct input value plus the effective quantity (representing all of the other data) $\Lambda_{\text{eff}} = 1.002044 \pm 15.5$ ppm. The consistency between the direct input datum and all of the other input data is measured by the difference $\Lambda_{\text{in}} - \Lambda_{\text{eff}} = (24 \pm 34)$ ppm.

A comparison of all the final input data of DC55 is given in Table I. Only Eq. (6-3) (the Bearden and Schwarz determination of the short-wavelength limit) is at all discordant, and even this discrepancy is only slightly larger than two probable errors (assuming a Gaussian distribution of errors).

It is also possible to make a direct comparison between each input datum and the value of the same quantity computed by a least-squares analysis which omits that item. This latter value is merely the effective datum mentioned previously. In terms of the input and output data, the effective quantity is given by

$$c_i' = c_i^* + \frac{\sigma_i^{*2}}{\sigma_i^2 - \sigma_i^{*2}}(c_i^* - c_i),$$

$$\sigma_i' = \sigma_i \sigma_i^* (\sigma_i^2 - \sigma_i^{*2})^{-1/2},$$

where c_i' is the value of c_i computed from a least-squares analysis which omits the direct observation, and σ_i' is its standard error. The comparison of c_i with c_i' gives a direct means for evaluating the consistency of any given measurement with all of the other data and in addition

TABLE I. Residues of least-squares data. All errors are computed on the basis of internal consistency.

Equation number (DC55)	Input value	Output value	Difference output-input
0-1	0.00 ± 3.00	1.94 ± 1.37	1.94 ± 2.68
1-1	3.50 ± 3.78	3.45 ± 3.46	-0.05 ± 1.51
2-1	4.00 ± 0.45	3.92 ± 0.44	-0.08 ± 0.07
3-1	-2.30 ± 2.29	-1.96 ± 1.34	0.36 ± 1.86
4-1	11.10 ± 1.31	11.35 ± 1.13	0.25 ± 0.66
5-2	13.50 ± 1.10	13.31 ± 0.99	-0.19 ± 0.47
6-3	-5.60 ± 8.16	7.86 ± 1.46	13.46 ± 8.04

¹ J. W. M. DuMond and E. R. Cohen, *Revs. Modern Phys.* **25**, 691 (1953).

² Cohen, DuMond, Layton, and Rollett, *Revs. Modern Phys.* **27**, 363 (1955); the article is referred to as DC55.

³ E. R. Cohen, *Revs. Modern Phys.* **25**, 709 (1953).

TABLE II. Direct and indirect values. Each indirect value is the result of a least-squares solution from which the direct measurement has been omitted and hence represents the value of the quantity which may be inferred from the totality of other measurements.

Equation number (DC55)	Direct value	Indirect value
0-1	0.00±3.00	2.45±1.53
1-1	3.50±3.78	3.19±8.66
2-1	4.00±0.45	0.76±2.83
3-1	-2.30±2.29	-1.77±1.86
4-1	11.10±1.31	12.08±2.24
5-2	13.50±1.10	12.47±2.32
6-3	-5.60±8.16	8.30±1.48

indicates to what extent the output value of a given function is determined by the indirect implications of that other data.

The direct input values and the indirect least squares values are presented in Table II. From this table we see for example that the indirect value of 0-1 (the conversion factor from x-units to milliangstroms) is somewhat more accurate than the direct value. On the other hand item 1-1 (the Siegbahn-Avogadro number, $N_s' = N\lambda^3$) is given much more accurately by the direct

data than by the indirect. That this was so has been established previously in more cumbersome ways.⁴

The directly measured value of item 2-1 (fine-structure splitting in deuterium) is more than six times as accurate, giving it almost forty times as much weight, as the indirect value. This demonstrates forcibly how important Dayhoff, Triebwasser, and Lamb's measurement of the fine-structure constant is in providing a crucial datum for the values of the atomic constants. On the other hand, the situation is reversed with respect to the h/e determinations, (6-3); in this case the indirect value is much more accurate than the direct measurement. If the direct measurement were omitted from the analysis, the weight assignable to the value of h/e would be changed only slightly and the output value would be altered by less than half the probable error. The need for further measurements of the short-wavelength limit of the continuous x-ray spectrum has of course been previously emphasized.^{2,5}

⁴ J. W. M. DuMond and E. R. Cohen, Phys. Rev. **94**, 1790 (1954); E. R. Cohen and J. W. M. DuMond, Phys. Rev. **98**, 1128 (1955).

⁵ J. A. Bearden and J. S. Thomsen, "A Survey of Atomic Constants," The Johns Hopkins University, Baltimore, 1955 (unpublished).

Field Dependence of Magnetoconductivity

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A theoretical calculation of the magnetic field dependence of the elements of the conductivity tensor has been performed for a crystal with a general electronic energy band structure. It was assumed that the Boltzmann equation is valid, and that an energy-dependent relaxation time exists. The results are the same as would be given by a superposition of electron gases, whose cyclotron frequencies are related harmonically. The strengths of the har-

monics depend upon the energy band structure; in particular, there are certain relations among them which are required by symmetry. The diagonal elements of the conductivity tensor are found to be monotonically decreasing functions of the magnetic field strength. Extension of the calculation to alternating electric fields reveals harmonics in the cyclotron resonance.

1. INTRODUCTION

UNTIL recently, calculations of the magnetic field dependence of the Hall effect and magnetoresistivity have been confined to materials with simple ellipsoidal band structures.¹ For general band structures, the limiting cases of very weak fields² and very strong fields³ have been studied. Zeiger has reported a calculation based on a particular (nonellipsoidal) model for the band structure of *p*-type germanium.⁴ This paper con-

sists of a calculation which applies, under restrictions which are discussed below, at all field strengths to general band structures. We show that certain new features found by Zeiger are to be expected in general.

In materials which contain more than one type of carrier, the field dependence of the Hall effect and magnetoresistivity may be used to separate the effects of the different carriers, and to obtain concentrations and mobilities for each type. Such analyses have been carried out for *p*-type germanium, in which the two carriers are light and heavy holes.^{5,6} The separation was accomplished by fitting the experimental data to theoretical formulas derived on the basis of spherical energy surfaces. To make a similar analysis on a material with

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¹ See, for instance, H. Jones, Proc. Roy. Soc. (London) **A155**, 653 (1936); B. Abeles and S. Meiboom, Phys. Rev. **95**, 31 (1954); and M. Shibuya, Phys. Rev. **95**, 1385 (1954).

² H. Jones and C. Zener, Proc. Roy. Soc. (London) **A145**, 268 (1934).

³ J. A. Swanson, Phys. Rev. **98**, 1534 (1955); **99**, 1799 (1955).

⁴ H. J. Zeiger, Phys. Rev. **98**, 1560 (1955).

⁵ Willardson, Harmon, and Beer, Phys. Rev. **96**, 1512 (1954).

⁶ Adams, Davis, and Goldberg, Phys. Rev. **99**, 625 (1955).