ANL Data Assimilation Methodology: GMADJ

For the data assimilation activities of WPEC Subgroup 33, Argonne will use the GMADJ code written primarily by W. P. Poenitz and used by ANL in the 1980's in support of design activities for the Clinch River Breeder Reactor (CRBR) and for the metal core of the Fast Flux Test Reactor (FFTF). Many papers and reports were published at that time describing both the methodology and the performance.

A code, GMA (for Gauss, Markov and Aitken), for the simultaneous evaluation of parameters by generalized least-squares was developed in 1980.[1,2] GMA provides for a first-step evaluation of n parameters for which an overdetermination or minimum determination exists with a large experimental data base. The code GMADJ[3] provides for the utilization of additional experimental data for the improvement of the n parameters or of quantities calculated with these parameters. With emphasis on the latter, the code can be used to obtain adjusted calculated quantities without explicit adjustments of the underlying parameter set. Uncertainties and correlations among the calculated quantities are provided. The present brief account is based on a summary by W. P. Poenitz.[4]

Parameter adjustment based on least-squares is due to Gauss[5] and modifications of the least-squares method in order to account for correlations as derived by Aitken[6] have been taken into account in recent work, e.g., in Ref. 7. Other approaches, e.g., based on Bayes' theorem, lead to the same formulation as the generalized least-squares method (GLS) which is used here. Uncertainty analysis is considered in detail, e.g., in Ref. 8.

We consider the vector of m calculated quantities, $\boldsymbol{Q} = (Q_1, Q_2, \ldots Q_m)$, which contains components from critical assemblies, as well as reactor designs. The calculations are based upon n prior evaluated parameters, $\boldsymbol{p} = (p_1, p_2, \ldots p_n)$, with covariance $\boldsymbol{C_p}$. The covariance of calculated quantities due to the parameter covariance then follows from error propagation, i.e.,

$$\boldsymbol{C_Q} = \boldsymbol{S}\, \boldsymbol{C_p}\, \boldsymbol{S^T} \tag{1}$$

where $\boldsymbol{S}$ is the $m \times n$ sensitivity matrix with components

$$\boldsymbol{S_{ij}} = \frac{\boldsymbol{p_j}}{\boldsymbol{Q_i}} \frac{\boldsymbol{\partial Q_i}}{\boldsymbol{\partial p_j}} \tag{2}$$

which are the percent changes of the $\boldsymbol{Q_i}$'s per percent changes of the parameters $\boldsymbol{p_j}$.

It is assumed that the prior evaluation of the n parameters was based upon ℓ (differential) experimental data ($\ell > n$) and that k additional (integral) experimental data are available which are uncorrelated with the ℓ values. Utilization of the additional k experimental data leads to adjustments on the prior evaluated parameters with the adjustment vector given by

$$\boldsymbol{\delta} = \boldsymbol{C_p}\, \boldsymbol{S^T}\, \boldsymbol{W^{-1}} \boldsymbol{E} \tag{3}$$

$$\boldsymbol{W} = \boldsymbol{S}\, \boldsymbol{C_p}\, \boldsymbol{S^T} + \boldsymbol{C_E} = \boldsymbol{C_Q} + \boldsymbol{C_E} \tag{4}$$

where $\boldsymbol{E}$ is the reduced measurement vector with covariance $\boldsymbol{C_E}$. It is with the weight matrix, $\boldsymbol{W^{-1}}$, that the relative importance of the prior information, contained in the pre-evaluated parameters, and the

additional information, contained in the k experimental values, is properly taken into account. The covariance matrix of the adjusted parameters is given by

$$\boldsymbol{C_p' = C_p - C_p S^T W^{-1} S C_p} \tag{5}$$

and is inserted in Eq.(1) in order to evaluate the uncertainties and correlations of the calculated quantities based upon the adjusted parameters. The latter can be obtained by recalculating $\boldsymbol{Q}$ with the adjusted parameters, or, alternatively, by directly adjusting the calculated quantities with

$$\boldsymbol{Q' = Q\,(I + S\,\delta)} \tag{6}$$

where $\boldsymbol{I}$ is the unit vector.

For the present considerations, the prior evaluated parameters are the cross sections and other parameters obtained from the evaluated nuclear data files which are reduced to group cross sections with a specified energy-group structure. The additional experimental data are the data obtained from critical assembly experiments. The corresponding quantities are functions of the parameters which require linearization which are obtained from the Taylor series expansion, broken off with its first-order term:

$$\boldsymbol{Q_i = Q_{io} + \sum_j \frac{\partial Q_i}{\partial p_j}\,(p_j - p_{jo})} \tag{7}$$

The neglect of the higher order terms in the Taylor series expansion leads to errors of the adjusted parameters which propagate to errors of the reactor quantities. However, if the adjustments are made on the calculated quantities based on the same linear Taylor Series expansion, instead of recalculating the quantities with adjusted parameters, one would expect a partial compensation of the errors made.

Some of the parameters are group cross sections and adjustments on infinite dilute cross sections are implied. However, the adjustments ought to be made on the underlying parameters, e.g., resolved resonance parameters, unresolved resonance parameters, pointwise cross sections, etc., labeled g. The linear term of the Taylor series expansion should therefore read

$$\boldsymbol{\sum_l \frac{g_l}{Q_i}\frac{\partial Q_i}{\partial g_l}\frac{g_l - g_{ol}}{g_{ol}}} \tag{8}$$

Using the chain rule one obtains

$$\boldsymbol{\sum_l \delta_l \sum_j \frac{p_j}{Q_i}\frac{\partial Q_i}{\partial p_j}\frac{g_l}{p_j}\frac{\partial p_j}{\partial g_l} = \sum_l \delta_l \sum_j S_{ij}\, D_{jl}} \tag{9}$$

where the $\boldsymbol{\delta_l}$ are the adjustments on the underlying parameters and the transformation matrix $\boldsymbol{D}$ contains the sensitivities of the group cross sections to the underlying parameters. This has been discussed in the context of higher order effects in sensitivity analysis by Greenspan *et al*.[9] As long as adjustments to the calculated quantities are small compared to one, uncertainties due to these effects should be small. Therefore, at present, they have been neglected, though efforts to introduce the transformation matrix may later be introduced.

The Taylor series expansion should involve all parameters, including those relating to the reactor model and methods approximation. The latter would be expressed as corrections (for example, for cell heterogeneity). However, most features involved in the models and most methods approximations are difficult to quantify and corresponding parameters are ignored. It is generally assumed that the model and methods approximations are fit into parameter adjustments. The uncertainties of the neglected parameters have been accounted for by replacing the covariance matrix of the experimental data $\boldsymbol{C_E}$, with $\boldsymbol{C_E} + \boldsymbol{C_M}$. It is interesting to note that the generalized $\boldsymbol{X^2}$ of the fit[10]

$$(\boldsymbol{Q'} - \boldsymbol{E})\, \boldsymbol{W^{-1}}\, (\boldsymbol{Q'} - \boldsymbol{E})^{\boldsymbol{T}} \qquad (10)$$

increases by about a factor of 10 if the model and methods uncertainties are not included in the covariance matrix for the reduced measurement vector $(\boldsymbol{E} - \boldsymbol{Q})$. This indicates that the model and methods approximations cannot be fit into parameter adjustments if such parameters are not provided for. Including the model and methods uncertainties, or not, with the uncertainties of the experimental data has only minor effects on the adjusted quantities.

References

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