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A proposed method for addressing large unphysical uncertainties in mubar

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Abstract. Mubar uncertainties in Section MF 34 MT 2 of ENDF/B-VIII.0 data are sometimes too large. Physical limitations of the bounds of mubar limit the maximum uncertainty to be < 1.0 and usually << 1.0. Two ad hoc methods are proposed to artificially constrain the randomly sampled values of mubar to allowable values. The application of NJOY's mubar covariance matrix to the "sandwich rule" is also discussed and a consistent way to apply sensitivity coefficients is described. Mubar uncertainties for the Jezebel k_{eff} were found to be 156 pcm – a value comparable to other evaluated cross section uncertainties.

1 Introduction

Elastic scattering mubar covariances are found in the MF 34 MT 2 section of the evaluated nuclear data files [1]. These uncertainties are given for mubar, the cosine of the lab scattering angle, from an elastic neutron scattering event. As calculated by NJOY [2], values are given in a groups by 1 vector for the Legendre P_1 out-scattering divided by the Legendre P_0 out-scattering for a given incident energy group. (Higher order mubar terms are not presently available from NJOY.) As such, the values of mubar are bounded between -1 (backward scattering) and +1 (forward scattering).

These physical limits on mubar also imply a constraint on the allowable values of the uncertainty of mubar. When the data found in the evaluation files for mubar uncertainty is too large, then the generation of correlated random samples of mubar becomes impossible without encountering unphysical (outside the -1 to 1 interval) values of mubar. A sampling technique used in NORTA [3] and Copula [4] methods is proposed as an ad hoc fix for the problems of large unphysical uncertainties in mubar. A second technique is also presented which uses a zscale-like transformation.

Additionally, a consistent application of NJOY produced mubar covariance data is presented for usage in the "sandwich rule" for the propagation of uncertainty. This is necessary, since NJOY produces a groups by 1 vector of relative variance values, while the relative sensitivity values produced by codes like SENSMG [5] and the "ksen" option of MCNP [6] are usually a matrix dimensioned as "groups by groups".

2 The constraints on the variance and standard deviation of mubar

For a distribution defined only between -1 and +1, the largest possible variance or standard deviation is 1.0. This occurs when ½ of the sampled points are at -1.0 and the other ½ are at 1.0. This configuration gives the largest possible spreading out of the points.

However, if a more realistic uniform (i.e., flat) mubar distribution is assumed, then the variance and the standard deviation are reduced further. For a uniform distribution between -1 and +1, the variance = 1/3 and the standard deviation = $1/\sqrt{3}$.

If a truncated normal distribution is forced into the interval, say at a 3 or 4 sigma truncation, then the standard deviation of mubar is even less.

Finally, as the scattering becomes very forward, then the allowable variance and standard deviations approach 0.0. Mubar = 1.0 implies that all mu values = 1.0. These uncertainty limits are shown in Figure 1.

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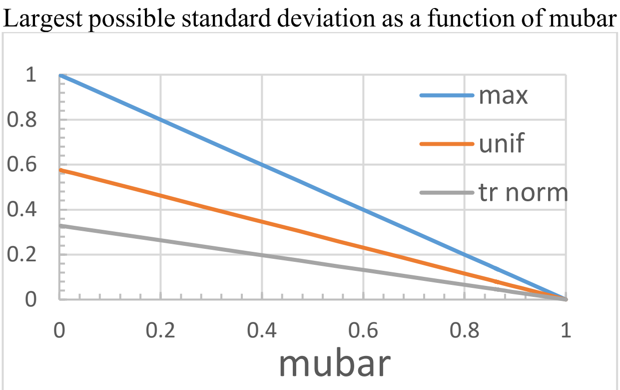

Fig 1: Constraints on mubar uncertainty due to the distribution and value of mubar

3 Proposed sampling techniques to limit the uncertainty on mubar

A version of a known statistical sampling method (NORTA – NORmal To Anything) has recently been employed to address these large uncertainties. The randomly sampled mubar points (which are initially drawn in a normal distribution) from the groups with large uncertainties are transformed into a uniform (i.e., flat) distribution which is constrained to fit inside of the allowable -1.0 to 1.0 interval in such a way as to preserve the average mubar. A CDF (cumulative distribution function) statistical function is used to transform the normal random samples to a uniform (i.e., flat) distribution (ranging initially from 0.0 to 1.0). This transformation imposes a hard limit on the variance of the group value of mubar of <1/3 and thus a limit on the standard deviation of <1/sqrt(3). For mubar = 0.0, the uniform CDF produced points between 0.0 and 1.0 are then scaled linearly to -1.0 to +1.0.

