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LUCAS HEIGHTS

REACTOR CALCULATIONS AND NUCLEAR INFORMATION

by

D.W. LANG

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ABSTRACT

The relationship of sets of nuclear parameters and the macroscopic reactor quantities that can be calculated from them is examined. The framework of the study is similar to that of Usachev & Bobkov. The analysis is generalised and some properties required by common sense are demonstrated. The form of calculation permits revision of the parameter set. It is argued that any discrepancy between a calculation and measurement of a macroscopic quantity is more useful when applied directly to prediction of other macroscopic quantities than to revision of the parameter set. The mathematical technique outlined is seen to describe common engineering practice.

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PREDICTION EQUATIONS; STATISTICAL MODELS; REACTORS; NUCLEAR DATA COLLECTIONS: STATISTICS

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1. INTRODUCTION

In reactor physics, detailed design studies often consider such quantities as reactivity of an assembly. The assembly may be constructed and measurements made. The experimental value of the k^{th} quantity would here be given the symbol E_k.

Repetition leads to a set of values with a mean $\langle E_k \rangle$ and a dispersion σ_k^2

$$\sigma_k^2 = \langle E_k^2 \rangle - \langle E_k \rangle^2 \quad . \tag{1}$$

The symbol $\langle E_k \rangle$, which is strictly a population mean, is used for convenience and no internal ambiguity arises here.

Calculations can also be made and the computed value C_k compared with E_k. Some quantities appearing in the computation are design dimensions of the assembly and would not vary if the computation was repeated for the same assembly. Other quantities come from nuclear experiments and the values used for these are revised as the experiments achieve greater accuracy.

With N such parameters making up a set $\{P_i\}$ it is sensible to write them in some standard order as a vector $\vec{P}$. It is conventional to treat the parameters as independent microscopic quantities measured in individual microscopic experiments. The restriction is not essential and discussion here proceeds without it. Calculation can proceed, as indicated in Appendix A, even if there is a correlation in the variation of directly measured experimental quantities.

Given a computation C_k and an experimental measurement E_k there is usually a discrepancy $E_k - C_k$, and a relative discrepancy r_k defined in relation to the standard deviation of the measurement

$$r_k = (E_k - C_k)/\sigma_k \quad . \tag{2}$$

If r_k^2 is near unity, agreement is indicated; and r_k^2 greater than three is taken as a warning that revision is needed somewhere. This report is concerned mainly with the possibility of a revision of the parameter set

$$\vec{P}' = \vec{P} + \vec{p} \quad , \tag{3}$$

where a correction term is given in a lower case to distinguish it from the accepted value which is given a capital. Other causes of discrepancy can often be found as discussed in more detail below. The discussion of

a revision of the parameter set is closely related to that of Usachev & Bobkov [1972,3]. The notation used here is mnemonic in English and some results are more general. The relationship is discussed in Appendix B.

A common cause of discrepancy not simply related to magnitudes in the parameter set is the systematic effect of approximations necessary for manageable computation. Where theory contains an integral, computation uses a finite summation. Any continuous independent variable in an integration is eventually replaced by a set of discrete values of that variable. Thus the neutron energy is replaced by a set of energy groups. The value of a continuous dependent variable such as neutron cross section is replaced by its mean value over the range of energies in a given neutron group.

More detailed consideration could indicate a dependence on the variance of the cross section as well, and so on.

In more mathematical notation if the quantity used for p_i is understood to be a mean quantity $\langle P_i(E) \rangle$ there may be a need to include dependence on the quantity Q_i defined by

$$Q_i^2 = \langle P_i^2(E) \rangle - P_i^2 \quad . \tag{4}$$

Where the original form of the calculation gave C_k

$$C_k = C_{k_0}(\vec{P}) \quad , \tag{5a}$$

it may be more appropriate or more accurate to write

$$C_k = C_{k_0}(\vec{P}) + C_{k_1}(\vec{P},\vec{Q}) \quad . \tag{5b}$$

It is a convenient starting point to assume that C_{k_1} is zero and use the relation

$$\frac{\partial}{\partial Q_i}(C_{k_0}) = 0 \quad , \tag{6}$$

for all k and all Q_i which are not included in the calculations actually used to obtain C_k, but which might appear in a more extensive calculation.

