A novel method of data analysis for hadronic physics

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A principal task in experimental and computational physics concerns the determination of the parameters of a theory (model) from experimental or simulation data. Examples are abundant: the determination of the parameters of the Standard Model in Particle Physics, the multipole amplitudes in Nucleon Resonance excitation in hadronic physics, the determination of the spectrum from correlators in lattice QCD calculations, the parameters of acoustic resonances in Cosmology, to mention a few.

The data from which information on parameters of the theory is to be extracted are characterized by statistical uncertainties and systematic errors, are typically of limited dynamic range and sensitive only to a few of the model parameters, rendering this task difficult and often intractable. Identifying which parameters of the model can be determined from the available data is often difficult to prejudge and their extraction without bias is often impossible. Particularly hard is the determination of the systematic and model uncertainties that ought to be assigned to the extracted values of the parameters.

We address this problem via a method, that we will refer to as the Athens Model Independent Analysis Scheme, "AMIAS", which is capable of extracting theory (model) parameters and their uncertainties from a set of data in a rigorous, precise, and unbiased way. The methodology is first presented and then subsequently applied to two problems in hadronic physics, which are used as demonstration cases. The two cases concern A) the extraction of the mass spectrum of hadrons from Euclidean time correlators in lattice QCD simulations and B) the extraction of the multipole excitation amplitudes for the Nucleon resonances and in particular that of the first excited state of the Nucleon, the $\Delta(1232)$ resonance.

The AMIAS method is applicable to problems in which the parameters to be determined are linked in an explicit way to the data through a theory or model. There is no requirement that this set of parameters are orthogonal; they can be subjected to constraints, e.g. by requiring that unitarity is satisfied. The method requires that a quantitative criterion for the "goodness" of a solution is chosen and thus far we have employed the $\chi^2$ criterion.

For a given theory any set of values for its parameters, satisfying its symmetries and constraints, provides a solution having a finite probability of representing reality. This probability can be quantified through a comparison to the data being analyzed. Based on these concepts AMIAS can be formulated as follows:

A set of parameters $A_1, A_2, \ldots, A_N \equiv \{A_\nu\}$ which completely and explicitly describes a process within a theory, can be determined from a data set $\{V_k \pm \varepsilon_k\}$, produced by this process, by noting that any arbitrary set of values $\{a_\nu\}$ for these parameters constitutes a solution having a probability $P(j)$ of representing "reality" which is equal to:

$$P(j) = G(\chi^2(j), \{a_\nu\})^j$$

where $G$ is a function of the data and the parameters of the model and of $\chi^2$, where,

$$\chi^2(j) = \sum_k \left(\frac{U_k^j - V_k}{\varepsilon_k}\right)^2$$

Thus $P(j)$ is a function of the $\chi^2$ resulting from the comparison to the data $\{V_k \pm \varepsilon_k\}$ of the predicted, by the theory, values $U_k^j$ by the $\{a_\nu\}$ solution.

In the case where we chose $G = e^{-\chi^2/2}$ the results obtained by AMIAS are related to those obtained by $\chi^2$ minimization methods and widely used and implemented in a number of codes (e.g. MINUIT [1]). The results become identical if correlations among the parameters of the theory are absent or ignored.

We call an ensemble $Z$ of such $a_\nu$ solutions Canonical Ensemble of Solutions, which has properties that depend only on the experimental data set. Similarly a Micro-canonical Ensemble of Solutions can be defined as the collection of solutions which are characterized by

$$\chi^2_A \leq \chi^2 \leq \chi^2_B$$

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where $\chi_A^2$ and $\chi_B^2$ define a sufficiently narrow range in $\chi^2$ space. A case of particular interest concerns the micro-canonical ensemble near the minimum $\chi^2$ value:

$$\chi^2 \leq \chi_{\text{min}}^2 + C$$  \hspace{1cm} (4)

where $C$ is usually taken to be the constant equal to the effective degrees of freedom of the problem.

The extraction of the model parameters $\{A_\nu \pm \delta A_\nu\}$ for a specific set of data can be accomplished by employing the following procedure:

- A canonical ensemble of solutions, is being constructed by randomly choosing values, $\{a_\nu\}$, for the set of parameters $\{A_\nu\}$ of the theory within the allowed physical limits and by imposing the required constraints. Each set $\{a_\nu\}$ constitutes a point in the ensemble which is labeled by the $\chi^2$ value this solution generates when compared with the data. In the absence of constraints, any given model parameter $A_\nu$ will assume all allowed values with equal probability (equipartition postulate).

- To each point of the ensemble $\{a_\nu\}$ a probability is assigned, equal to $P(j)$. Following standard statistical concepts, the probability $\Pi(a_\nu)$ of a parameter $A_\nu$ assuming a specific value $a_\nu$ in the range $(a_\nu, a_\nu + \Delta a_\nu)$ is equal to:

$$\Pi(a_\nu) = \frac{\int_{a_\nu}^{a_\nu+\Delta a_\nu} \sum_j dA_j P(j)}{\int_{-\infty}^{+\infty} \sum_j dA_j P(j)}$$  \hspace{1cm} (5)

This expression defines the Probability Distribution Function (PDF) of any parameter of the theory for representing "reality". It thus contains the maximum information that can be obtained from the given set of data. Having obtained the PDF, numerical results can be derived, usually moments of the distribution. The mean value is normally identified as the "solution" and the corresponding variance as its "uncertainty".

