Error Estimates of Theoretical Models: a Guide

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Abstract. This guide offers suggestions/insights on uncertainty quantification of nuclear structure models. We discuss a simple approach to statistical error estimates, strategies to assess systematic errors, and show how to uncover inter-dependencies by correlation analysis. The basic concepts are illustrated through simple examples. By providing theoretical error bars on predicted quantities and using statistical methods to study correlations between observables, theory can significantly enhance the feedback between experiment and nuclear modeling.
1. Introduction

“Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful.” [1] This quote, by George E.P. Box, a statistician and a pioneer in the areas of quality control and Bayesian inference, well applies to the nuclear many-body problem. When it comes to nuclear modeling, uncertainties abound. Indeed, the nuclear interaction, strongly influenced by in-medium effects, is not perfectly known, and the same can be said about many operators associated with observables. In addition the many-body equations are difficult to crack, which forces nuclear modelers to introduce simplifying assumptions.

The need for uncertainty estimates in papers involving theoretical calculations of physical quantities has been long recognized in the atomic-physics community. The current situation has been well captured by an Editorial in Physical Review A [2]:

It is all too often the case that the numerical results are presented without uncertainty estimates. Authors sometimes say that it is difficult to arrive at error estimates. Should this be considered an adequate reason for omitting them? [...] There is a broad class of papers where estimates of theoretical uncertainties can and should be made. Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances: (1) If the authors claim high accuracy, or improvements on the accuracy of previous work; (2) If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements. (3) If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

This demand applies equally well, if not even more so, in nuclear theory, where we have not a well settled ab-initio starting point at hand. We are dealing almost everywhere with effective theories justified in terms of general arguments, but whose parameters are basically unknown and often cannot be deduced from ab-initio modeling. Consequently, those parameters are often determined by fits to empirical data. This immediately raises the question of the predictive power of such phenomenologically adjusted theories; hence, there is a need for error estimates of the predicted values.

We have here particularly in mind effective interactions or energy functionals for nuclear structure and dynamics. These are usually fitted to large sets of experimental data. The technique of least-squares fitting, involved in these adjustments, opens immediately the door to the well developed strategies for error estimates from statistical (or regression) analysis [3 4]. This is the least we can do, and should do, towards delivering error estimates. Besides mere error estimates, statistical analysis is a powerful instrument to acquire deeper insights into models, e.g., by determining weakly and strongly constrained parameters or correlations between different observables.

However, a purely statistical analysis is not sufficient, as it does not cover what is called the systematic errors, that is, missing aspects of the modeling. Thus a broad
discussion of extrapolation errors must also address systematic errors. Unfortunately, systematic errors are just those which cannot be dealt with in systematic manner. It takes a deep insight into the related exact and approximate theories to have a presentiment of possible pitfalls in a fit.

In the following, we address all three aspects: error estimates by statistical analysis, attempts to assess systematic errors, and uncovering inter-dependencies by correlation analysis. A number of examples will be provided. Some of the questions addressed are:

(i) How to estimate systematic and statistical errors of calculated quantities?
(ii) What is model’s information content?
(iii) How to validate and verify theoretical extrapolations?
(iv) What data are crucial for better constraining current nuclear models?

A secondary objective of this guide is to set the stage for the upcoming Focus Issue of Journal of Physics G on “Enhancing the interaction between nuclear experiment and theory through information and statistics,” which will contain many excellent examples of uncertainty quantification in nuclear modeling.

We hope that these notes will serve as a useful guide for nuclear theorists, especially those who have not yet embarked on the uncertainty-quantification journey. In this context, we strongly recommend a recent essay by Saltelli and Funtowicz [5] on modeling issues at the science/policy interface; we found their checklist to aid in the responsible development and use of models particularly insightful. The proposed seven-rule checklist helps understanding the different sources of uncertainty and their relative importance [5]:

Rule 1: Use models to clarify, not to obscure. Many-parameter descriptions can be used at an interim stage on the way to understanding but a fit seldom provides an answer. Remember the quote by von Neumann: “With four parameters I can fit an elephant, and with five I can make him wiggle his trunk”? Models should explain and simplify, but not make a situation more confused.

Rule 2: Adopt an “assumption hunting” attitude. Are model assumptions expressly stated or implicit/hidden? What in the model is assumed to be irrelevant?

Rule 3: Detect pseudoscience. Be sure that uncertainties have not been twisted to provide desired results.

Rule 4: Find sensitive assumptions before they find you. Carry out technically sound sensitivity studies.

Rule 5: Aim for transparency. Fellow scientists should be able to replicate the results of your analysis.

Rule 6: Don’t just “Do the sums right,” but “Do the right sums” – to address the relevant uncertainties.

Rule 7: Focus the analysis. Sensitivity analysis of a many-parameter system cannot be done by merely changing one parameter at a time.
These notes are structured as follows. In Sec. 2 we discuss the notion of statistical and systematic errors. Section 3 summarizes the technique of least-squares optimization and shows how to estimate statistical errors. In Sec. 4 we discuss systematic errors and employ two pedagogical models to illustrate basic concepts. In Sec. 5 we come back to statistical analysis and show how it allows us to acquire deeper insights into model’s information content. Section 6 contains selected examples from recent work.

2. Systematic and statistical model errors

In general, there are no surefire prescriptions for assigning error bars to theory. Model uncertainties have various sources, some are rooted in experimental errors, some in model deficiencies. As well put by Albert Tarantola:

The predicted values cannot, in general, be identical to the observed values for two reasons: measurement uncertainties and model imperfections. These two very different sources of error generally produce uncertainties with the same order of magnitude, because, due to the continuous progress of scientific research, as soon as new experimental methods are capable of decreasing the experimental uncertainty, new theories and new models arise that allow us to account for the observations more accurately.

While the mutual interaction between experiment and theory resulting in a mutual reduction of uncertainties better applies to atomic theory, as theoretical uncertainties usually dominate experimental ones in nuclear modeling, the positive feedback described in the above quotation constitutes the situation we all should be striving to.

