Best linear unbiased estimation of the nuclear masses

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Abstract

This paper presents methods to provide an optimal evaluation of the nuclear masses. The techniques used for this purpose come from data assimilation (DA) that allows combining, in an optimal and consistent way, information coming from experiment and from numerical model. Using all the available information, it leads to improve not only masses evaluations, but also to decrease uncertainties. Each newly evaluated mass value is associated with some accuracy that is sensibly reduced with respect to the values given in tables, especially in the case of the less well-known masses. In this paper, we first introduce a useful tool of DA, the Best Linear Unbiased Estimation (BLUE). This BLUE method is applied to nuclear mass tables and some results of improvement are shown. Then finally, some post validation diagnostics, demonstrating that the method has been used in optimal conditions, are described and used to validate the results.

Keywords: Data assimilation, Best Linear Unbiased Estimation, BLUE, nuclear masses, mass tables

1 Introduction

The mass tables provide an evaluation of the mass for every known and forecasted nuclei that are very important in nuclear physics. Information gathered inside those table by experimentalist and various nuclear mass models (for example "Finite-Range Liquid-Drop Model" [1, 2] or "Finite-Range Droplet Model" [3]) is used for reaction planning and nuclear reactions simulations. Thus, an accurate knowledge of masses of the nuclei permits to realize high quality calculations and planning.

The purpose of this paper is to present a method to optimally evaluate masses of known nuclei, as well as the accuracy associated. The aim is to

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produce an improved set of data for nuclear masses, with better accuracy respect to tabulated ones. This general approach is already applied in other fields of science, as for example in meteorology, climatology or oceanography. The procedure proposed here is the same as the one climatologists use to obtain high accuracy meteorological data. This is the case for example of the widely used meteorological re-analysis ERA-40 [4].

Despite a frontier often exists between experimental results and theoretical ones, both provide pieces of information on the same reality. With an extreme point of view, two positions can be assumed. The first one is that only theory is valuable and then all experiences are useless. The complete antagonist position claims that only experience is meaningful, so there is no need to do simulation for forecasting or explaining within a theoretical framework. Obviously, both points of view are too restrictive, and ideally both information (theoretical and experimental) need to be merged to describe more accurately the physic. Data assimilation (DA) is precisely a general method to handle jointly experimental data and numerical modelling information to estimate the optimal values. Moreover, DA techniques allow at the same time to improve accuracy of the estimation with respect to the original data.

In this paper, we will first develop some aspects on the theory and the basics concepts of DA. In fact DA covers a large number of techniques. Here we will focus on the Best Linear Unbiased Estimation (BLUE) technique, that fits very well to the present problem. We will use this BLUE technique to estimate the nuclear masses of the known nuclei found in the classical mass tables. This will lead to a new set of nuclear masses with improved accuracy. The evaluation we obtain by this procedure could always be claimed to be dominated by some assumption. Thus, in the last part of this paper, we will focus on the post validation of DA method. That permits to show that the optimal estimation obtained by DA is not dominated by intrinsic assumptions.

2 Data assimilation

We briefly introduce the theory of DA. However, DA is a wide domain and we will not present here the advanced techniques that include dynamics of the process, that are for example the basis of the nowadays-meteorological operational forecast. This is through advanced DA methods that long-term weather forecasting has been drastically improved in the last 30 years. Improvement in this field are constant, and nowadays 3-day weather forecasts are as reliable as 1-day forecasts twenty years ago. Such a procedure use all the recently available data, such as satellite measurements, as well as sophisticated numerical models. Some interesting information on these approaches can be found in the following references [5, 6, 7].

The ultimate goal of DA methods is to be able to figure out the inaccessible true value of the system state, so called $x^t$ with the $t$ index for "true". The basic idea of DA is to put together information coming from an $a$ priori on the state of the system (usually called $x^b$, with $b$ for "background"), and information
coming from measurements (referenced as \( y \)). The result of DA is called the analysis \( x^a \), and it is an estimation of the true state \( x^t \) we want to find.

Some tools are necessary to achieve such a goal. As the mathematical space of the background and the one of observations are not necessary the same, a bridge between them needs to be built. This is the so called observation operator \( H \), with its linearization \( H \), that transforms values from the space of the background to the space of observations. The reciprocal operator is the adjoint of \( H \), which in the linear case is the transpose \( H^T \) of \( H \).