A formal theory of the corrections indicated in equation 3 is developed and afterwards it can be modified in the light of equation 5b.

In Section 2, a least square requirement is imposed to select best values of parameters. A formal solution is given with linear variations of the specified set of parameters. Central in the formal least squares solution is the inverse of a sensitivity matrix. Its structure is examined in Section 3.

In Section 4 the impact of a particular experimental result on prediction/s of the result/s of related experiment/s is considered. A mathematical description of the resemblance between macroscopic experiments is formulated. As expected, it is found that strong resemblance leads to strong predictive power.

2. FORMULATION AND FORMAL SOLUTION OF LEAST SQUARES PROBLEM

For small changes in $\vec{P}$ small linear corrections can be made to C_k;

$$\Delta C_k = \sum_i S_{ki} p_i \quad . \tag{7}$$

Then

$$C_k = \overleftarrow{S}_k \cdot \vec{p} + C_{k_0}(\vec{P}) \quad , \tag{8}$$

where the i^{th} element of the column vector $\vec{p}$ is p_i and of the row vector $\overleftarrow{S}_k$ is S_{ki}, and

$$S_{ki} = \frac{\partial}{\partial p_i} C_{k_0}(\vec{P}) \quad . \tag{9}$$

For a set of quantities to be calculated an order can be established so that a vector $\vec{C}$ can be written with k^{th} element C_k. Then

$$\vec{C} = S\vec{p} + \vec{C}_0 \tag{10}$$

and the k^{th} row of the matrix S is $\overleftarrow{S}_k$; the k^{th} element of the column vector $\vec{C}_0$ is C_{k_0}. The quantity C_{k_0}, and the use of a small magnitude vector $\vec{p}$, are made necessary by the non-linear nature of the problem. Each element of the matrix S may be the result of an extensive calculation and it should be remembered that the correction in equation 10 is only the first term of a usually non-linear set.

All the differential experiments can be and are assumed to be incorporated into equation 5. An experiment depending on only p_ℓ of the $\vec{p}$ can be described by the row vector $\overleftarrow{S}_\ell$ with only one non-zero element

$$S_{\ell i} = \delta_{\ell i} \quad . \tag{11}$$

If all the quantities involved in the matrix calculation were well known, a least squares technique could be used to evaluate the N elements of the vector $\vec{p}$. Chi-squared, defined by

$$\chi^2 = \sum_k (E_k - C_k)^2/\sigma_k^2 \quad , \tag{12}$$

could be minimised over the experimental set. Chi-squared can be written

$$\chi^2 = (\overleftarrow{E} - \overleftarrow{C})\omega^2(\vec{E} - \vec{C}) \quad , \tag{13}$$

and from equation 12, ω^2 is a diagonal matrix,

$$\omega^2_{jk} = \delta_{jk}\sigma_k^{-2} \quad . \tag{14}$$

Implicit in equations 12, 13 and 14 is the assumption that the set of experimental data is independent, i.e.

$$\langle E_k E_\ell \rangle = \langle E_k \rangle \langle E_\ell \rangle + \delta_{k\ell}\sigma_k^2 \quad . \tag{15}$$

The basis of this assumption is discussed briefly in Appendix A. From equations 10 and 13

$$\chi^2 = (\overleftarrow{E} - \overleftarrow{C}_0 - p\overleftarrow{S}^T)\omega^2(\vec{E} - \vec{C}_0 - S\vec{p}) \quad . \tag{16}$$

A minimum of chi-squared with respect to every element of $\vec{p}$ is obtained by differentiation, leading to

$$S^T\omega^2 S\vec{p} = S^T\omega^2(\vec{E} - \vec{C}_0) \quad , \tag{17}$$

or

$$\vec{p} = (S^T\omega^2 S)^{-1} S^T\omega^2(\vec{E} - \vec{C}_0) \quad . \tag{18}$$

3. EVALUATION AND STRUCTURE OF THE LEAST SQUARES INVERSE MATRIX

The matrix $S^T\omega^2 S$ can conveniently be written, by use of equation 15, as a sum of symmetric rank one terms. This property and the method of rank annihilation [Wilf 1959] permit study of the effect on the inverse matrix of individual experiments. Where there are N+M experimental measurements incorporated so that it makes sense to assume that the N elements of $\vec{p}$ are considerably over-determined, we write

$$(S^T\omega^2 S)_{M+N} = \sum_{k=1}^{M+N} \vec{S}_k \omega_k^2 \overleftarrow{S}_k \quad . \tag{19}$$

