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NUCLEAR PHYSICS

No need to decide

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To test the validity of theoretical models, their predictions must be compared to experimental data. Instead of choosing one out of many to describe mass measurements of zirconium, Bayesian statistics allows to average over a variety of models.

One of the most spectacular quantum effects in atomic nuclei is the emergence of a shell structure. Protons and neutrons are interacting through the strong force, and rearrange themselves into a shell structure that is similar to the one observed in the electronic structure of atoms. Since Maria Goeppert Mayer's pioneering work[1], which earned her the Noble Prize in Physics in 1963, nuclear physicists have gained a better understanding of the shell structure. However, important questions such as the origin of an additional binding energy, named the Wigner energy, in nuclei, where neutrons and protons occupy the same shell orbitals[2,3], remain open. Now, writing in Nature Physics, Alec Hamaker and colleagues have provided answers to this question by performing accurate mass measurements of zirconium isotopes[4].

The mass measurements are then combined with an advanced statistical analysis in order to shed light on the underlying shell structure. Hamaker and colleagues used a theoretical approach based on energy density functional theory. Originally developed in the field of condensed matter physics by Pierre Hohenberg and Walter Kohn[5], this theory has been successfully applied to nuclear physics[6] and moreover, has become a common tool for describing the properties of atomic nuclei.

As alluded to in its name, the key element of density functional theory is the functional of the density that describes the properties of the system under scrutiny. Knowing the exact functional would allow to determine the actual ground state properties of the system at a given density. As the ideal functional is not known, one needs to use approximations that are often based on different hypotheses. Given their phenomenological nature, most of the available functionals are characterised by a number of adjustable parameters, which can be extracted from a fit to the experimental data.

Although the majority of available functionals tend to reproduce the nuclear observables reasonably well, their extrapolations to unchartered territories of the nuclear chart lead to different results. This raises the questions on how one can rely on such a variety of extrapolations and which functional one should use to compare new experimental results to?

The answer Hamaker and colleagues have employed is rather simple and illuminating[7]. Instead of selecting one particular model to compare their measurements to, they averaged over a pool of models using Bayesian statistics. Figure 1 illustrates the procedure: given two models trained on a set of data, a new model can be built by using a weighted average of the original two. According to the Bayesian model average procedure, the weights are calculated by using the data of a validation set. Such a data-driven approach allows to combine the best out of a family

of models by obtaining results that are less dependent on the choices underlying the model, for example, the optimization of a certain parameter of a given functional.

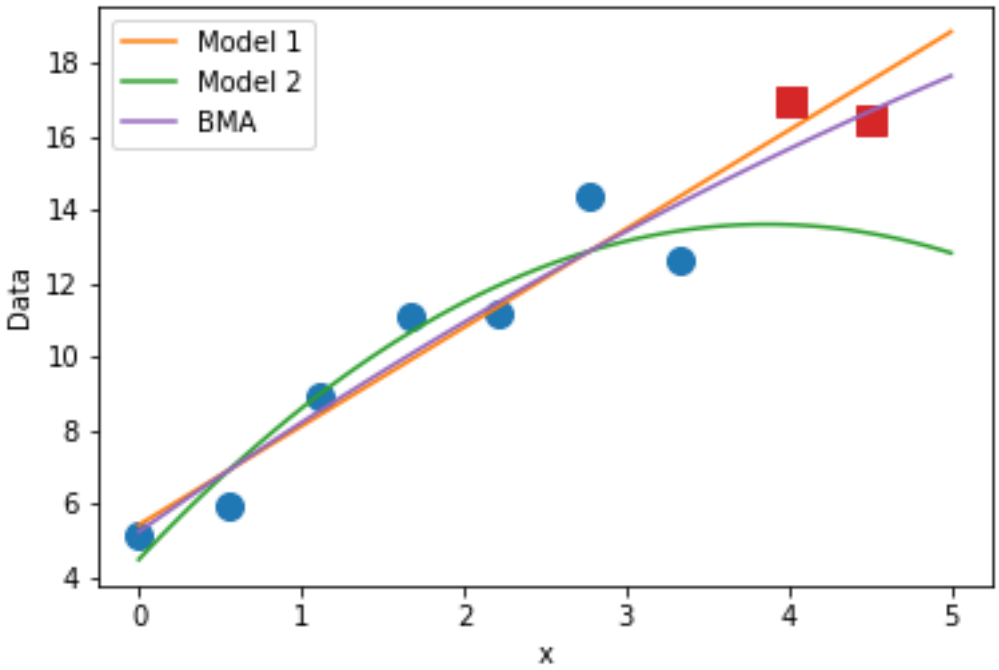

Figure 1 Schematic representation of Bayesian model averaging). Two models (orange and green lines) are trained on a given data set (blue circles). Bayesian model averaging provides a new model (purple line) from the weighted average of models 1 and 2. Hereby, the weights are calculated by using a validation data set (red squares).

On top of each individual model considered for the Bayesian model averaging (BMA), Hamaker and colleagues suggested the use of a simple Gaussian process[8] to compensate for possible deficiencies of a given model in reproducing some given observable. The main advantage of using a Gaussian process instead of a more sophisticated neural networks[9] is the reduced number of adjustable parameters and the straightforward definition of error bars. Thanks to the use of BMA, Hamaker and colleagues provide a solid conclusion concerning the missing physics in the adopted nuclear models that can not simply taken into account by slightly readjusting the underlying coupling constants.

When compared to the mass measurements, the authors find a discrepancy between theory and experiment with a significance of more than one standard deviation. This represent a clear challenge for current theoretical models, and thus this work proves that in not sufficient to perform better adjustement of functional in order to better describe the data, but new physics should be explored as for example the competition between deformation effects, isospin breaking effects, and proton-neutron pairing[10].

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Competing interests:

The author declares no competing interests.