Statistical significance of theoretical predictions: 
A new dimension in nuclear structure theories (II)

B SZPAK\textsuperscript{1}, J DUDEK\textsuperscript{2}, M-G PORQUET\textsuperscript{3} and B FORNAL\textsuperscript{1} 

\textsuperscript{1}The Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences, ul. Radzikowskiego 152, Pl-31-342 Kraków, Poland
\textsuperscript{2}Institut Pluridisciplinaire Hubert Curien, Département de Recherches Subatomiques UMR7178, IN2P3-CNRS and Université de Strasbourg, 23 rue du Loess B.P. 28, F-67037 Strasbourg Cedex 2, France
\textsuperscript{3}Centre de Spectrométrie Nucléaire et de Spectrométrie de Masse, IN2P3-CNRS and Université Paris-Sud, Bâtiments 104 et 108, F-91405 Orsay Campus, France

E-mail: Bartlomiej.Szpak@ifj.edu.pl, Jerzy.Dudek@IReS.in2p3.fr, Marie-Genevieve.Porquet@csnsm.in2p3.fr, Bogdan.Fornal@ifj.edu.pl

Abstract.
We present examples and illustrate associated tests of statistical significance of the parameter fitting procedures in the nuclear mean-field context using a phenomenological toy-model based on the spherical Woods-Saxon Hamiltonian. We calculate the variance-covariance matrix and compare the standard estimates of the confidence intervals (and more generally - the uncertainty distributions) based on the standard $\chi^2$-fitting as opposed to a more general Monte-Carlo simulations. We give arguments for the superiority of the latter approach.

1. Introduction
In [1] further on referred to as (I) we have introduced the problem of uncertainties of theoretical predictions as well as those of the parametrizations of the theory Hamiltonians. Such uncertainties originate not only from the experimental errors but first of all from the inexact character of the theoretical models. These considerations brought us to the notion of the probability distributions accompanying the usual numerical theory predictions. In other words: Within the new formulation, the theories are expected to provide not only the pure numerical prediction (as it was the case so far) but also the probability with which we might expect this prediction to represent the real physical system under considerations. At present we are not able to provide the full solution of this type of the problem (the whole approach is under construction); instead we will focus on illustrating the functioning of the most elementary mathematical tools that will be used in the future to fully solve the problem.
2. Elements of the formalism - a short summary
Suppose we have found the minimum of the $\chi^2(p)$ as in (4) or (7) in (I). We may introduce the so-called unbiased estimator for the root-mean-square deviation

$$\Delta^2_{rms} \equiv \frac{\chi^2}{n_d - n_p}$$

where as before $n_d$ is the number of data points and $n_p$ the number of fitted parameters. In probability theory one shows that $\Delta^2_{rms}$ has the properties of the so-called $\chi^2$ probability-distribution with $\nu \equiv n_d - n_p$ degrees of freedom. With the help of the Jacobian matrix introduced in (6) of (I), a number of statistical properties of a system can be obtained using the variance-covariance matrix $M$ and the correlation matrix $\rho$ defined by

$$M = \Delta^2_{rms}(J^T J)^{-1} \quad \text{and} \quad \rho_{ij} = M_{ij}/\sqrt{M_{ii}M_{jj}}.$$ (2)

Consider $(M_{ii})^{1/2}$, the standard error for the $i^{th}$ parameter. The $100\% - \alpha$ confidence interval for the least-square estimator $\hat{p}_i$ of the parameter $p_i$ is given as usual by:

$$p_i \in (\hat{p}_i - t_{\alpha/2,\nu}\sqrt{M_{ii}}, \hat{p}_i + t_{\alpha/2,\nu}\sqrt{M_{ii}}),$$ (3)

where $t_{\alpha/2,\nu}$ denotes Student $t$–distribution. In the following examples we are interested in $90\%$ confidence intervals thus setting $t_{0.05,\nu}$ in (3).

Alternatively, one can obtain the variance-covariance matrix and the confidence intervals for the model parameters using Monte-Carlo techniques. Assuming that the value of $\sigma$ for each experimental data point is given by the $\Delta_{rms}$ (obtained from a fit to a set of experimental data) we add the gaussian random noise with variance equal to $\Delta_{rms}$ to each experimental point and repeat the minimization thousands of times. The Monte-Carlo method has a number of advantages over the method based on single least-square fit, cf. [2].