A sequence of inverse matrices is defined with L^{th} member D_L

$$D_L(S^T\omega^2 S)_L = (S^T\omega^2 S)_L D_L = I \quad , \tag{20}$$

and

$$D_{L+1} = D_L - d_{L+1} \quad . \tag{21}$$

From equation 20

$$I = (D_L^{-1} + \vec{S}_{L+1}\omega^2_{L+1}\overleftarrow{S}_{L+1})(D_L - d_{L+1}) \quad . \tag{22}$$

From equation 19, D_{L+1}^{-1} is real and symmetric. It is also clear that the diagonal matrix element $\overleftarrow{x}D_{L+1}^{-1}\vec{x}$ is non-negative for any real vector $\vec{x}$. For non-zero weights ω_ℓ^2, D_{L+1}^{-1} has as many positive eigenvalues as it contains linearly independent vectors $\vec{S}_\ell$. If any D_L^{-1} is non-singular,

i.e. if all diagonal matrix elements $\overleftarrow{x}D_L^{-1}\overrightarrow{x}$ are positive, then all subsequent D_{L+M}^{-1} are also non-singular.

Rearranging equation 22

$$d_{L+1} = D_L \overrightarrow{S}_{L+1}\omega_{L+1}^2\overleftarrow{S}_{L+1}(D_L - d_{L+1}) \quad . \tag{23}$$

Where d_{L+1} appears in the right hand side of equation 23 it may be replaced by the entire right hand side, giving

$$d_{L+1} = D_L \overrightarrow{S}_{L+1}\omega_{L+1}^2\overleftarrow{S}_{L+1}(D_L - \omega_{L+1}^2\overleftarrow{S}_{L+1}D_L\overrightarrow{S}_{L+1}(D_L - d_{L+1})) . \tag{24}$$

The matrix element $\overleftarrow{S}_{L+1}D_L\overrightarrow{S}_{L+1}$ is a scalar, and simple algebraic elimination between equations 23 and 24 then yields the rank-one form

$$d_{L+1} = f_{L+1}\, D_L\overrightarrow{S}_{L+1}\omega_{L+1}^2\overleftarrow{S}_{L+1}D_L \tag{25}$$

where the scalar quantity f_{L+1} is given by

$$f_{L+1} = (1 + \overleftarrow{S}_{L+1}D_L\overrightarrow{S}_{L+1}\omega_{L+1}^2)^{-1} \quad . \tag{26}$$

An extension of this process can incorporate several rank-one components into the inverse at one step. We write

$$D_{L+J} = D_L - \sum_{\ell,k=1}^{J} g_{\ell k}D_L\overrightarrow{S}_\ell\omega_\ell\omega_k\overleftarrow{S}_k D_L \tag{27}$$

as in equation 21, and substitute in a modified form of equation 22. The coefficients of quantities $\omega_j\omega_k\overrightarrow{S}_j\overleftarrow{S}_k D_L$ must vanish there, giving

$$\delta_{jk} = g_{jk} + \sum_{\ell=1}^{J} g_{\ell k}\omega_j\omega_\ell\overleftarrow{S}_j D_L\overrightarrow{S}_\ell \tag{28}$$

$$= \sum_{\ell=1}^{J} g_{\ell k}(\delta_{\ell j} + \omega_j\omega_\ell\overleftarrow{S}_j D_L\overrightarrow{S}_\ell) \tag{29}$$

for all values $1 \leqslant (j,k) \leqslant J$.

Equation 29 shows that the (JxJ) matrix with elements $g_{\ell k}$ is the inverse of the commensurate matrix with elements

$$\delta_{j\ell} + \omega_j\omega_\ell\overleftarrow{S}_j D_L\overrightarrow{S}_\ell \tag{30}$$

and equation 26 follows as a special case. It can be seen that for all positive values of J, all eigenvalues of the matrix in expression 30 are greater than zero, so that the inverse is guaranteed to exist.