It is manifestly obvious that AMIAS has minimal assumptions and that it introduces no methodological bias to the solution. It determines the theory/model parameters that exhibit sensitivity to the data yielding PDFs that allow only a restricted range of values usually with a well defined maximum and a narrow width. If the data do not contain physical information to determine some of the parameters, then the resulting PDFs are featureless. The underlying stochastic approach allows easy scalability to a very large number of parameters even with limited number of data.

The method is computationally robust and stable; obviously it could not have been implemented without the advent of powerful computers. We have developed algorithms that can be implemented efficiently and produce results to realistic and demanding problems within reasonable computation times. It is also apparent that the method is amenable to trivial computational parallelism. Description of its algorithmic implementation, is beyond the scope of this paper and it will be presented elsewhere.

A validation of the method and demonstration of its capabilities has been extensively studied in a number of toy models and in two physical problems in hadronic physics both of current interest: A) The extraction from lattice simulation data of the masses of the spectrum of mesons and baryons and B) The extraction of multipole amplitude strength from nucleon electroexcitation spectra. In all cases studied the AMIAS method recovered with the expected statical accuracy the input parameters in the case of pseudodata. The derived uncertainties are compatible with those obtained using the "jackknife" technique in the case of toy models and the lattice data.

We present below results with pseudodata to demonstrate the validity for the two cases mentioned above; analysis of physical data or simulations corresponding to these case have been published elsewhere.

**A. Extraction of Mass Spectrum of Baryons from Euclidean Time Correlators**

There has been impressive progress in lattice QCD calculations where new algorithms and faster computers make feasible high-precision simulations close to the physical parameters. As in the case of experimental data, simulation data are characterized by statistical uncertainties and systematic error. To extract physical quantities from lattice simulations such as masses of hadrons, decay constants and form factors, fits to the simulated data are performed. As in other fields, various approaches have been explored in order to extract the physics of interest.

We have successfully applied the AMIAS method to the analysis of two-point correlators which result from calculations in Lattice QCD. Its generalization to more complicated objects such as three-point correlators is under study. Results extracted from lattice QCD simulations have been presented and compared to traditional methods elsewhere.

In Lattice Gauge theories, the Euclidean time correlator $C(t)$ of an interpolating operator $J(x,t)$ and its spectral decomposition for zero three-momentum is:

$$C(t) = \sum_x < J(x,t) J^\dagger(0,0) > = \sum_{n=0}^{\infty} A_n e^{-m_n t}$$  \hspace{1cm} (6)

where the brackets denote the vacuum expectation value. The exponential dependence is correct for Dirichlet boundary conditions. In the large $t$ limit the state with the lowest mass (ground state) dominates the time dependence of the correlator. Fitting the asymptotic behavior of $m_{eff}(t) = -\log\{C(t)/C(t+1)\}$ to a constant yields the lower mass of the hadron while determination of higher masses gives the excitation energies of states of the same quantum numbers as the ground state.
The case of lattice QCD simulations present an excellent case for AMIAS. As required, a framework that connects the data and the model parameters of interest, the masses \( m_j \) and the overlap amplitudes \( C_j \), is explicit and in this case is given by Eq. [1].

We present here a simple case employing pseudodata so as to demonstrate the validity and some features of the method. Pseudodata were generated for a system for a theory with \( f(t) = C_0 \exp(-m_0 t) + C_1 \exp(-m_1 t) \) and relative errors that grow with time resembling lattice data. We have arbitrarily chosen \( C_0 = 1.0, m_0 = 0.500, C_1 = 3.0 \) and \( m_1 = 1.00 \). We have demonstrated that the extracted values have a precise meaning through the analysis of pseudo-data generated with predetermined statistical accuracy.

The extracted results are statistically compatible irrespective of whether they were derived by taking \( n = 2 \) or \( n \geq 3 \). The uncertainty of the fitted parameters grows as the number of the (a priori unknown) terms fitted is increased. We adopted an ansatz whereby the number of terms employed is greater by one to those that can be extracted with finite uncertainty. Similarly the size of the phase volume that the Monte-Carlo method is sampling does not affect the solution provided that the volume is sufficiently large to include all "good solutions". By "good solutions" we denote solutions with small or reasonable \( \chi^2/(\text{degrees of freedom}) \). As shown in Fig. 1 the parameters are accurately extracted, in complete agreement with the generator values within the stated statistical accuracy. As expected, search for \( M_2 \) yields a null result.

AMIAS has been used to analyze lattice simulation data and the derived results [2] that compare favorably to those derived by traditional methods considered as defining the "state of the art" in the lattice community [3].