The statistical model error is usually quantifiable for many models. Namely, when the model is based on parameters that were fitted to large datasets, the quality of that fit is an indicator of the statistical uncertainty of the model’s predictions. The commonly employed tool to estimate statistical errors is the regression analysis. Section 3 shows how to estimate statistical errors by means of weighted least squares.

The systematic model error is due to imperfect modeling: deficient parametrizations, wrong assumptions, and missing physics due to our lack of knowledge. Since in most cases the perfect (exact, reference) model is not available, systematic errors are extremely difficult to estimate. Especially in the context of huge extrapolations, no perfect strategy exists to assess systematic errors, as some model features that are unimportant in the known regions may become amplified, or even dominant, in the new domains. Some commonly used ways to assess systematic model errors are discussed in Sec. 4.

In all optimization problems, the key element of the approach is the appropriate definition of the so-called penalty function. This function, which depends on model parameters, experimental data, and most often also on pre-defined parameters specified by the modelers, gives us a one-dimensional measure of the quality of the fit. By definition, model parameters leading to a smaller value of the penalty function are
considered to be superior to those leading to a larger value. The optimization process is thus reduced to a minimization of the penalty function. One cannot underestimate, and one should never forget about, a possible fundamental influence of the definition of the penalty function on the results of the optimization process. Through this definition, a researcher may indeed exert influence on the modeling – this effect is as ubiquitous and fundamental as the influence of an observer on a quantum system investigated.

For an exact model, the task is reduced to the optimization problem, in which model’s parameters are determined by comparing predicted observables with carefully selected set of data. For such a perfect model, the systematic error is zero, and the total error is statistical, that is, it is given predominantly by the quality of the measurement of the key data determining the model. Moreover, exact models are characterized by an independence, or a weak dependence, of the final result on the definition of the penalty function [7].

In practice, nuclear models are imperfect, as most effective models are, and the total uncertainty is usually dominated by systematic effects. How useful is it, therefore, to compute statistical uncertainties of an imperfect model? There are, in fact, several good reasons to embark on such a task:

(i) Statistical analysis yields uncertainties of model parameters. In particular, by studying statistical errors on parameters one can assess whether the dataset used to constrain the model is adequate (in terms of quality and quantity).

(ii) Statistical analysis can be used to compare different mathematical formulations/assumptions and benchmark different approaches. In this case, it is essential to use the same set of fit observables.

(iii) The covariance matrix of the parameters tells us whether adding more data makes sense. If the dataset is sufficiently diverse (that is, it allows us to probe all directions in the model’s parameter space) and large, the model may become over-constrained, and the resulting statistical uncertainties may become small. In such a case, by inspecting the non-statistical behavior of residuals (which are the differences between the observed and the estimated values) one can assess sources of missing model features leading to systematic errors.

(iv) Statistical method allows one to estimate the maximum model’s accuracy on a class of observables. If a higher accuracy is required, further model refinements are needed.

(v) By assessing statistical errors of extrapolated quantities, one can make a statement whether a model carries any useful information content in an unknown domain.

(vi) By using Bayesian inference, one can test model’s adequacy as additional data are added, or additional evidence is acquired (for some recent nuclear examples, see, e.g., Refs. [8, 9, 10]).

(vii) The covariance matrix of the parameters enables one to compute correlations between various observables predicted within a model. This is a very useful tool when making new predictions and guiding future experiments [11].
A comparison of propagated statistical errors with residuals can be one of the most powerful indicators of presence of missing aspects of the model [12, 13].

3. Estimating statistical errors

Let us consider a model having \( N_p \) parameters \( \mathbf{p} = (p_1, ..., p_{N_p}) \) that are fitted to \( N_d \) measured observables \( O_i \) \((i = 1, ..., N_d)\). The steps are: define a penalty function, minimize it with respect to the parameters \( \mathbf{p} \), construct the covariance matrix of the parameters, and then apply the covariance matrix to estimate errors of predictions by associating them with uncertainties in the parameter values. The commonly used penalty function is the \( \chi^2 \) objective function, by which we begin.

3.1. The \( \chi^2 \) function

We define the \( \chi^2 \) function for the parameter fit as [3, 4, 6]

\[
\chi^2(\mathbf{p}) = \sum_{i=1}^{N_d} \frac{(O_i(\mathbf{p}) - O_i^{\text{exp}})^2}{\Delta O_i^2},
\]

where \( O_i(\mathbf{p}) \) stands for the calculated values, \( O_i^{\text{exp}} \) for experimental data, and \( \Delta O_i \) for adopted errors. (It is to be noted, that when dealing with observables that change by orders of magnitude (yields, half-lives), one must use \( \log(O) \) rather than \( O \) in Eq. (1).)

The model is thus defined not only by the equations that are used to calculate the predicted observables (that is, mathematical formulation and assumed model space), but also by the dataset \( \{O_i^{\text{exp}}, i = 1...N_d\} \) and adopted errors \( \{\Delta O_i, i = 1...N_d\} \) used to determine the parameters.

The adopted errors are determined as follows. Each one is the sum of three components:

\[
\Delta O_i^2 = (\Delta O_i^{\text{exp}})^2 + (\Delta O_i^{\text{num}})^2 + (\Delta O_i^{\text{the}})^2.
\]

Since the set of fit observables is usually divided into types (masses, radii, ...), errors are adopted for each data type separately. The experimental error, \( \Delta O_i^{\text{exp}} \), is whatever the experimentalists or evaluators quote in their datasets. The numerical error associated with the chosen computational approach, \( \Delta O_i^{\text{num}} \), is also generally small, but may not be such for models based on, e.g., basis expansion methods [14]. In those cases, the numerical error needs to be estimated. The remaining part, \( \Delta O_i^{\text{the}} \), is the theoretical error due to inherent deficiencies of the model.