4. INTERPRETATION OF FORMAL RESULTS

We now assign a meaning to the standard deviation of the quantity

C_k. For any set of experimental measurements $\vec{E}$, there is a predicted value of C_k. If each of the members of $\vec{E}$ varies randomly and independently with the correct mean and standard deviation given by equation 1, a mean and standard deviation can be found for the consequent values of C_k. From equations 18 and 8

$$C_k = C_{k_0} + \overleftarrow{S}_k (S^T\omega^2 S)^{-1} S^T\omega^2 (\vec{E} - \vec{C}_0) \quad , \tag{31}$$

$$\langle C_k \rangle = C_{k_0} + \overleftarrow{S}_k (S^T\omega^2 S)^{-1} S^T\omega^2 (\langle \vec{E} \rangle - \vec{C}_0) \quad . \tag{32}$$

Since the approximation used is linear, the mean of C_k is obtained by substituting the mean for each experimentally measured quantity. Further, in the case of the variance

$$\langle C_k^2 \rangle - \langle C_k \rangle^2 = \sum_\ell \overleftarrow{S}_k (S^T\omega^2 S)^{-1} \vec{S}_\ell \omega_\ell^2 (\sigma_\ell^2) \omega_\ell^2 \overleftarrow{S}_\ell (S^T\omega^2 S)^{-1} \vec{S}_k \tag{33}$$

$$= \overleftarrow{S}_k (S^T\omega^2 S)^{-1} \vec{S}_k \quad . \tag{34}$$

The prediction depends on how many measurements have been incorporated

$$\langle C_k^2 \rangle_L - \langle C_k \rangle_L^2 = \overleftarrow{S}_k D_L \vec{S}_k \quad . \tag{35}$$

In general the predicted values of quantities C_k and C_m are correlated. The quantity M_{km} is defined by

$$M_{km} = \langle C_k C_m \rangle_L - \langle C_k \rangle_L \langle C_m \rangle_L = \overleftarrow{S}_k D_L \vec{S}_m \quad . \tag{36}$$

Consider now the incorporation of a further measurement E_ℓ, which has an associated standard deviation σ_ℓ and predicted value C_ℓ, into the measurement set. There is a new value C_k' in place of C_k, and M_{km}' replaces M_{km}.

$$C_k' = C_{k_0} + \overleftarrow{S}_k (D_L - f_\ell \omega_\ell^2 D_L \vec{S}_\ell \overleftarrow{S}_\ell D_L) \; [S^T\omega^2 (\vec{E} - \vec{C}_0) +$$

$$\vec{S}_\ell \omega_\ell^2 (E_\ell - C_{\ell_0})] \tag{37}$$

$$= C_k - f_\ell \omega_\ell^2 M_{k\ell} (C_\ell - C_{\ell_0}) + f_\ell \omega_\ell^2 M_{k\ell} (E_\ell - C_{\ell_0}) \tag{38}$$

$$= C_k + f_\ell \omega_\ell^2 M_{k\ell} (E_\ell - C_\ell) \quad , \tag{39}$$

where use has been made of the equation

$$(D_L - f_\ell \omega_\ell^2 D_L \vec{S}_\ell \overleftarrow{S}_\ell D_L) \vec{S}_\ell = D_L \vec{S}_\ell f_\ell \quad . \tag{40}$$

Also

$$M_{km}' = M_{km} - \omega_\ell^2 f_\ell M_{k\ell} M_{\ell m} \quad . \tag{41}$$

We note that

$$f_\ell \omega_\ell^2 M_{\ell\ell} = 1 - f_\ell \quad , \tag{42}$$

and, for the special case of $k = \ell$, we obtain in place of equation 39

$$C'_\ell = (1-f_\ell)E_\ell + f_\ell C_\ell \quad , \tag{43}$$

and in place of equation 41, with $k = \ell$

$$M'_{\ell m} = f_\ell M_{\ell m} \quad , \tag{44}$$

which can be specialised still further

$$M'_{\ell\ell} = f_\ell M_{\ell\ell} \quad . \tag{45}$$

Equations 43 and 45 are the standard results obtained for the value and standard deviation of the quantity C'_ℓ by combining the independent evaluations as a quantity E_ℓ with standard deviation σ_ℓ and as a quantity C_ℓ of standard deviation $(\overleftarrow{S}_\ell D_L \overrightarrow{S}_\ell)^{\frac{1}{2}}$. The weight f_ℓ is then

$$f_\ell = \sigma_\ell^2 / (\sigma_\ell^2 + \overleftarrow{S}_\ell D_L \overrightarrow{S}_\ell) \quad , \tag{46}$$

and equation 45 shows that the prediction of C_ℓ is refined by the inclusion of a measurement of it.