Two other ingredients are necessary. The first one is the covariance matrix \( R \) of observation errors, which are \( \epsilon_o = y - H(x^t) \). It can be obtained from the known errors on the unbiased measurements. The second one is the covariance matrix \( B \) of background errors, which are \( \epsilon_b = x^b - x^t \). It represents the error on the a priori, assuming it to be unbiased. There are many ways to obtain these observation and background error covariance matrices. However, this is commonly the output of a model and an evaluation of its accuracy, or the result of expert knowledge.

To find this optimal value \( x^a \) the underlying idea is to minimise the variance of the error \( \epsilon_a = x^a - x^t \) associated to this value. Then it can be proved that, within this formalism, the Best Unbiased Linear Estimator \( x^a \) is given by the following equation:

\[
x^a = x^b + K(y - Hx^b)
\]

where \( K \) is the gain matrix:

\[
K = BH^T(BH^T + R)^{-1}
\]

Moreover we can obtain the analysis error covariance matrix \( A \), characterising the analysis errors \( \epsilon_a \). This matrix can be expressed from \( K \) as:

\[
A = (I - KH)B
\]

with \( I \) the identity matrix. Note that one way to prove equation 2 is to minimise the trace of the matrix \( A \), leading also to prove \( x^a \) is the optimal value we are looking for. The demonstration is detailed in the reference [7]. It can equivalently be proven through a maximum likelihood hypothesis.

It is worth noting that solving equation 1 is equivalent to minimising the following function \( J(x) \), \( x^a \) being the optimal solution:

\[
J(x) = (x - x^b)^TB^{-1}(x - x^b) + (y - Hx)^TR^{-1}(y - Hx)
\]

If we assume that the background \( x^b \) is given by a model, and that the covariance matrix \( B \) comes from an error evaluation of the model, then we can make some interesting remarks concerning equation 4. If we recall the extreme assumptions on model and experiments mentioned in the introduction, we notice that these cases are covered by the minimizing of this function \( J \). If we assume that the model is completely wrong then the covariance matrix \( B \) is
∞ (or equivalently $B^{-1}$ is 0), and minimum of $J(x)$ is given by "$x^a = H^{-1}y$", it corresponds directly to information given only by data. With the opposite assumption that data are useless, implying that $R$ is $\infty$, we obtain $x^a = x^b$. Such an approach covers the whole range of assumptions we can state with respect to data.

Then the main work is to evaluate as well as possible the observation operator $H$ and the two covariance matrices $B$ and $R$. We will proceed with this task within the framework of the mass tables.

### 3 Application of data assimilation to the nuclear mass evaluation

To build the Best Linear Unbiased Estimation of the mass tables, we will work on masses excess instead of masses themselves. The mass excess of a nucleus is the difference between its actual mass and its mass number ($A \times u$) with $u$ the atomic mass unit, or "unified atomic mass" (see Table A in [8] for information on this unit) and $A$ the number of nucleons.

For the background $x^b$, we will take the reference data of mass excess values proposed in [9, 10] by P. Moller, J.R. Nix, W.D. Myers, and W.J. Swiatecki, focusing on the masses obtained from the Finite-Range Droplet Model [3] with shell energy correction. Note the results are very similar to the ones obtained from the Finite-Range Liquid-Drop Model [1] [2]. In those theoretical tables, we will limit ourselves to the known nuclei heavier than oxygen, that is with protons number $Z \geq 8$, which is the lowest reliable value for the model.

The experimental mass excess values are the one from G. Audi and all reference tables [11, 8, 12, 13]. This remarkable collection of data also includes the error associated to each measurement. This represents the observation, denoted $y$ in the previous section.

These two data series of mass excess values $x^b$ and $y$ are in the same space. Then the required observation operator $H$ is obviously reduced to identity $I$.

The covariance matrix $R$ on observation errors is chosen to be a diagonal matrix. On the diagonal, we put the known value of the uncertainties given in experimental tables [11, 8, 12, 13].

The evaluation of the background errors covariance matrix $B$ is more complicated. The first assumption is that background errors are independent the one from the other. Then $B$ reduces to a diagonal matrix. As no information yet exists on the model accuracy, it is also assumed as a second assumption that this accuracy is independent of each nuclei we consider. Thus we only need one global value of accuracy denoted as $\sigma_b^2$. It remains to evaluate this unique value $\sigma_b^2$ on the diagonal. For this purpose, we made a statistical study. The error between $x^b$ and $x^t$ is over estimated by the error between $x^b$ and $Hx^t = y$, that is globally more variable. Thus, considering that, last relative error gives a penalty to the accuracy on model evaluation. This is the third assumption we make to obtain model error evaluation. To evaluate a value for the diagonal
of $B$, we calculate the mean square of $x^b - y$ over all the available nuclei. The mean square is $\sigma_b^2 = 0.652904$, that is $\sigma_b = 0.808024$ MeV. This is the value that we will put on the diagonal of $B$.