A judicious choice of the adopted errors \( \Delta O_i^{\text{the}} \) is the crucial ingredient to the \( \chi^2 \) method for model development. In practice, the residuals of predicted observables should be confined to the range defined by \( \Delta O_i^{\text{the}} \). If only statistical errors are present, the residuals are stochastically distributed. Since nuclear models are not perfect, however, trends in the residuals will appear due to systematic errors.

If different types of observables are present in the dataset, adopted errors have to be defined for each type. For example, typical nuclear fits use one value of \( \Delta O_i^{\text{the}} \) for...
binding energies, another one for r.m.s. radii, and so forth. Each $\Delta O_i^{\text{the}}$ carries the same dimension as the observable $O_i(p)$ thus rendering each contribution to $\chi^2$ dimensionless. In this way, different types of observables are combined into one penalty function. The inverse square root $W_i = 1/\sqrt{\Delta O_i}$ defines the relative weight, wherewith the observable $O_i(p)$ enters the optimization problem. By changing the values of $W_i$, one can control the impact of a particular observable, or a type of observables, on the resulting parametrization.

It needs hardly be said that a certain degree of arbitrariness in choosing the weights $W_i$ is inevitable, as they can be set individually for every observable. In some cases, the weights vary from datum to datum [15, 16], while in many cases equal weights $W_i$ are chosen for all observables of a given type. Clearly, there is no “obvious” choice here [7], and various optimization protocols (driven by physics strategies) are possible. This ambiguity is one of the primary reasons for a proliferation of parametrizations in nuclear structure theory.

Fortunately, there is one guiding principle that comes to the rescue. Remember that in the case of statistical fluctuations there is a consistency between the distribution of residuals and the adopted error. Namely, the rules of statistical analysis require that the total penalty function at the minimum should be normalized to $N_d - N_p$, i.e., the average $\chi^2(p_0)$ per degree of freedom should be one:

$$\frac{\chi^2(p_0)}{N_d - N_p} \rightarrow 1.$$  

(3)

This condition provides an overall scale for the normalization of the penalty function at the minimum and removes some of the arbitrariness in choosing the weights.

Now, the basic idea is to tune the $\Delta O_i^{\text{the}}$ so that it is consistent with the distribution of residuals, even if this distribution is non-statistical. The relative weights between the types of observables can thus be determined by requiring that the average $\chi^2$ for each type is

$$\sum_{i \in \text{typ}} \frac{(O_i(p) - O_i^{\text{exp}})^2}{\Delta O_i^2} \rightarrow \frac{N_d - N_p}{N_d}.$$  

(4)

where $N_{\text{typ}}$ is the number of data points of a given type.

It is thus clear that the values $\Delta O_i \approx \Delta O_i^{\text{the}}$ obeying the normalization condition (4) cannot be chosen from the onset, but have to be determined iteratively during the optimization process. In practice, the conditions (3) or (4) are seldom fulfilled exactly. For example, it often happens that one wants to study variations of a fit while keeping the adopted errors fixed [17], which inevitably changes the normalization condition (3). In order to deal with such situations, we introduce a global scale factor $s$ such that

$$\chi^2_{\text{norm}}(p_0) = \frac{\chi^2(p_0)}{s} = N_d - N_p.$$  

(5)

This amounts to a global readjustment $\Delta O_i \rightarrow \Delta O_i \sqrt{s}$ which establishes correct normalization for $\chi^2_{\text{norm}}$, but leaves the relative weights untouched. If experimental and numerical errors are small compared to theoretical uncertainties, i.e., $\Delta O_i = \Delta O_i^{\text{the}}$,
assumption (5) defines a trivial scale factor, which does not impact the minimum $p_0$. In the following, we shall carry through all expressions with the scale factor $s$. This means that the standard rules of statistical analysis will apply to the normalized $\chi^2_{\text{norm}}$.

Assumption (5), through its triviality is, in fact, the only one that does not depend on the researcher’s choice. In this way, the normalization of $\chi^2$ at its minimum value at $p_0$ is fixed by definition. This implies that one deals here with a model that is fundamentally inaccurate and cannot describe simultaneously all the data within the experimental and numerical errors alone. As it has been noted previously, in the case of negligible experimental and numerical errors, the minimization of $\chi^2$ does not depend on the condition (5); hence, the scale $s$ can be computed after determining $p_0$.

In principle, an auxiliary scale factor $s_{\text{typ}}$ can be introduced for each data type, if the adopted theoretical errors are being adjusted during the optimization process. This amounts to a readjustment $\Delta O_i \rightarrow \Delta O_i \sqrt{s_{\text{typ}}}$ for $i \in \text{typ}$ in each optimization step. The situation is particularly simple if one assumes the same weights for each data type. In this case the value of $s_{\text{typ}}$ in a given step can be obtained directly from the condition (4). Such an iterative adjustment, leading eventually to $s_{\text{typ}} = 1$, is recommended if the researcher has no intuition about the expected theoretical error, and/or experimental and numerical errors are not negligible (see Ref. [15] for a practical realization of an iterative adjustment of $\Delta O_{\text{the}}$ using the maximum likelihood method.)

In practical situations, however, this is seldom the case, and a global scaling (5) following the minimization is fully adequate.

Another extreme case is the one when experimental/numerical errors are so large that they mask the theoretical error entirely, and thus one can set $\Delta O_{\text{the}} \equiv 0$. This case is often encountered in curve fitting of experimental data. In such a situation the value of $\chi^2/(N_d - N_p)$ provides a direct estimate of the quality of the fit.

### 3.2. Optimization

The optimum parametrization $p_0$ is the one that minimizes the penalty function, in particular, the $\chi^2$ function, with the minimum value of $\chi^2_0 = \chi^2(p_0)$.