Another important special case of equation 41 is obtained by putting $k = m$. In this case

$$M'_{kk} = M_{kk} - \omega_\ell^2 f_\ell M_{k\ell}^2 \tag{47}$$

so that any measurement either refines the accuracy of any prediction or leaves it unchanged.

Some insight may be gained into the effects of measurement by writing

$$\overrightarrow{S}_k = \alpha \overrightarrow{S}_\ell + \overrightarrow{S}_m \tag{48}$$

where $\overrightarrow{S}_m$ is conjugate to $\overrightarrow{S}_\ell$ with respect to the matrix D_L, i.e.

$$M_{\ell m} = \overleftarrow{S}_m D_L \overrightarrow{S}_\ell = 0 \quad . \tag{49}$$

Then

$$\alpha = M_{k\ell} / M_{\ell\ell} \tag{50}$$

and

$$\overrightarrow{S}_m = \overrightarrow{S}_k - \alpha \overrightarrow{S}_\ell \quad . \tag{51}$$

We define C_{m_0} by

$$C_{k_0} = \alpha C_{\ell_0} + C_{m_0} \tag{52}$$

Then $C_k = \alpha C_\ell + C_m$. (53)

Similarly

$$M_{kk} = (\alpha \overleftarrow{S}_\ell + \overleftarrow{S}_m) D_L (\alpha \overrightarrow{S}_\ell + \overrightarrow{S}_m) \quad (54)$$

$$= \alpha^2 M_{\ell\ell} + M_{mm} \quad . \quad (55)$$

An additional measurement of E_ℓ is now made, and the value of the standard deviation for this measurement is σ_ℓ. We calculate the effect on C_k and on M_{kk}

$$C_k' = \alpha C_{\ell_0} + C_{m_0} + (\alpha \overleftarrow{S}_\ell + \overleftarrow{S}_m)(D_L - f_\ell D_L \overrightarrow{S}_\ell \overleftarrow{S}_\ell D_L \omega_\ell^2)[S^T \omega^2 (\overrightarrow{E} - \overrightarrow{C}_0) + \overrightarrow{S}_\ell \omega_\ell^2 (E_\ell - C_{\ell_0})] \quad (56)$$

$$= C_m + \alpha C_{\ell_0} + \alpha f_\ell (C_\ell - C_{\ell_0}) + \alpha f_\ell \overleftarrow{S}_\ell D_L \overrightarrow{S}_\ell \omega_\ell^2 (E_\ell - C_{\ell_0}) \quad (57)$$

$$= C_m + \alpha f_\ell C_\ell + \alpha (1 - f_\ell) E_\ell \quad (58)$$

$$= C_m + \alpha C_\ell' \quad . \quad (59)$$

Also $$M_{kk}' = (\alpha \overleftarrow{S}_\ell + \overleftarrow{S}_m)(D_L - f_\ell D_L \overrightarrow{S}_\ell \omega_\ell^2 \overleftarrow{S}_\ell D_L)(\alpha \overrightarrow{S}_\ell + \overrightarrow{S}_m) \quad (60)$$

$$= M_{mm} + f_\ell \alpha^2 M_{\ell\ell} \quad . \quad (61)$$

The separation of components of S_k is equivalent to a separation of available information. There is a component of C_k that is fully determined by measurement of the ℓ^{th} reactor constant C_ℓ, and a component C_m that is unchanged in magnitude and in accuracy by measurements E_ℓ.

Design studies of reactor experiments can make use of such information. To predict C_k, a quantity is needed that is cheaper to measure, substantially similar to C_k in its dependence on the parameter set, and such that the difference component C_m is easily calculated. The argument here is basically a description of standard engineering practice involving scale models, etc. In the extreme case no calculated form of C_k or C_ℓ exists, but calculations can be performed on what appears to be a correction term C_m; also the factor α can be calculated from the design of the experiments. Equation 61 can be rewritten using equations 26 and 36 as

$$M_{kk}' = M_{mm} + \alpha^2 (\sigma_\ell^{-2} + M_{\ell\ell}^{-1})^{-1} \quad . \quad (62)$$

In the extreme case of no measurement, σ_ℓ^{-2} tends to zero and we return to the form of equation 55. At the other extreme, where C_ℓ is not calculated, or where E_ℓ has been measured much more accurately than is

possible in the calculation of C_ℓ,

$$M'_{kk} = M_{mm} + \alpha^2\sigma_\ell^2 \quad . \tag{63}$$

The extension to the case where S_k can be split into several components corresponding to simply measured quantities follows naturally.

