CONF-850507--11

CONF-850507--11

DE85 011937

UNCERTAINTY PROPAGATION FROM RAW DATA TO FINAL RESULTS

N. M. LARSON
Oak Ridge National Laboratory*

Abstract Reduction of data from raw numbers (counts per channel) to physically meaningful quantities (such as cross sections) is in itself a complicated procedure. Propagation of experimental uncertainties through that reduction process has sometimes been perceived as even more difficult, if not impossible. At the Oak Ridge Electron Linear Accelerator, a computer code ALEX[1] has been developed to assist in the propagation process. The purpose of ALEX is to carefully and correctly propagate all experimental uncertainties through the entire reduction procedure, yielding the complete covariance matrix for the reduced data, while requiring little additional input from the experimentalist beyond that which is needed for the data reduction itself. The theoretical method used in ALEX is described, with emphasis on transmission measurements. Application to the natural iron[2] and natural nickel[3] measurements of D. C. Larson is shown.

INTRODUCTION

For any experiment, it is necessary to reduce raw data (counts per channel) to physically meaningful quantities (cross sections, transmissions). In the reduction process, one wishes to use all available experimental information, but spend a minimum of time and effort communicating this information (i.e., programming the computer). Desired output includes, in addition to the reduced data, a meaningful uncertainty for each data point and the complete covariance matrix for the entire data set.

The computer code ALEX[1] was developed to fill this need: ALEX is a black-box code into which the experimentalist can feed all the information he already has (raw data, deadtime corrections, backgrounds, etc.) and from which he can learn the uncertainties on the corrected data and the correlations among data points. The code handles the intermediate steps, determining necessary derivatives and propagating uncertainties to produce the final result. Moreover, the code produces, stores, and displays results in an efficient manner, without requiring the entire resources of the computer. In this paper we deal with the specific case of a sample-in, sample-out measurement from which transmissions and cross sections are extracted.

*Research sponsored by the U.S. Department of Energy under Contract No. DE-AC05-84OR2140 with Martin Marietta Energy Systems, Inc.

METHOD USED IN ALEX

The method used in ALEX is as follows: from user-supplied input, ALEX generates the five functions β_{ni}, where

$$\begin{aligned}
&\beta_{1i} = \eta_i = \text{normalization for time–channel i}\\
&\beta_{3i} = b_i = \text{background counts for sample–in}\\
&\beta_{2i} = d_i = \text{deadtime correction for sample–in}\\
&\beta_{4i} = D_i = \text{deadtime correction for sample–out}\\
&\beta_{5i} = B_i = \text{background counts for sample–out}
\end{aligned} \tag{1}$$

In addition, ALEX generates $\partial\beta_{ni}/\partial P_k$, the derivatives of the β_{ni} with respect to any parameter P_k, where $\{P_k\}$ represents the data-reduction parameters.

If c_i (C_i) represents sample-in (-out) counts, ALEX calculates the transmission

$$\tau_i = \eta_i \frac{d_i c_i - b_i}{D_i C_i - B_i} \tag{2}$$

and the partial derivatives of the transmission with respect to the parameters P_k,

$$\frac{\partial \tau_i}{\partial P_k} = \sum_{n=1}^{5} \frac{\partial \tau_i}{\partial \beta_{ni}} \frac{\partial \beta_{ni}}{\partial P_k}. \tag{3}$$

Expressions for the partial derivations $\partial\tau_i/\partial\beta_{ni}$ are found directly from Eq. (2) using (1); the partial derivatives $\partial\beta_{ni}/\partial P_k$ are found from user-supplied input. Partial derivatives of τ_i with respect to c_i and C_i are also found from Eq. (2).

To obtain the uncertainty on data point i (and the covariance between points i and j), consider a small increment $\delta\tau_i$ on the transmission τ_i. This increment can be expressed in terms of increments in c_i, C_i, and P_k as

$$\delta\tau_i = \frac{\partial \tau_i}{\partial c_i}\delta c_i + \frac{\partial \tau_i}{\partial C_i}\delta C_i + \sum_k \frac{\partial \tau_i}{\partial P_k}\delta P_k \tag{4}$$

The expectation value of the product $\delta\tau_i\delta\tau_j$ is then the covariance matrix element between data points i and j:

$$\langle \delta\tau_i \delta\tau_j \rangle = \left[\left(\frac{\partial \tau_i}{\partial c_i}\right)^2 c_i + \left(\frac{\partial \tau_i}{\partial C_i}\right)^2 C_i\right]\delta_{ij} + \sum_{kk'} \frac{\partial \tau_i}{\partial P_k} \langle \delta P_k \delta P_{k'} \rangle \frac{\partial \tau_j}{\partial P_{k'}} \tag{5}$$

which has been simplified using the Poisson statistics of the raw counts. In this expression, δ_{ij} is the Kronecker delta function and $\langle \delta P_k \delta P_{k'} \rangle$ represents the covariance matrix for the parameters. Note that $(\Delta P_k)^2 = \langle \delta P_k \delta P_k \rangle$ is the square of the uncertainty on parameter P_k, and $(\Delta\tau_i)^2 = \langle \delta\tau_i \delta\tau_i \rangle$ is the square of the uncertainty on transmission τ_i.