Using an EXCEL® function:

uniform points = NORM.S.DIST(z,'true') (1)

Where z = the standard scores for the normal random points

Using a MATLAB® function:

uniform points = normcdf(z) (2)

The uniform points are distributed between 0 and 1 (based on the area under the normal curve measured from the left hand side). A large negative score for the normal random point is transformed to a value close to 0, while a large positive score is transformed to a value close to 1. The uniform points can then be scaled linearly to a range of -1 to 1 (for mubar = 0) or more generally to a subset of -1 to 1.

The basic transformation is illustrated in Figure 2 below. Notice how the pattern of distances between the adjacent points on the normal curve is mostly preserved in the uniform curve.

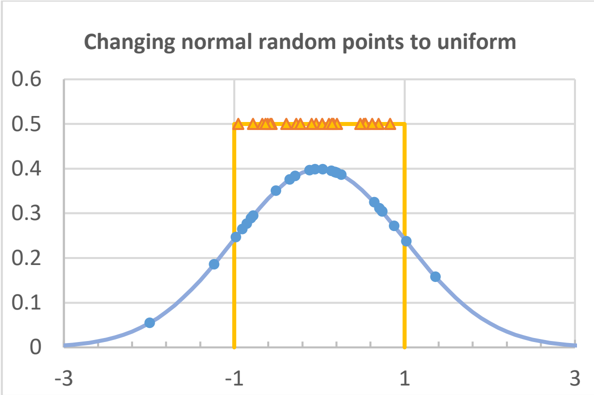

Fig. 2: Transformation of normal random points to a uniform distribution

If the value of mubar is not 0.0, then the limits of the uniform distribution are linearly scaled to a symmetric (i.e., about mubar) sub-interval that preserves mubar. For example, if mubar = 0.2, the uniform limits are -0.6 and 1.0. These results are illustrated in Figure 3.

Consistent with Figure 1, the standard deviation of the uniform distribution with mubar = 0.2 is smaller (0.46188) than the mubar = 0.0 distribution (0.57735). These values come from the formula for the standard deviation of uniform distributions.

$$\sigma = (b-a) / 2\sqrt{3} \tag{3}$$

where b = the right hand limit.
a = the left hand limit.

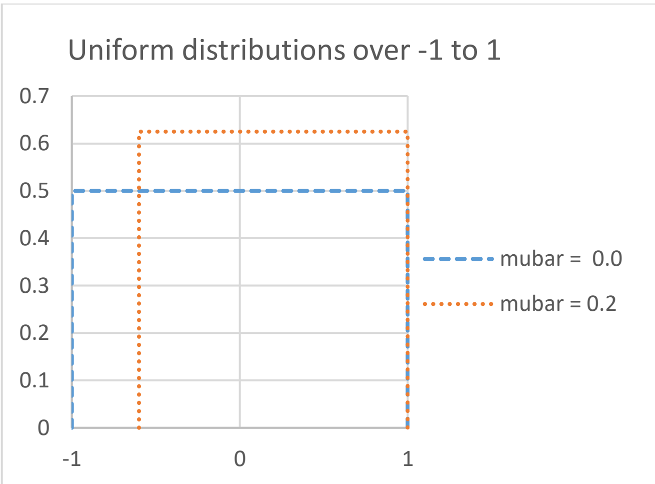

Fig 3: Comparison of mubar = 0 and 0.2 distributions

Fortunately, this transformation preserves the rank correlation (e.g., the largest and smallest points are still at their same locations in the vector) of the randomly sampled points – though it does not exactly preserve the linear correlation between the mubar data samples. However, the transformed samples all fit inside the allowed interval and the average group value of mubar is preserved.