#### 3.2.1. Pre-optimization

A global model optimization becomes very involved when several categories of fit-observables are considered. Such optimization procedures are expensive, as they require a large number of model evaluations. Consequently, it is always useful for the global optimization to have preliminary estimates for the parameter values and their errors. An efficient pre-optimization method, particularly convenient if observables are linear functions of model parameters, is the linear regression algorithm employing the singular value decomposition (SVD). This method has been used in the context of mass fits [18] [7], single-particle energies [19], and pre-optimization of novel functionals [20]. The advantage of the SVD approach is that it can provide an efficient and accurate assessment of model’s error pertaining to a selected category of observables. In addition, it provides an estimate of the effective size of the model parameter space [18].
Many least-square solvers included in optimization packages contain an SVD truncation of the parameter space.

3.2.2. Reasonable domain of model parameters. Usually, most of the model space produces observables which are far from reality. Therefore, one needs to confine the model space to a “physically reasonable” domain around the minimum \( p_0 \). Within this domain there is a range of “reasonable” parametrizations \( p \) that can be considered as delivering a decent fit, that is, \( \chi^2_{\text{norm}}(p) \leq \chi^2_{\text{norm}}(p_0) + 1 \) (see Sec. 9.8 of Ref. [4]). As this range is usually rather small, we can expand \( \chi^2 \) as

\[
\chi^2(p) - \chi^2_0 \approx \sum_{\alpha, \beta=1}^{N_p} (p_\alpha - p_{0, \alpha}) M_{\alpha \beta} (p_\beta - p_{0, \beta}),
\]

that is, \( M \) is the Hessian matrix of \( \chi^2 \) at the minimum \( p_0 \). The reasonable parametrizations thus fill the confidence ellipsoid given by

\[
\frac{1}{8} (p - p_0)^T \hat{M} (p - p_0) \leq 1,
\]

see Sec. 9.8 of Ref. [4] and Fig. 1.

3.3. Statistical error

Given a set of parameters \( p \), any observable \( A \) can be within the model uniquely computed as \( A = A(p) \). The value of \( A \) thus varies within the confidence ellipsoid, and this results in some uncertainty \( \Delta A \) of \( A \). Let us assume, for simplicity, that the observable varies weakly with \( p \), such that one can linearize it in the relevant range, that is,

\[
A(p) \approx A_0 + G^A \cdot (p - p_0) \quad \text{for} \quad A_0 = A(p_0) \quad \text{and} \quad G^A = \partial_{p_0} A_{|p_0}. \quad (9)
\]
Let us, furthermore, associate a weight \( \propto \exp \left( -\chi_{\text{norm}}^2(p) \right) \) with each parameter set \([4, 6]\).

The prescription for assigning an error to the predicted value \( A(p_0) \) is the following formula:

\[
\Delta A^2 = \sum_{\alpha\beta} G_A^\alpha \hat{C}_{\alpha\beta} G_A^\beta, \tag{10}
\]

where \( \hat{C} \) is the covariance matrix. Upon the assumption that the fitted observables \( O_i \) depend only linearly on parameters \( p \), the covariance matrix is simply related to the Hessian matrix as

\[
\hat{C} = s \hat{M}^{-1} = s \left( \hat{J}^T \hat{J} \right)^{-1}, \tag{11}
\]

where

\[
\hat{J}_{i\alpha} = \left. \frac{\partial p_\alpha}{\partial O_i} \right|_{p_0} \Delta O_i \tag{12}
\]

is the Jacobian matrix, which is inversely proportional to the adopted errors. If the condition \([5]\) is met with \( s = 1 \), the expression for the covariance matrix simplifies to \( \left( \hat{J}^T \hat{J} \right)^{-1} \), see Table [A1] middle column. In particular, by taking \( A(p) = p_\alpha \), one obtains the expression for the statistical error of the model parameter \( p_\alpha \):

\[
\Delta p_\alpha = \sqrt{s \hat{C}_{\alpha\alpha}}.
\]

We note that if the fitted observables weakly depend on some parameters, the Hessian matrix becomes almost singular and the covariance matrix becomes ill-conditioned. In such a case, errors or all predicted values \([10]\) become unreasonably large. This shows again that observables that weakly depend on model parameters should not be fitted and parameters that have small impact on the results should be removed from the model by proper pre-optimization procedures, see Sec. 3.2.1 and discussion in Sec. II.B of Ref. [21].

The Hessian (\( \hat{M} \)), covariance (\( \hat{C} \)), and Jacobian (\( \hat{J} \)) matrices constitute the basic ingredients of the statistical-error analysis, and thus should be routinely computed following the optimization process.

### 3.4. Dependence on the number of data points and on adopted errors

It is worth noting that the Hessian matrix, \( \hat{M} = \hat{J}^T \hat{J} \), increases linearly with the number \( N_d \) of data points constraining the model. This is best visible in the case of identical observables \( O_i \equiv O \) accompanied with identical adopted errors \( \Delta O_i \equiv \Delta O \), whereupon one has

\[
\hat{M}_{\alpha\beta} = \frac{N_d}{\Delta O^2} \left( \left. \frac{\partial p_\alpha}{\partial O} \right|_{p_0} \right) \left( \left. \frac{\partial p_\beta}{\partial O} \right|_{p_0} \right). \tag{13}
\]

Therefore, the statistical uncertainty \([10]\) does decrease with the number \( N_d \) of data points constraining the model. Indeed, if our model were exact (\( \Delta O_i^{\text{num}} = \Delta O_i^{\text{the}} = 0 \)), by taking a very large number \( N_d \) of fit observables, the model observables would be determined with an arbitrary accuracy, that is,

\[
\Delta A = \sqrt{\Delta A^2} \sim \frac{\Delta O^{\exp}}{\sqrt{N_d}}, \tag{14}
\]
and the precision would improve as the square root of the number of measurements (data points), see Eq. (4.12) of Ref. [3]. In general, as the number of uncorrelated data points grows and the number of parameters stays fixed, the confidence intervals become tighter. This does not mean, of course, that by increasing \( N_d \) we can make predictions more accurate. At some point, adding more fit observables makes little sense as the model error becomes dominated by the systematic error, see Sec. 4.