The knowledge of full variance-covariance matrix is essential for obtaining information about the first elements of the predictive power of a model: the confidence intervals for parameters and the detection of the possible parameter correlations [for the importance of the latter cf. (I)]. Under certain simplifying assumptions that are not specified here the Probability Distribution Function of the model parameters can expressed by a multivariate Gaussian distribution:

$$P(p) \propto \exp \left[ -\frac{1}{2}(p - \hat{p})M^{-1}(p - \hat{p}) \right],$$ (4)

where $M^{-1}$ is the inverse of the variance-covariance matrix and $\hat{p}$ is the estimation of $p$ obtained in a least-square fit. This distribution can be sampled using a Monte-Carlo method to obtain the mean and confidence intervals for parameters of the Hamiltonian and/or physical observables.

3. Illustrations: Single-particle levels within a toy-model
To illustrate our considerations we will use a phenomenological Woods-Saxon Hamiltonian whose parameters are fitted to a set of neutron single particle levels in $^{208}$Pb. In this schematic presentation we assume equal weights for all experimental levels. The toy-model Hamiltonian is $H = T + V_c + V_{so}$ where the central potential $V_c$ and the spin-orbit one, $V_{so}$, are defined by

$$V_c \equiv \frac{V_0}{1 + \exp[(r - R_0)/a_0]} \quad \text{and} \quad V_{so} \equiv \frac{1}{r} \frac{d}{dr} \left\{ \frac{V_{0}^{so}}{1 + \exp[(r - R_0^{so})/a_0^{so}]} \right\}.$$ (5)

It turns out that the solutions to the Schr"{o}dinger equation depend very regularly on diffuseness of the spin-orbit close to the $\chi^2$-minimum and to simplify the otherwise schematic illustrations
we set \( a_0^{s_0} = 0.6 \) fm. Accordingly, the 5-dimensional parameter vector takes the form \( \{ p \} \equiv \{ V_0, r_0, a_0, V_0^{s_0}, r_0^{s_0} \} \). The experimental single-particle states are taken from [2]; they are \( \{1a_9/2, 2f_7/2, 1i_{13/2}, 3p_3/2, 2f_5/2, 3p_{1/2}, 2g_9/2, 1f_{11/2}, 1j_{15/2}, 3d_{5/2}, 4s_{1/2}, 2g_{7/2}, 3d_{3/2} \} \) with the corresponding experimental energies \( \{ \varepsilon \} \) /MeV given by

\[
\{-10.784, -10.3, -9.8, -8.27, -7.94, -7.37, -3.94, -3.160, -2.517, -2.37, -1.9, -1.44, -1.4 \}.
\]

An essential element of the analysis consists in evaluating the stability of the obtained solution. For instance when increasing the number of experimental data points we may be able to find out whether the parameters-solutions of the \( \chi^2 \)-minimisation change a lot (or just to the contrary whether they are already stabilised) and/or if the theoretical energies lie systematically close to the corresponding experimental values. However, such an option is seldom at our disposal. Obtaining each new experimental point usually requires a non-trivial instrumental effort so that the experimental points are never in excess. Therefore the only easy option consists in decreasing the number of experimental data points taken to the fit and verifying the stability properties in this way.

Formally, by decreasing the number of experimental data points we approach the situation of having too few such points to constrain the number of parameters that is fixed a priori - in this way we approach the limit of model’s ill-posedeness. For the test purposes we can make ourselves independent of the limitation imposed by the actual experimental situation: we may generate the theoretical spectrum using a reasonable (i.e. close to the empirical values) set of parameters and then try to re-obtain the Hamiltonian parameters using an arbitrarily selected number of those theoretical levels treated as experimental. We will use 7 data points \( \{1i_{13/2}, 3p_{3/2}, 2f_{5/2}, 3p_{1/2}, 2g_{9/2}, 1f_{11/2}, 1j_{15/2} \} \) to approach an ill-posed problem. The set of 13 levels represents the realistic scenario (this is the actually known number of experimental neutron levels in \(^{208}Pb\)). By using 21 levels we will be able to estimate how the knowledge of extra levels can constrain the confidence intervals for parameters and observables. Figure 1 illustrates the

\[ \sigma = 0.35 \text{ MeV} \]

![Figure 1. The Probability Distribution Function for the \( V_0 \) (left) and \( V_0^{s_0} \) (right) parameters as obtained from the Monte-Carlo simulation assuming common Gaussian random noise with \( \sigma = 0.35 \) MeV.](image)

‘speed’ with which an increase in the number of data points constrains more and more the parameters - here the central potential depth and the spin-orbit strength parameters. Observe a characteristic difference: the fitting of spin-orbit strength parameter is influenced by the double-valued structure in the \( \chi^2 \)-minima - see below and also in (I) - the distributions for 13 and 21 levels remain similar in that case.