For design of an experiment to measure E_ℓ, statistical criteria must be mixed with economics. Apart from economics, not much information is obtained unless σ_ℓ^2 is less than, say, five times $M_{\ell\ell}$ and not much more can be obtained if σ_ℓ^2 is less than one fifth of $M_{\ell\ell}$ and of $\alpha^{-2}M_{mm}$. Since the quantity E_ℓ is assumed to be a simply measurable part of E_k it would be expected that good design would easily give σ_ℓ^2 less than $M_{\ell\ell}$.

Finally, since the quantity C_{k_1} of equation 5b is unknown, it is unprofitable to discuss it in too much detail. We can observe the following three points.

1. There is an effect on the parameter set. The result of a series of calculations that neglects effects of a non-zero $\vec{C}_1$, adds a term to the vector $\vec{p}$

$$\vec{p}_1 = (S^T\omega^2 S)^{-1}S^T\omega^2\vec{C}_1, \tag{64}$$

since $\vec{C}_1$ is omitted from consideration in equation 18. The added term is an artefact of calculation rather than a natural contribution. The nuclear parameter set used in reactor calculation is subject to correction by incorporation of macroscopic experiments, but because of equation 64 the process should be operated cautiously. A large correction from use of equation 18 can be treated as a flag to signal for re-examination of the microscopic measurement and the macroscopic calculation.

2. We can endeavour, in special cases, to cope with the effects of $\vec{C}_1$ in a linear fashion. Descriptions of quantitative physics experiments from an elementary level onwards, include lists of approximate corrections for small effects. Such corrections can compensate for deficiencies in calculation or measurement.

3. In a case where similar experiments are being compared, as in equation 48 and the following discussion, it is plausible as well as desirable to expect the uncalculated parts of C_k and

C_ℓ to show a similar overlap to the part that is actually calculated. In two experiments where it is reasonable to expect the relevant neutron flux spectrum and all cross sections to be identical, the difference between results is unlikely to depend strongly on the number of neutron groups used. We should be alert to allow for any term C_{m_1} in the difference between two reactor quantities, and incorporate any such uncertainties into the quantity M_{mm} that appears in equation 55, *et seq*.

Because of points 1 and 3, the formalism is likely to be much more useful in the standard engineering application than in extrapolating from large scale integral measurements to correction of microscopic parameters. There is a halfway procedure, to be treated with caution, in which a parameter set is built up that gives good agreement with macroscopic reactor constants, and is adjusted to correct any discrepancies that arise. The set is used only for reactor calculations and is not required to be consistent with nuclear data measurements. The result appears to be an *ad hoc* approximation to the discussion given above.

5. SUMMARY

The formalism developed by Usachev and Bobkov depends on the ability to express an integral quantity so that it has a linear dependence on small corrections to the parameter set from which it was calculated. Even if the linear dependence cannot be calculated, the formalism gives common sense answers to some simple questions and describes the essentials of common modelling procedures.

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APPENDIX A

THE ASSUMPTION OF INDEPENDENCE

Even in microscopic quantities, nuclear experiments often measure a single number which depends on several members of the parameter set. A simple case to understand involves a normalisation that applies to nuclear cross sections over a range of energies. The cross sections may be considered as primary measurements, in which case the errors are correlated, or preferably the measurement of the normalisation can be included so that with one more measurement, all measurements are independent.

The separation into independent measurements is assumed complete in the form given to equation 14. The correlation of values of the parameter set still makes itself felt in equation 19. It is tentatively assumed in section 2 of Usachev & Bobkov [1974] that the N x N matrix of the equation analogous to equation 19 is diagonal for just N measurements. The simplicity is not strictly necessary, and correlations arising out of constants of normalisation make it unlikely.