Naturally, the precision of an exact model also improves when all experimental data are determined with smaller and smaller uncertainties \( \Delta \mathcal{O}_{\text{exp}} \). However, when the model is inaccurate and the theoretical errors dominate, the normalization condition (5) applied to observables of the same type, assuming identical weights, gives:

\[
\left( \Delta \mathcal{O}^{\text{the}} \right)^2 = \frac{N_d}{N_d - N_p} \left( \mathcal{O}(p_0) - \mathcal{O}_{\text{exp}} \right)^2.
\]

That is, typical adopted theoretical errors are of the order of a typical residual, and cannot be further decreased.

4. Estimating systematic errors

A systematic error of a theoretical model is a consequence of missing physics and/or poor modeling. Since in most cases the perfect model is not available, systematic errors are very difficult to estimate. To get some idea about systematic uncertainties, especially in the context of extrapolations, one can adopt the following strategies:

**Analysis of residuals** Study the distribution of residuals for a given observable. For a perfect model, one should see a statistical distribution. In most practical cases, however, one does see systematic trends. These often allow us to guess the underlying missing physics, see Sec. [for examples.

**Analysis of inter-model dependence** Make a number of predictions \( \mathcal{O}_j \) of an observable \( \mathcal{O} \) using a set of \( N_m \) reasonable and sufficiently different models \( M_j \) \( j = 1, ..., N_m \), well calibrated to existing data and based on different theoretical assumptions/optimization protocols. Assuming that the biases introduced in different models are independent, one hopes that some randomization of systematic errors would take place. The predicted model-averaged value of an observable \( \mathcal{O} \) can be written as:

\[
\overline{\mathcal{O}}_m = \frac{1}{N_m} \sum_{j=1}^{N_m} \mathcal{O}_j,
\]

with the corresponding systematic error

\[
\Delta \mathcal{O}_{\text{syst,m}} = \sqrt{\frac{1}{N_m} \sum_{j=1}^{N_m} (\mathcal{O}_j - \overline{\mathcal{O}}_m)^2},
\]

which provides the scale of the model uncertainty.
Comparison with existing data The systematic errors of fit observables can be estimated by optimizing the model using a large number data points to guarantee that the statistical error is small. Then compute the r.m.s. deviation $\Delta O_{\text{rms}}$ from the known experimental data for a given type of observables (e.g., masses or radii). The systematic error of a predicted observable $O$ belonging to this type should be at least of the order of $\Delta O_{\text{rms}}$. It is recommended to combine the strategies above by investigating both $\Delta O_{\text{syst},m}$ and $\Delta O_{\text{rms}}$. Having estimated the systematic and statistical error $\Delta O$, the predicted observable $O$ can be written as

$$O = \bar{O} \pm \Delta O_{\text{stat}} \pm \Delta O_{\text{syst}}.$$  \hspace{1cm} \text{(18)}

Let us emphasize again that the proposed analysis of adopted errors (and hidden systematic errors) does not fully allow us to estimate the contribution of the systematic error to extrapolations, as the available data usually constrain only a limited region of the model parameter space.

4.1. Illustrative examples

In this section, methodologies used to estimate statistical and systematic errors are illustrated by means of schematic examples. Those are followed in Sec. 6 by references to recent studies aiming at uncertainty quantification in the context of realistic nuclear modeling.

4.1.1. Odd-Even Staggering Model. In this example, we illustrate the concept of statistical and systematic errors using theoretically generated pseudo-data \[22\]:

$$O_{\text{exp}}(i) = \delta(-1)^i + \varepsilon(i), \quad (i = 1, 2, \ldots N_d),$$  \hspace{1cm} \text{(19)}

where $\delta$ stands for a magnitude of an odd-even staggering of a physical quantity (mass, radius,...), $\varepsilon(i)$ represents a white noise with zero mean (for both $i$-even and $i$-odd) and finite variance

$$\sigma^2 = \frac{1}{N_d} \sum_{i=1}^{N_d} \varepsilon^2(i),$$  \hspace{1cm} \text{(20)}

and $N_d$ (an even number) is a number of data points. It is assumed that $\delta \gg \sigma$ and $N_d \gg 1$. To interpret the dataset \[19\] we employ two models of one fitted observable:

**Model A:** $O_{\text{i}=1}(p) = p_{\alpha=1} (N_p = 1)$.

**Model B:** $O_{\text{i}=1}(p) = p_{\alpha=1} + p_{\alpha=2}(-1)^i (N_p = 2)$.

Let us begin with Model A. It corresponds to a typical situation, in which the nuclear model is imperfect, and experimental errors are small. The minimization of $\chi^2$ yields $p_1 = 0$, and the condition \[5\] yields $\Delta O_1 = \Delta O \approx \sqrt{\delta^2 + \sigma^2} \approx \delta$. The resulting Jacobian matrix \[12\] is $\hat{J}_{11} = 1/\delta$; hence, the covariance matrix \[11\] becomes $(\hat{N}^{-1})_{11} = \delta^2/N_d$. This is consistent with the discussion in Sec. 3.4, the statistical
uncertainty\footnote{10} decreases with the number $N_d$ of data points constraining the model. The estimated statistical error on the odd-even staggering, $\Delta O_{\text{stat}} = \delta / \sqrt{N_d}$, can become very small if one takes very many data points. This of course does not mean that our prediction is accurate. Indeed, by inspecting the residuals of Model A shown in Fig. 2(a), one immediately concludes that their distribution is \emph{not} statistical. This suggests the presence of a large systematic error that can be estimated as $\Delta O_{\text{rms}} = \delta$. Consequently, for Model A, $\Delta O_{\text{stat}} \ll \Delta O_{\text{syst}}$.