Next, results are rebinned as needed, yielding the transmission for bin I

$$T_I = N_I \sum_{i=Imin(I)}^{Imax(I)} \tau_i \Delta_i \tag{6}$$

and partial derivatives thereof

$$\frac{\partial T_I}{\partial P_k} = N_I \sum_{i=Imin(I)}^{Imax(I)} \frac{\partial \tau_i}{\partial P_k} \Delta_i \tag{7}$$

Here Δ_i is the width of channel i, and the normalization N_I is given by

$$N_I = \left[\sum_{i=Imin(I)}^{Imax(I)} \Delta_i \right]^{-1} \tag{8}$$

The quantity T_I of Eq. (6) is the desired reduced data. The *statistical* contribution to the uncertainty on T_I is the sum, in quadrature, of the sample-in and the sample-out contributions, where the sample-in statistical uncertainty is given by

$$\Delta T_I^{in} = N_I \left[\sum_{i=Imin(I)}^{Imax(I)} \left(\frac{\partial \tau_i}{\partial c_i} \right)^2 c_i \Delta_i^2 \right]^{1/2} \tag{9}$$

and similarly for sample-out. The covariance matrix C_{IJ} for the reduced data is the sum of statistical plus *systematic* contributions:

$$C_{IJ} = \left[\left(\Delta T_I^{in} \right)^2 + \left(\Delta T_I^{out} \right)^2 \right] \delta_{IJ} + \sum_{k,k'} \frac{\partial T_I}{\partial P_k} <\delta P_k \delta P_{k'}> \frac{\partial T_J}{\partial P_{k'}} \tag{10}$$

Finally, conversions from transmission to cross section are made via

$$\sigma_I = -\frac{1}{n} \ln T_I \tag{11}$$

where n is sample thickness. Derivatives of σ are found by taking derivatives of Eq. (11).

EXAMPLE: NATURAL IRON

A straight-forward application of these techniques is provided by the natural iron measurement of D. C. Larson[1,2], for which the five functions β_{ni} of Eq. (1) have the form

$$\begin{aligned} \beta_{1i} &= M/m & \beta_{4i} &= D_i \\ \beta_{2i} &= d_i & \beta_{5i} &= G \\ \beta_{3i} &= g \end{aligned} \tag{12}$$

where m (M) represents the monitor counts for sample-in (-out), d_i (D_i) the deadtime correction factor for sample-in (-out), and g (G) the constant background for sample-in (-out). In addition, n represents the sample thickness. Because the deadtime correction is assumed to be exact for this measurement, these are the only parameters P_k. Values and uncertainties are given by

$$P_1 = n = 0.42960 \pm 0.2\% \qquad P_4 = g = 2.7422 \pm 5.0\%$$
$$P_2 = m = 877039. \pm 0.5\% \qquad P_5 = G = 2.5587 \pm 5.0\%$$
$$P_3 = M = 7060770. \pm 0.5\% \tag{13}$$

The output generated by ALEX for this iron measurement is summarized in the table below. Because g and G are added directly to the counts $d_i c_i$ and $D_i C_i$ (which are larger), the contributions to the uncertainties due to g and G are small, and have therefore been omitted from the table. Contributions due to m and M are constant, equal to 0.012 in both cases, and are also omitted from the table. Note that, because bin sizes are so large, the dominant contributors to the overall uncertainties are not the statistical errors $(\Delta\sigma)^{in}$ and $(\Delta\sigma)^{out}$ but rather are the systematic errors due to the monitor counts.

Table. Cross sections and contributions to uncertainties for iron

Energy range (MeV)	σ	$\Delta\sigma$	$(\Delta\sigma)^{in}$	$(\Delta\sigma)^{out}$	$\frac{\delta\sigma}{\delta n}\Delta n$	correlation, times 100
2.0- 2.4	3.147	.023	.012	.007	.006	100
2.4- 3.0	3.424	.022	.011	.006	.007	65 100
3.0- 4.5	3.531	.019	.006	.003	.007	74 77 100
4.5- 8.0	3.586	.018	.003	.002	.007	77 81 92 100
8.0-11.0	3.121	.018	.003	.002	.006	77 80 91 97 100
11.0-25.0	2.379	.017	.001	.001	.005	78 81 92 97 98 100
25.0-50.0	2.402	.017	.002	.002	.005	77 80 91 96 97 98 100
50.0-79.8	2.343	.020	.008	.005	.005	69 71 81 86 86 87 86 100

EXAMPLE: NATURAL NICKEL

The natural nickel measurement of D. C. Larson et al[3] is a far more complicated example of the techniques available in ALEX. For this measurement, the correct background description requires twenty-six parameters. One additional parameter (σ^2) is needed to describe the variation in the magnitude of the flux intensity from one burst to the next (producing an adjustment in the deadtime correction factor as described in the appendix to the nickel report[3]). These plus the sample thickness (n) and the sample-in and -out monitor counts (m and M) give a total of thirty parameters, many of which have non-zero correlations. Uncertainty propagation via ALEX shows that the four parameters n, m, M, and σ^2 provide the largest contributions to the total uncertainty, exceeding even the statistical contributions for large energy bins. For details, see Ref. 3.

REFERENCES

1. N. M. Larson, ORNL/TM-8676, ENDF-332 (1984).
2. D. C. Larson, Symposium on Neutron Cross Sections from 10 to 50 MeV, BNL-NCS-51245, pg. 277 (1980).
3. D. C. Larson, N. M. Larson, J. A. Harvey, N. W. Hill, C. H. Johnson, ORNL/TM-8203 (1983).

DISCLAIMER