What is necessary is that at some stage of building up equations similar to equation 19, a positive definite N x N matrix is achieved. Once achieved, as noted in the text of this report, subsequent additional data built into enlargement of equation 19 preserve the positive definite property. It is not usually easy to establish the property by inspection, but one special case can arise. If the measurements and data sets can be so ordered that the first contribution to equation 19 is diagonal and that when n measurements are incorporated, all non-zero elements are contained in an n x n region of the matrix with n positive elements on the diagonal, the n x n matrix is positive definite and develops to a positive definite N x N matrix.

The equation 15 is used as a basis for discussion in the body of the report, and may be achieved, as discussed above, even where superficial indications are otherwise. Even in the absence of such simplicity it may still be useful to define chi-squared. Off-diagonal correlations in an equivalent to equation 15 lead to off-diagonal elements in a weight matrix replacing ω^2 of equation 14. Using the same symbol, equation 18 is still valid. The analysis in Section 3 is concerned with the addition of symmetric rank-one terms to a symmetric matrix. In

Section 4 an equation similar to equation 33 is valid but more complicated to write down. The equations replacing 34 and 35 are formally identical in terms of the more complicated weight matrix.

The assumption of addition of symmetric rank-one terms used in the body of the report can also be dispensed with. A completely general matrix U of rank r can be added to a matrix T^{-1} with an inverse T. The extended inverse T-t, if it exists, satisfies

$$(T-t)(T^{-1}+U) = (T^{-1}+U)(T-t) = I \quad . \tag{A1}$$

The matrix U can always be written explicitly to exhibit its rank r.

$$U = \sum_{a,b=1}^{r} \vec{L}_a \, \overleftarrow{R}_b \, B_{ab} \quad . \tag{A2}$$

Clearly,

$$t = TUT - tUT = TUT - TUt \tag{A3}$$

and hence

$$t = TUT - TUTUT + TUtUT \quad . \tag{A4}$$

It follows that t can also be written in an explicitly rank-r form

$$t = \sum_{a,b=1}^{r} T \vec{L}_a \, \overleftarrow{R}_b \, T \, Q_{ab} \tag{A5}$$

where the coefficients, Q_{ab} remain to be evaluated. Writing

$$G_{mn} = \overleftarrow{R}_m \, T \, \vec{L}_n \tag{A6}$$

and combining equations A2, A3, A5 and A6 yields a set of equations for the coefficients Q_{ab}

$$\begin{aligned} Q_{ab} &= B_{ab} - \sum_{m,n=1}^{r} Q_{am} \, G_{mn} \, B_{nb} \\ &= B_{ab} - \sum_{m,n=1}^{r} B_{am} \, G_{mn} \, Q_{nb} \quad . \end{aligned} \tag{A7}$$

The coefficients make up r x r matrices and from equation A7

$$Q(I+GB) = B = (I+BG)Q \tag{A8}$$

so that

$$Q = B(I+GB)^{-1} = (I+BG)^{-1} \, B = (B^{-1}+G)^{-1} \quad . \tag{A9}$$

The matrix operations are defined in terms of an r x r space for which the coefficients B make up a non-singular matrix. Thus B^{-1} exists, but even so there is a possibility that $B^{-1}+G$ is singular. If so, the equations A8 hold but the derivation of A9 fails.

APPENDIX B

COMPARISON WITH USACHEV AND BOBKOV [1972,3,4]

When mathematical treatment of statistics is written in English, the symbol σ usually denotes a standard deviation. In nuclear parameter sets, cross sections also appear with the same symbol. In this report the statistical basis is essential. The nuclear information is a starting point, but what matters is the useful combination of a large parameter set with experiments that depend on a large segment of the parameter set. Accordingly, the notation of this report has little relevance to the particular data sets that give rise to the problem described.

It is convenient to distinguish between references to equations occurring in the Russian work and to those in the body of this report. The form '[1972] Eqn 2' gives the year of the relevant report and the capital E is further confirmation of the external origin. The form 'equation 2' refers to an equation from this report. Values of quantities such as discrepancies are also used here rather than manifestly dimensionless ratios. This is the author's preference to avoid the artificial complications associated with the predicted value of a quantity being zero or close to it. The quantity f_x from Usachev & Bobkov [1973], is given by them as $(\delta\sigma/\sigma)$. It would appear here as p_x/P_x. The quantity g_x would appear as σ_x/P_x so that f_x/g_x is p_x/σ_x. The capitalised P_x indicates an accepted value of a parameter and the lower case p_x an adjustment arising from the calculation, and the corresponding standard deviation has the symbol σ_x.