By inspecting the pattern of the residuals of Model A, one concludes that this model is not adequate, and this leads to a two-parameter Model B. Here, the minimization of $\chi^2$ yields $p_1 = 0, p_2 = \delta$, and the condition\footnote{5} gives $\Delta O_1 = \Delta O \approx \sigma$. The resulting Jacobian matrix\footnote{12} is $\hat{J}_{11} = 1/\sigma, \hat{J}_{12} = (-1)^i/\sigma$; hence, the covariance matrix\footnote{11} becomes $\hat{M}^{-1} = \sigma^2/N_d \hat{I}$, where $\hat{I}$ is a $(2 \times 2)$ unity matrix. Figure 2(b) shows the corresponding residuals: they are statistically distributed around zero. This tells us that Model B is perfect, and its error is statistical: $\Delta O_{\text{stat}} = \sigma$.

4.1.2. Liquid Drop Model. In this example, we test the $\chi^2$-optimization by using theoretically-generated pseudo-data. To this end, $N_d = 516$ even-even nuclei with $6 \leq Z \leq 106$ listed in the Audi-Wapstra mass tables were computed with the Skyrme functional SV-bas\footnote{17} using the axial HF+BCS approach. Their binding energies were taken as pseudo-data to which a four-parameter ($N_p = 4$) LDM model for the total binding energy,

$$E(Z, N) = a_{\text{vol}} A - a_{\text{surf}} A^{-2/3} + a_{\text{sym}} \frac{(N - Z)^2}{A} + a_C Z^2 A^{-1/3},$$  \hspace{1cm} (21)

was optimized. The adopted theoretical error on $E$ of 3.8 MeV was tuned according to Eq. 3.

Table 1 compares the optimal parameters of the LDM model\footnote{21} with the LDM parameters of SV-bas obtained by means of the leptodermous expansion\footnote{23}. Due to the huge sample, one obtains fairly small statistical errors (see Sec. 3.4). The deviation of the fit from the SV-bas LDM values is much larger. This is by no means surprising; to use the leptodermous expansion on bulk and surface properties, one needs huge nuclei ($A \approx 1000 - 10000$)\footnote{23}. The very incorrect fitted symmetry energy demonstrates
Table 1. Parameters of the LDM mass model \([21]\) optimized to SV-bas masses ("fitted") compared to SV-bas LDM constants obtained by means of the leptodermous expansion \([23]\). All values in MeV.

| parameter \(a\) | SV-bas | fitted | \(\sigma_{\text{stat}}\) |
|-----------------|--------|--------|----------------|
| \(a_{\text{vol}}\) | -15.904 | -15.47 | 0.06 |
| \(a_{\text{surf}}\) | 17.646 | 16.68 | 0.18 |
| \(a_{\text{sym}}\) | 30.00 | 22.82 | 0.15 |
| \(a_C\) | 0.702 | 0.004 | 0.004 |

an additional problem with the dataset used. While it covers a large range of mass numbers thus providing sufficient constraints on isoscalar properties, the isospin range is fairly limited, which results in a poor determination of isovector properties. The lesson learned from this exercise is that the dataset used is clearly inadequate: the mass surface of known nuclei alone does not allow for a reasonable extraction of \(a_{\text{sym}}\) \([17]\).

![Figure 3](image)

Figure 3. Total binding energy residuals obtained with the LDM mass formula \([21]\). Isotopic chains are connected by lines. The shaded area marks the r.m.s deviation from SV-bas masses, \(\pm 3.8\) MeV.

Figure 3 shows the distribution of the resulting binding energy residuals. The shaded area marks the band corresponding to the final r.m.s error of 3.8 MeV. It is immediately seen that the binding energy residuals are not statistically distributed: there is a systematic trend due to the missing shell energy. It is now clear, that the error of the model \([21]\) on predicted masses is dominated by the systematic component,
which is at least 3.8 MeV. Of course, it is well known that systematic behavior of energy
residuals can be partly cured by adding shell corrections, and this makes the model
quantitative (see, e.g., Fig. 1 of Ref. [15]).

5. Correlation analysis

In this section, we come back to the rich information contained in the least-squares fits
that provides worthwhile insights into the actual (imperfect) model. We discuss here
two aspects: correlations between predicted observables and probing the sensitivity of
model parameters.

5.1. Covariances

A weighted average over the parameter space yields the covariance between two
observables $\hat{A}$ and $\hat{B}$, which represents their combined uncertainty:

$$\Delta A \Delta B = \sum_{\alpha\beta} G^A_{\alpha} \hat{C}_{\alpha\beta} G^B_{\beta}.$$  \hspace{1cm} (22)

For $A=B$, Eq. (22) gives the variance $\Delta^2 A$ that defines a statistical uncertainty (error)
of an observable [10]. In addition, one can introduce a useful dimensionless product-
moment correlation coefficient [4]:

$$c_{AB} = \frac{|\Delta A \Delta B|}{\sqrt{\Delta A^2 \Delta B^2}}.$$  \hspace{1cm} (23)

A value $c_{AB} = 1$ means fully correlated and $c_{AB} = 0$ – uncorrelated. Variance,
covariance, and the correlation coefficient are useful quantities that allow us to estimate
the impact of an observable on the model and its parametrization.

Since the number of parameters is usually much smaller than the number of
observables, there must exist correlations between computed quantities. Moreover, since
the model space has been optimized to a limited set (and type) of observables, there must
also exist correlations between model parameters. Figure 4 shows covariance ellipsoids
for two pairs of observables in $^{208}$Pb that nicely illustrate the cases of strong (neutron
skin and isovector dipole polarizability; $c_{AB}=0.98$) and weak (neutron skin and effective
nucleon mass $m^*/m$ in symmetric nuclear matter; $c_{AB}=0.11$) correlation.