Indeed, fitting to 13 levels results in two local minima which differ mainly in terms of \( r_0^{s_0} \) parameter, see Table 1; the \( r_0^{s_0} = 1.231 \) fm solution is referred to as ‘non-compact’ and the
one with \( r_0^{so} = 0.924 \text{ fm} \) as ‘compact’. Although the ‘non-compact’ solution has a smaller value of \( \Delta_{rms} \) one should remember that the value obtained from a single fit to a certain set of experimental data represents only one single point on the x-axis of the \( \chi^2 \)-distribution\(^1\) which describes \( \Delta_{rms} \) estimator. Therefore the difference of 0.076 keV between the two results may be a single-point effect which has no statistical significance. This hypothesis is confirmed by a Monte-Carlo simulation tests performed independently which indicates that both solutions are almost equally probable. In the case of fit to 7 levels there also exist two local minima, the ‘compact’ solution has a smaller value of \( \Delta_{rms} \) estimator in this case.

### Table 1. The values of the Woods-Saxon Hamiltonian parameters as obtained in the fit to 7 or 13 neutron single particle levels in \(^{208}\text{Pb}\). The confidence intervals are defined as \( 2t_{0.05,v} \sqrt{M_{ii}}. \)

| Quantity | \( V_0 \) | \( r_0 \) | \( a_0 \) | \( V_0^{so} \) | \( r_0^{so} \) |
|----------|----------|----------|----------|----------|----------|
| **Non-compact solution \( \Delta_{rms} = 0.349 \text{ MeV (13 levels)} \)** |
| Mean value | −42.025 | 1.320 | 0.694 | 24.781 | 1.231 |
| Standard error | 1.217 | 0.023 | 0.031 | 2.639 | 0.050 |
| Confidence interval | 2.264 | 0.043 | 0.058 | 4.907 | 0.093 |
| **Compact solution \( \Delta_{rms} = 0.425 \text{ MeV (13 levels)} \)** |
| Mean value | −41.653 | 1.328 | 0.670 | 24.007 | 0.924 |
| Standard error | 1.494 | 0.029 | 0.036 | 2.075 | 0.035 |
| Confidence interval | 2.777 | 0.053 | 0.066 | 3.859 | 0.066 |
| **Compact solution \( \Delta_{rms} = 0.151 \text{ MeV (7 levels)} \)** |
| Mean value | −42.923 | 1.294 | 0.616 | 26.692 | 0.890 |
| Standard error | 0.912 | 0.018 | 0.027 | 1.030 | 0.021 |
| Confidence interval | 2.664 | 0.052 | 0.079 | 3.007 | 0.061 |

The calculated Jacobian matrix allows to estimate the confidence intervals for the model parameters. In the case of the fit to 13 levels the confidence intervals calculated with the relations (2) and (3) agree with the results of Monte-Carlo calculations - compare the widths of Probability Density Functions presented in Figure 1 with the confidence intervals widths from Table 1. In the case of ill-posed problems the variance-covariance matrix can be unreliable and so will be the confidence intervals. The fit performed to 7 levels results in \( \Delta_{rms} = 0.151 \text{ MeV} \) which is more then a factor of 2 smaller then in the fit employing 13 levels. This suggest an effect called over-fitting of parameters: a small change in one of experimental data may strongly influence the resulting values of optimal parameters. Observe that the confidence intervals obtained in the fit to 7 levels are of the same size as those obtained in the fit to 13 levels, an abnormal situation for the case of the stable fit. Indeed, the Monte-Carlo simulations performed with \( \Delta_{rms} = 0.35 \text{ MeV} \) give confidence intervals which are an order of magnitude bigger in the case of 7 levels used in the fit. This observation supports the thesis about the superiority of the Monte-Carlo tests that contain a global-type information as opposed to a single-point test based on (2).