These constructions of $B$ and $R$ matrices are based on some hypothesis that are realistic but one can always claim they are not correct or to lousy. To comfort them, in section 4 we will present a post validation of the matrix $B$ and $R$ that prove they are reliable in the context of this framework and the known data.

For informative purpose, it is interesting to look at the calculated mean value of $x^b - y$, which it is equal to $-0.058326$ MeV. It is fairly close to 0, and then comfort the implicit hypothesis to be in a quasi-unbiased case for background error estimation.

Note that the choice done to build the $B$ and $R$ as diagonal matrix imply that only nuclei included in DA procedure are affected by it.

All the required data are then available to build the DA analysis as described in section 2 by simply applying formula 1. The differences between the experimental results $y$ and the analysed results $x^a$ obtained with DA are shown on Figure 1 in percentage of change of mass excess for all the nuclei in function of their protons and neutrons numbers.

On Figure 1 it can be noticed that the relative modification of the masses could be as lower as $10^{-10}\%$ up to $80\%$ in absolute value. This wide range
of modification can be explain easily within an assimilation process. On one hand, in case nuclei masses are known very accurately, like for stable nuclei, then information provided by the background (model) do not contribute a lot, masses excess to not change, and the relative modification is around $10^{-100}\%$.

On the other hand, if nuclei masses excess are not known very accurately masses excess given by the model give a lot more information. Thus, information on physical property of nuclei included in the model permits to drive the measured value toward a new value that is more likely (in the sense of the maximum likelihood principle include in DA method) and then modification can be up to 80%. Thus, as we notice on Figure 1, the more we go far from stability valley the more modification of the nuclei masses excess could be important because the less the measurement are accurate.

Considering those notable modification it is worth taking into account the new results for mass excess. We have checked that all results are correctly enclosed between the background previsions and the experimental values. This mean that we never overshoot either experimental value or the one given by the model. So the analysed value respects information provided by both. To understand better this point let’s assume analysed value is not enclosed between data and models value. This means that some information was given to the procedure to push it towards another unknown value. As there are no other source of information, even no correlation between nuclei errors in the present case, the analysis values need to be enclosed between experimental value and model prediction. Thus whatever is the estimated value, it is somehow consistent with the provided information.

A key point is on the accuracy, as, by construction of the method, DA improves it. The diagonal of the matrix $\mathbf{A}$ (which, in the present case, is a diagonal matrix) contains the variance $\sigma_a^2$ of the analysis $x^a$ for each nuclear nuclei. We are looking at the percentage of evolution of the accuracy, with respect to the experimental accuracy $\sigma_y$ for each nuclei. Thus we can construct the following accuracy indicator $\frac{\sigma_y - \sigma_a}{\sigma_y}$, observed in percents.

With such a definition, an improvement of the accuracy (that is a decrease of $\sigma_a$ with respect to $\sigma_y$) is a positive percentage. As we are only interested in the evolution of this value, we will make a histogram plot where each bin represent the accuracy indicator for one nuclei to get a 1D representation of all the results. To obtain such mono dimensional plot we consider the nuclei ordered in the same way as in the reference file [13]. Thus the first bin correspond to the first nuclei of the G. Audi and all table, and so on. The results are presented on the Figure 2.

From Figure 2 we confirm that all values are positive, which means that there is always an improvement of the accuracy. The improvement can be up to roughly 70% in some cases. As for the analysed value themselves, this means that when an experimental value is known very accurately, a lot of effort is required to do better. On the contrary, if original accuracy on data is no so good, it is easy to improve it providing only little additional information.

Considering Figure 2 from an experimental point of view, we notice that
DA provides value with better accuracy specially on the weak points when the experimental value are inaccurate due to the difficulties of measurements.

Then, globally speaking, we can say DA method applied to nuclear mass tables is very successful, and leads within a simple framework to some significant improvements of nuclei masses excess and their associated error.