An example of the correlation analysis for the symmetry energy $a_{sym}$ is given in
Fig. 5 taken from the survey, which compared predictions of Skyrme-Hartree-Fock (SHF)
and Relativistic-Mean-Field (RMF) energy density functionals (EDFs) [25]. The first
four entries concern the basic nuclear matter properties. It is only for $L$, the density
dependence of symmetry energy, that a strong correlation with $a_{sym}$ is seen. The
remaining two entries are $\alpha$-decay energy in yet-to-be-measured super-heavy nucleus
$Z = 120, N = 182$ and the fission barrier in $^{266}$Hs. The data on $Z = 120, N = 182$
consistently do not correlate with $a_{sym}$. The correlation with fission barrier in $^{266}$Hs
exhibits an appreciable model dependence with some correlation in SHF and practically
none in RMF.
5.2. Post-optimization: sensitivity tests

As discussed in Refs. [26, 27], it is useful to study the overall impact of each data type in the $\chi^2$ function on the obtained parameter set $p_0$. To this end, one can employ the $N_p \times N_d$ sensitivity matrix

$$S(p) = \left[ J(p) J^T(p) \right]^{-1} J(p).$$

(24)
For each row in the sensitivity matrix (each parameter), one can compute the partial
sums over each type of data. This gives us a measure of the change of the parameter
under a global change of all the data of a given type. Figure 6, produced in the
context of UNEDF1 functional optimization \( (N_p = 10, N_d = 115) \), shows the relative
change of parameter \( p_\alpha \) when such an average datum of an observable is changed. The
total strengths for each parameter were normalized to 100% and only relative strengths
between various data types (masses, proton radii, odd-even binding energy staggering,
and fission isomer energies) are shown. A large percentage contribution from a given
data type tells that \( p_\alpha \) is very sensitive to changes in these data, and other data types
have little impact on it at the convergence point. Note that in the example considered
the fission isomer excitation energies represent less than 4% of the total number of data
points but account for typically 30% of the variation of the parameter set. This kind
of analysis, however, does not address the importance of an individual datum on the
optimal solution.

\[
\frac{||\delta p/\sigma||}{\sum_{\alpha} \left( \frac{\delta p_{\alpha}}{\Delta p_{\alpha}} \right)^2} = 25
\]

for the optimal parameter set when data points \( O_i^{(\text{exp})} \) are changed by an amount of
0.1\( \Delta O_i \) one by one. As can be seen, the variations are small overall, assuring us that
the dataset was chosen correctly. The masses of the double magic nuclei \( ^{208}\text{Pb} \) and \( ^{58}\text{Ni} \)
seem to have the biggest relative impact on the optimal parameter set. One can also

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{sensitivity.png}
\caption{Sensitivity of UNEDF1 energy density functional parametrization to
different types of data entering the \( \chi^2 \) function. (From Ref. \[27\].)}
\end{figure}
see that the sensitivity of the parameters on the new fission isomer data is larger than the average datum point. By contrast, the dependence of the parametrization on the masses of deformed actinides and rare earth nuclei is weaker.

![Figure 7. Overall change in $p$ for the UNEDF1 when the datum $O_i^{(\text{exp})}$ is changed by an amount of $0.1\Delta O_i$ one by one. The four rightmost data points marked FI correspond to excitation energies of fission isomers. (From Ref. [27].)](image)

6. Examples of recent work

In this section, we list examples of some recent theoretical work involving advanced optimization, error estimates, and covariance analysis.

Optimization of nuclear energy density functionals (EDFs) using different data categories were carried out for nuclei [17, 26, 27, 21] and for nuclei and neutron stars [28]. Figure 8 shows the predicted mass-radius relation of neutron stars for SV-min [17] and TOV-min [28] EDFs. In addition, the estimated statistical uncertainty band for a prediction using SV-min is shown. As both observables are correlated, it is not possible to estimate the uncertainty for mass and radius separately. For this reason, the error band is obtained by calculating the covariance ellipsoid for each point of the $M(R)$ curve as indicated in Fig. 8. The area covered by all covariance ellipsoids can be viewed as the error band for a prediction using SV-min. Based on this exercise, we can conclude that the low-density part of the neutron matter equation of state, as given by the commonly used nuclear EDFs optimized around the saturation density carries no information on the high-density region. Therefore, EDFs optimized to nuclear ground-state data cannot be used to predict, e.g., maximum mass of the neutron star; scrutinizing existing functionals with respect to this quantity makes little sense. This
example nicely illustrates the point made earlier that by assessing statistical errors of extrapolated quantities, one can make a statement whether a model carries any useful information content in an unknown domain. Here it does not.

![Mass-radius neutron star relation](image)

**Figure 8.** Mass-radius neutron star relation obtained for SV-min and TOV-min EDFs [28]. The uncertainty band for SV-min is shown. This band is estimated by calculating the covariance ellipsoid for the mass $M$ and the radius $R$ at each point of the SV-min curve as indicated by the ellipsoid. Also depicted (dotted lines) are uncertainty limits for the newly developed functional TOV-min optimized using exactly the same protocol as in earlier studies pertaining to nuclei but now including neutron star data.

The first solid attempt to carry out optimization of the nucleon-nucleon interaction from chiral effective field theory at next-to-next-to-leading order was done in Refs. [16, 29, 30]. In the phase-shift analysis of Ref. [16], it was assumed that the weights $W_i$ corresponding to phase shifts $\delta(q)$ decrease with the relative momentum $q$ – to be consistent with the assumed order of the effective field theory. This is a good example of a situation, in which physical arguments can impact a form of the penalty function. The covariance analysis for the chiral constants in Refs. [29, 30] enabled the uncertainty quantification of the interaction, parameter correlation, and predictions with error bars for deuteron static properties.