The results obtained with (2) for fits with 7 and 13 levels are given in the lower left and upper right ‘triangles’ of Table 2, respectively. One can read from the table a very strong

---

\(^1\) We wish to make the reader attentive to the existence of two meanings of the term ‘chi-square’: a. The \( \chi^2 \)-probability distribution studied in the domain of probabilities (as needed in this paragraph) and b. The \( \chi^2 \) as the minimised function.
Table 2. The correlation matrix for the Woods-Saxon Hamiltonian parameters. The upper right ‘triangle’ presents the correlation coefficients for ‘compact’ solution for 13 levels whereas the lower left ‘triangle’ represents the same information for the ‘compact’ solution with 7 levels.

|       | $V_0$ | $r_0$ | $a_0$ | $V_{0}^{so}$ | $r_{0}^{so}$ |
|-------|-------|-------|-------|--------------|--------------|
| $V_0$ | 0.990 | −0.028| 0.044 | 0.341        |              |
| $r_0$ | 0.991 | 0.056 | 0.068 | 0.323        |              |
| $a_0$ | 0.609 | 0.689 | 0.218 | −0.123       |              |
| $V_{0}^{so}$ | −0.161 | −0.146 | 0.110 | −0.588      |              |
| $r_{0}^{so}$ | 0.784 | 0.787 | 0.526 | −0.547      |              |

correlation between the depth and radius parameters for both central and spin-orbit potentials; these are roughly independent of the number of data points used in the fit. On the contrary, the correlation coefficient between the $r_0$ and $a_0$ parameters decreases from 0.743 to 0.092 when the number of experimental levels changes from 7 to 13. These results are confirmed by Monte-Carlo calculations. Figure 2 presents indeed strong correlations between $V_0$-$r_0$ and $V_{0}^{so}$-$r_{0}^{so}$ pairs of parameters, here for the 13 levels in the fit.

Figure 2. Left: The correlation between the $V_0$ and $r_0$ parameters as obtained from the Monte-Carlo simulation assuming $\sigma = 0.35$ MeV in the fit to 13 levels. Right: Same as on the left but for the $V_{0}^{so}$ and $r_{0}^{so}$ parameters. Observe the ‘compact’ and ‘non-compact’ correlations coexisting independently in the second case. The diagrams contain 10,000 points each.

The proper estimation of a variance-covariance matrix is essential for the reliable predictions of observables and analysis of a predictive power of a model. The importance of correlations between the parameters can be illustrated by comparing the predictions which utilise full variance-covariance matrix with the results of calculations when only diagonal elements (standard errors of parameters) are used. The results of these two kinds of calculations are presented in Figure 3. In the presented calculations the variance-covariance matrix obtained from (2) is sampled with Monte-Carlo method. One clearly sees that neglecting the correlation can significantly increase the variance of predictions.

In the case of a well-posed problem the predictions obtained from Monte-Carlo sampling of variance-covariance matrix and Monte-Carlo simulation should be similar. Indeed, comparison of Figures 3 and 4 shows that this is the case in the analysed example. Complications arise
Figure 3. Left: The Probability Density Function for the neutron levels in $^{132}$Sn obtained from the extrapolation of parameters given in the first part of Table 1. Right: same as on the left assuming no correlation between the Hamiltonian parameters.

Figure 4. The Probability Density Function for the neutron levels in $^{132}$Sn obtained from the extrapolation of parameters obtained in the Monte-Carlo simulation assuming common Gaussian noise with $\sigma = 0.35$ MeV and the fit to 13 levels.

when multiple local $\chi^2$-minima exist. The variance-covariance matrix is calculated only in one minimum while in Monte-Carlo analysis all local minima are taken into account. This explains the different widths of $1h_{9/2}$ levels whose position strongly depends on the spin-orbit parameters. The reader may wish to compare these with more simulation results in [3] and [4].

4. Summary
In this article we have presented and discussed a few elements of the analysis of the statistical significance in determination of the parameters of theory Hamiltonians using a toy-model in the form of a phenomenological (Woods-Saxon) nuclear mean field. Analyses using variance-covariance matrix and the Monte-Carlo simulations were compared pointing out to the superiority of the latter.

Acknowledgements
This work is supported by the Polish Ministry of Science and Higher Education, under contract N-N202-263238, by the LEA COPIGAL and by the COPIN-IN2P3 agreement No.06-126.

References
[1] Dudek J, Szpak B, Porquet M-G and Fornal B 2010 *J. Phys.: Conference Series* This Issue
[2] Dudek J, Szpak B, Porquet M-G, Molique H, Rybak K and Fornal B 2010 *J. Phys. G: Nucl. Part. Phys.* 37 064031
[3] Dudek J, Rybak K, Szpak B, Porquet M-G, Molique H, and Fornal B 2010 *Int. J. Mod. Phys. E* 19 652
[4] Szpak B, Dudek J, Porquet M-G, Rybak K, Molique H, and Fornal B 2010 *Int. J. Mod. Phys. E* 19 665