The quantity C_I of [1973] Eqn 2, would be written here as C_{I_0}, and the adjusted value C_I' in the same Eqn is C_I here, i.e. in equation 8,

$$C_I = C_I' \text{ [Usachev \& Bobkov]} = C_{I_0}(\vec{P}) + \overleftarrow{S}_I \cdot \vec{P} \quad .$$

The quantity e_I is seen to be σ_I/C_I . Such terms as Z_{Ii} appear in [1973] Eqn 4 where i is the label of a member of the parameter set and I the label of a member of the set of macroscopic experiments.

From the connection between [1973] Eqn 4 and [1973] Eqn 5

$$Z_{Ii} = \frac{\partial C_I'}{\partial f_i}$$

$$= P_i/C_{I_0} \quad \frac{\partial C_{I_0}}{\partial p_i}$$

$$= P_i \, C_{I_0}^{-1} \, S_{Ii} \quad \text{in the notation here.}$$

In addition there is no distinction in the formalism here between microscopic and macroscopic experiments. It is convenient but not essential that in the limit of equation 11 there are experiments that depend only on a single member of the parameter set. Even in such a case, the value used in the parameter set may be different from the result of a particular experiment. The value used then gives a prediction for the result of the experiment and there is a discrepancy, incorporated in the vector on the right hand side of equation 17 of this report.

The corresponding quantity in [1973] appears in the right hand side of Eqn 5

$$Y_i = \sum_{I=1}^{N_o} \left[\frac{(E_I - C_I)}{C_I}\right] \frac{1}{e_I^2} \, Z_{Ii}^T \quad . \qquad \text{Eqn 5}$$

In matrix notation the order of quantities in the square brackets would be reversed and the set of quantities Y_i incorporated into a vector $\vec{Y}$

$$\vec{Y} = Z^T \, e^{-2} \, C^{-1} \, (\vec{E} - \vec{C})$$

where e^{-2} and C^{-1} are diagonal matrices of dimension $N_o \times N_o$, $\vec{E} - \vec{C}$ is a column vector, i.e. dimension $1 \times N_o$, and Z is the sensitivity matrix of dimension $N_o \times N_1$, so that Z^T has dimension $N_1 \times N_o$. The number N_1 is the size of the parameter set and has been called N elsewhere in this report.

The vector $\vec{Y}$ is not quite the same as that on the right hand side of equation 17. To obtain that right hand side, the discrepancy vector must first be lengthened from $1 \times N_o$ to $1 \times (N_o + N_1)$ incorporating any discrepancies between the parameter set and the corresponding set of microscopic experiments. It then follows that the matrix S has dimension $(N_1 + N_o) \times N_1$ so that

$$S_{Ii} = C_{Io} \, Z_{Ii} / P_i \quad \text{for } I \leq N_o$$

and $$S_{I+N_o\,i} = \delta_{Ii} \, , \qquad 1 \leq I \leq N_1 \quad .$$

First, $\vec{Y}$ must be multiplied by a diagonal matrix P^{-1} with ij element $\delta_{ij} P_i^{-1}$ for $i < N_1$ to obtain a quantity comparable with the right hand side of equation 17.

The diagonal style of structure given for the final N_1 rows of the

matrix S is consistent with that implied by Usachev & Bobkov [1973] Eqn 4 for the structure of the matrix M. It is, however, as discussed in Appendix A, a bit optimistic. The matrix corresponding to M in equation 17 would be composed of the sum of $N_1 + N_o$ terms each of rank one and contained within the dimensions $N_1 \times N_1$ of M.

$$M = P\, S^T\, \omega^2\, S\, P$$

and $$P\vec{f} = \vec{p} \quad .$$

Thus equation 17 is closely related to [1973] Eqn 6 but is generalised in a minor way.

In passing, it should be noted that there is an error that runs through a sequence of [1973] Eqns. The denominator in [1973] Eqns 10, 13 and 14 is a scalar. The form given, $1+WGD(N_o)G^T$, should be altered to read $1+WG^TD(N_o)G$.

NOTES

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