In a number of recent papers, propagation of statistical uncertainties in EDF models for separation energies and drip lines [31], radii [13], and various structural properties [12] was carried out. A correlation testing analysis can be found in Ref. [32]. The recent papers [26, 27, 13] contain sensitivity analysis and statistical error budget for various observables. Of particular importance to fission studies was a development of the UNEDF1 parametrization [27] that is suitable for studies of strongly elongated nuclei. A sensitivity analysis carried out for UNEDF1 has revealed the importance of states at large deformations in driving the final fit.
There are some studies, involving inter-model analysis, of correlations and statistical
and systematic errors for nucleon-nucleon potentials and few-body systems [33], drip
lines [31, 34] (see Fig. 9), neutron skins and dipole polarizability [35, 36, 37],
nucleon densities [12], weak-charge form factor [11], and neutron matter equation of
state [8, 38, 24, 39, 40, 41, 42, 28].

Examples and tests of statistical significance of the parameter fitting procedures
in the nuclear mean-field context using phenomenological toy-models can be found in
Refs. [43, 44, 45]. Finally, an application of the statistical likelihood analysis in the
evaluation of fission neutron data is described in Ref. [46].

7. Summary

“One important idea is that science is a means whereby learning is achieved, not by mere
theoretical speculation on the one hand, nor by the undirected accumulation of practical
facts on the other, but rather by a motivated iteration between theory and practice.” [47]
The essence of the scientific method is to explore the positive feedback in the loop
“experiment-theory-experiment-...” Based on experimental data, the theory is modified
and can be used to guide future measurements. The process is then repeated, until
the predictions are consistent with observations. The process can be enhanced if care
is taken to determine parameter uncertainties and correlations, the errors of calculated

Figure 9. Map of bound even-even nuclei as a function of the proton number \(Z\) and
and the neutron number \(N\) [31]. Mean drip lines and their uncertainties (red) were obtained
by averaging the results of different Skyrme-EDF models. (For a similar analysis using
covariant-EDF models, see Ref. [34].) The two-neutron drip line of SV-min (blue) is
shown together with the statistical uncertainties at \(Z=12, 68,\) and \(120\) (blue error bars).
The \(S_{2n} = 2\text{ MeV}\) line is also shown (brown) together with its systematic uncertainty
(orange).
observables, and the uniqueness and usefulness of an observable, that is, its information content with respect to current theoretical models.

Since every nuclear model aiming at addressing the actual reality contains some parameters, the main source of statistical errors in nuclear modeling is optimization of those parameters to experimental data. The good news is that various methods have been developed to assess model misfits. Unfortunately, since “Essentially, all models are wrong” [1], there is no perfect way to assess systematic uncertainties. One option is to use high performance computing to make predictions using many models based on different assumptions. By means of an inter-model analysis and by comparing with existing data, some information about systematic errors can be deduced.

This guide and the references cited contain good illustrations of the seven rules of Ref. [5], quoted in the introduction, when it comes to nuclear modeling. More illuminating examples will soon appear in the upcoming Focus Issue of Journal of Physics G on “Enhancing the interaction between nuclear experiment and theory through information and statistics.”

Numerous contributions from G.F. Bertsch are gratefully acknowledged. We would like to thank A.N. Andreyev, D. Higdon, J. Rosiński, W. Loveland, and S. Wild for useful comments. This work was finalized during the Program INT-13-3 “Quantitative Large Amplitude Shape Dynamics: fission and heavy ion fusion” at the National Institute for Nuclear Theory in Seattle; it was supported by the U.S. Department of Energy under Contract No. DE-FG02-96ER40963 (University of Tennessee), No. DE-FG52-09NA29461 (the Stewardship Science Academic Alliances program), No. de-sc0008499 (NUCLEI SciDAC Collaboration); by the Academy of Finland and University of Jyväskylä within the FIDIPRO programme; by the Polish National Science Center under Contract No. 2012/07/B/ST2/03907; and by the the Bundesministerium für Bildung und Forschung (BMBF) under contract number 05P09RFFT.

Appendix A. Different normalizations of $\chi^2$

There are various forms of the least-squares function $\chi^2$ used in the literature. Two of the most widely used options and their consequences for Jacobian and variances are summarized in Table A1. The “simple” version (middle column) incorporates the basic assumption of properly scaled $\chi^2$, namely $\chi^2(p_0) \approx N_d$ and ignores $N_p$ in the scaling assuming $N_d \gg N_p$, i.e., $s \approx 1$. 

$$
\chi^2(p_0) \approx N_d 
$$
Table A1. Different versions of the $\chi^2$ function and related quantities. The scale factor $s$ is given by Eq. (5): $s = \frac{\chi^2(p_0)}{N_d-N_p}$.

| quantity       | direct $\chi^2$ | direct $\chi^2$, simple | normalized $\chi^2$ |
|----------------|-----------------|--------------------------|---------------------|
| penalty function | $\sum_i \frac{(O_i-O_i^{(exp)})^2}{\Delta O_i^2}$ | $\sum_i \frac{(O_i-O_i^{(exp)})^2}{\Delta O_i^2}$ | $\frac{1}{N_d-N_p} \sum_i \frac{(O_i-O_i^{(exp)})^2}{\Delta O_i^2}$ |
| Jacobian $J_{\alpha}$ | $\frac{\partial O_i}{\partial p_{\alpha}} \frac{1}{\Delta O_i}$ | $\frac{\partial O_i}{\partial p_{\alpha}} \frac{1}{\Delta O_i}$ | $\frac{\partial O_i}{\partial p_{\alpha}} \frac{1}{\Delta O_i}$ |
| variance $\Delta^2 p_{\alpha}$ | $s \left( (\dot{J}^{T} \dot{J})^{-1} \right)_{\alpha \alpha}$ | $\left( (\dot{J}^{T} \dot{J})^{-1} \right)_{\alpha \alpha}$ | $\chi^2(p_0) \left( (\dot{J}^{T} \dot{J})^{-1} \right)_{\alpha \alpha}$ |
| covariance $\hat{C}$ | $s \left( \dot{J}^{T} \dot{J} \right)^{-1}$ | $\left( \dot{J}^{T} \dot{J} \right)^{-1}$ | $\chi^2(p_0) \left( \dot{J}^{T} \dot{J} \right)^{-1}$ |

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