**B. Extraction of Multipole Amplitudes from electroexcitation Spectra**

The problem of extracting multipole amplitudes from electroexcitation spectra with reduced model uncertainty motivated the work that is reported here. In particular, the verification of the conjecture that hadrons are non spherical [10, 11] has been demanding the isolation with high precision of the small resonant quadrupole amplitudes in the \( N \rightarrow \Delta \) transition. It was observed that increased accuracy in the experimental data would not yield more precise results [10], which were inherently limited by the limitations of the analysis methods employed. This important case provides a typical problem of high complexity, amenable to being solved by the AMIAS method.

The parameters of the model \( \{ A_\nu \} \), are the multipole amplitudes such as the \( M_{1/2}^{1/2}, M_{3/2}^{3/2} \) using standard spectroscopic notation. They relate to the data, cross sections and polarization observables in electroexcitation experiments, through the CGLN formulation of the resonance electroexcitation [12]. They are infinite in number, so a truncation is needed and they are related to the data through a very complex convoluted scheme, unlike the case of masses in QCD lattice data. Furthermore, in this case, the parameters of the problem are subjected to the constraint of unitarization.

The validity of the AMIAS method was demonstrated with the employment of pseudodata generated through the well established MAID scheme [13] (which implements the CGLN formalism). AMIAS derived results have been demonstrated to have a precise meaning through the analysis of pseudodata which were generated with predetermined statistical accuracy. In the cases presented below, we have frozen the \( A_{3/2}^3 \) and we have varied the \( A_{3/2}^3 \) helicity amplitudes. Few demonstrative cases of the pseudodata validation are presented below.

We use pseudodata with kinematics of the \( Q^2 = 0.127 \text{ (GeV/c)}^2 \) Bates and Mainz \( N \rightarrow \Delta \) data [14] to demonstrate the validity of the analysis. The data set is published, is well understood and it is well described by MAID. Two sets of pseudodata were generated using MAID, characterized by different statistical accuracy: "Set A" with statistical accuracy similar to that of the experimental values and "Set B" with statistical accuracy hundred times better than that of the experimental values. These data were analyzed and the multipoles were extracted which are tabulated and compared with the generator values in the Table. We have tabulated only extracted values which are derived with uncertainties better than 100% for "Set A". It can be seen that the
TABLE I: The multipole values extracted, in units of $10^{-3}/m_\pi$, from two pseudodata sets are compared to the generator (modified MAID) values. They are shown to be entirely compatible with increasing precision in the extracted parameters as the statistical accuracy of the data increases.

| Multipole | Generator | Set A | Set B |
|-----------|-----------|-------|-------|
| $M_{1+}$  | 27.248    | 27.23 ± 0.13 | 27.249 ± 0.001 |
| $L_{0+}$  | 3.500     | 3.70 ± 0.23  | 3.502 ± 0.002  |
| $L_{1+}$  | 1.048     | 1.03 ± 0.08  | 1.048 ± 0.001  |
| $E_{1+}$  | 1.481     | 1.49 ± 0.18  | 1.482 ± 0.002  |
| $E_{0+}$  | 4.225     | 3.68 ± 1.02  | 4.248 ± 0.013  |
| $M_{1-}$  | 4.119     | 4.47 ± 1.31  | 4.124 ± 0.013  |
| $L_{1-}$  | 1.205     | 1.05 ± 0.43  | 1.203 ± 0.008  |
| $E_{2-}$  | 1.024     | 1.07 ± 0.45  | 1.027 ± 0.006  |
| $L_{2+}$  | 0.007     | 0.02 ± 0.01  | 0.008 ± 0.001  |
| $E_{2+}$  | 0.006     | 0.01 ± 0.01  | 0.007 ± 0.001  |

AMIAS extracted multipole values are in complete agreement with the generator values within the stated statistical accuracy. Also, as required, the quoted uncertainties are reduced in set "B" (hundredfold), proportionally to the statistical accuracy of the pseudodata sets. For comparison, in Fig. 2 the probability distributions is shown for the most sensitive amplitudes of the Bates/Mainz experimental data set analyzed with AMIAS.

To verify the ability of AMIAS to extract uncertainties which have precise statistical interpretation is generally more difficult. The scaling behavior exhibited by the two sets of pseudodata, discussed above, is a necessary but not sufficient condition. The definitive validation was achieved by introducing an arbitrary uncertainty, a "generator uncertainty" to the nominal generator multipole values. Multiple sets of data generated by randomized input within the allowed uncertainties of the generator parameters are recovered by AMIAS. This demonstration exercise was performed both for simple functional forms (e.g. polynomial functions) and complicated cases such as this one (multipole amplitudes in a CGLN formalism), results of which have been presented in [15]. Furthermore, in the case of polynomial functions and lattice QCD two-point functions, deriv'd jackknife errors are found to be statistically compatible with AMIAS uncertainties.

In summary: a novel method of analysis is shown to offer significant advantages over existing methods in determining physical parameters from experimental or simulation data: it is computationally robust, it provides methodology independent answers with maximal precision in terms of the derived Probability Distribution Function for each parameter.

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