Furthermore, iterative improvement of the linear correlation properties of the random samples is often possible. See the recently published tutorial on random sampling for nuclear data [7].

Another ad hoc sampling technique which could be used is to take the normal distribution random samples (which are spread out beyond the -1.0 to 1.0 interval) and reduce their standard deviation in a zscale-like fashion so that all the sampled points fit in between -1.0 and 1.0. Even though the normal distribution is infinite in extent, the random samples will very seldom be found beyond 3 or 4 sigma's away from the mean.

This zscale-like procedure preserves the mubar mean and the rank correlations, and also preserves the linear correlations of the original random samples. The drawback is that only very small values of the standard deviation can be accommodated. See Figure 1. The maximum value of the standard deviation would be (assuming mubar > 0) (1.0 – mubar) / (3 or 4) for 3 or 4 sigma's, respectively. These values are smaller than the uncertainty values accommodated by a uniform distribution.

4 A consistent application of mubar covariances in the sandwich rule

As produced by NJOY, mubar variances include values for each incoming group but with all outgoing groups summed together. Group to group covariance data is also given for the incident groups. Covariances may be produced in absolute or in relative form or even in correlation form.

Application of this mubar covariance data (traditionally used in relative form) in the "sandwich rule" requires elastic scattering P_1 sensitivities which are also calculated for each incoming group and with all the outgoing groups summed together. However, SENSMG [5] only produces P_1 elastic sensitivities in group-by-group form. The "ksen" option of MCNP [6] can produce groupwise P_1 elastic scattering sensitivities with or without group-by-group binning of the output groups. Sensitivities are also usually produced in relative form to be consistent with the relative covariance data.

If the sensitivities are given in group-by-group (i.e., doubly differential) form, then the sum of the P_1 elastic scattering outgoing group sensitivities for each incoming group should be used in the sandwich rule.

A thirty group ENDF/B-VIII.0 analysis of Jezebel k_{eff} uncertainty due to mubar uncertainty was carried out using MF 34 MT 2 elastic scattering mubar uncertainties for Pu-239. P_1 elastic sensitivities from SENSMG were group summed over the output groups for each input group, and the result of the sandwich rule was an uncertainty of 156 pcm. This is certainly comparable to the other Jezebel uncertainties studied in the CIELO project [see Table VIII of Reference 8].

For the simple summing of output group elastic P_1 sensitivities for each input group to be used consistently, the individual values of the P_1 out-scatter cross sections used in Sn calculations must each be changed by the same ratio of new mubar / old mubar. This consistency has been established by Jeff Favorite and verified by comparison with second order accurate central differencing estimates of the sensitivity coefficients [9]. (This has not yet been officially published.) He has also shown that if the change in mubar is allocated in other ways to the P_1 elastic scattering cross sections, then the sum of the output group sensitivities must be modified accordingly – usually in the form of a weighted sum.

It should also be noted that changing the elastic scattering P_1 cross sections in a S_n code library can be somewhat laborious. The elastic scattering cross sections are usually mixed in with inelastic, n2n, n3n, etc. cross sections in the combined Legendre scattering matrix.

5 Summary

Two ad hoc workarounds for limiting the bad effects of unphysical ENDF/B-VIII.0 mubar uncertainties in the context of random sampling have been proposed. The methods preserve mubar and ensure that all sampled points are within the desired valid interval or sub-interval. The variances and standard deviations of mubar are limited to physically valid values while preserving rank correlation. Linear correlation of the randomly sampled points is approximately preserved for the uniform method and exactly preserved for the zscale-like approach.

Hopefully, the physical constraints on the size of mubar uncertainties discussed here will be respected in future MF 34 MT 2 elastic scattering mubar evaluated data.

In connection with this proposal and these constraints, a consistent way to use the NJOY produced mubar covariance data in the sandwich rule with group-by-group sensitivities has been described. Further publications will follow.

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