4 Post validation of the hypothesis

Establishing the $\mathbf{R}$ and $\mathbf{B}$ matrices is globally speaking a difficult task. This is already known for long time in the meteorology, oceanography and other domains. The construction of those matrices are fundamental for the DA process. Thus, checking methods have been developed to make post validation of those important components. The details of those methods and some applications are presented in references [14, 15]. We introduce them here to discuss their application and results.

We define the difference between measurements and observations by:

$$\mathbf{d} = \mathbf{y} - \mathbf{Hx}^b$$  

It can be proved that:

$$\mathbb{E}(\mathbf{dd}^T) = \mathbf{R} + \mathbf{HBH}^T$$
where \( \mathbb{E} \) is the mathematical mean. Then, from that formula, two other come rather directly:

\[
\mathbb{E}((I - HK)dd^T) = R
\]  

(7)

and:

\[
\mathbb{E}(Kdd^T) = BH^T
\]  

(8)

From those two formulas \(^7\) and \(^8\) we can check and validate the hypothesis we did. First, it is assumed that the best \( R \) matrix is proportional to the originally established one that we will call \( (R_0) \). Because the diagonal of the matrix contains variances, we need a positive coefficient, chosen to be a square term \( s_o^2 \). Thus, we have:

\[
R = s_o^2 R_0
\]  

(9)

To obtain that coefficient, using traces of both matrices leads (see \(^{14},^{15}\) for details) to the following result:

\[
s_o^2 = \frac{\mathbb{E}(d^T(y - Hx^a))}{\text{Trace}(R_0)}
\]  

(10)

We can do a similar process with background error matrix \( B \), assuming that:

\[
B = s_b^2 B_0
\]  

(11)

In this case, the situation is different, as we do not got direct equation on \( B \) but only on \( BH^T \). Thus, we will work on the \( HBH^T \) matrix assuming, equally to the previous equation, that:

\[
\text{Trace}(HBH^T) = s_b^2 \text{Trace}(HB_0B^T)
\]  

(12)

According to equation \(^{8}\) we have:

\[
\text{Trace}(HBH^T) = s_b^2 \text{Trace}(\mathbb{E}(HKdd^T))
\]  

(13)

The left side of the equation can be rewritten as:

\[
\mathbb{E}(d^T H \delta_a) = \mathbb{E}(d^T H (x^a - x^b))
\]  

with \( \delta_a = x^a - x^b \). Then we can express \( s_b^2 \):

\[
s_b^2 = \frac{\mathbb{E}(d^T H \delta_a)}{\text{Trace}(HB_0H^T)}
\]  

(15)

From equation \(^{9}\) and \(^{11}\) we notice that, if \( s_o^2 \) and \( s_b^2 \) are equal to 1, estimations of \( B \) and \( R \) are perfectly balanced with respect to BLUE equations. This method can be applied iteratively to improve the quality of the matrix until it converges to a steady state with both values of \( s_o^2 \) and \( s_b^2 \) close to 1.

Let’s first evaluate the quality of the modelling on the first step. The results are the following \( s_b = 0.97445 \) and \( s_o = 1.3007 \). If we go on in the iterations, a satisfactory converged state is reached at the 6\(^{th}\) one. Looking only at the first
step results, we can already claim that modelling of $B$ matrix is very satisfactory. For the case of the $R$ matrix the result is not so good, but still very correct in an assimilation procedure. It is worth recalling that the values $s_b$ and $s_o$ are linked together, so modification on $R$ or on $B$ impacts both of them. Globally speaking, results of the post processing are satisfactory and do not enlighten a discrepancy of several order of magnitude as it can happen in such process. Especially, we are deeply comforted about the rightfulness of the most delicate hypothesis done on the $B$ matrix.

5 Conclusion

DA technique applied on the mass tables appears to be very successful. The new set of mass data produced is reliable:

- it shows to be within the limit previously given by theory and experience,
- the accuracies on the mass excess are lower than the one previously known, which makes them more suitable to use,
- the post validation is satisfactory and validate the hypothesis done to build data set.

Thus here is described the generation of an optimal set of masses that can be used when needing mass tables information, as it was done in climatology by ERA-40 re-analysis [4].

However, as a perspective, the present application is showing only some limited aspects of the possibility of DA. Especially, the improvement of the $B$ matrix can be studied in order to open the way for forecasting more accurately masses of yet unknown nuclei. This is still a tiny improvement among the huge number of possibilities that DA can provide to nuclear physic field.

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