Machine learning algorithms for the interpolation of nuclear Potential Energy Surfaces

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Motivations

The microscopic description of the fission process can be done using a two-step approach with the Hartree-Fock-Bogoliubov (HFB) formalism and the Time-Dependent Generator Coordinate Method (TDGCM). First, a Potential Energy Surface (PES) is calculated using the HFB method in a given deformation subspace, then a dynamical propagation of a wave packet is performed using the TDGCM with a Gaussian Overlap Approximation (GOA) using the previously calculated PES as a set of TDGCM basis states. Since the HFB method we are using relies on the implicit minimization of the total binding energy under the action of several deformation constraints, some neighboring HFB solutions in the deformation subspace can in fact be quite different in the whole deformation space, and this can lead to the presence of discontinuites in the PES. One possible way to get rid of some of these discontinuites, in order to improve the description, is to increase the number of deformation constraints, i.e. use a bigger deformation subspace for the PES. However, increasing this number implies that the number of constrained HFB calculations needed to span the deformation subspace in a dense enough way for the subsequent use of the TDGCM method grows exponentially, and so do the numerical resources needed to produce the corresponding PES.
This study aims at comparing the capabilities of several machine learning methods to reduce the numerical cost of the production of a 3-dimensional PES. In the present study, we do not focus on one specific algorithm. Instead, we compare several very different methods and discuss their specificities in a given physical context (the description of nuclear low-energy fission). Our goal is that such a comparative study may emphasize some of the possible uses of diverse machine learning approaches in nuclear physics.

Goals

Let us consider a complete fission potential-energy surface for three shape coordinates $E[MeV] = f(q_{20}, q_{30}, q_{40})$ where $q_{20}[b]$ (elongation), $q_{30}[b^{3/2}]$ (mass asymmetry) and $q_{40}[b^2]$ (hexadecapolar moment) are the multipole-moments constraints constituting a database of 389 440 HFB energy values.
The corresponding PES is drawned in 3D according to the collective variable q_{20} between 0 b and 30 000 b and q_{30} between 0 $b^{3/2}$ and 100 000 $b^{3/2}$ and for the energies below -1943 MeV.

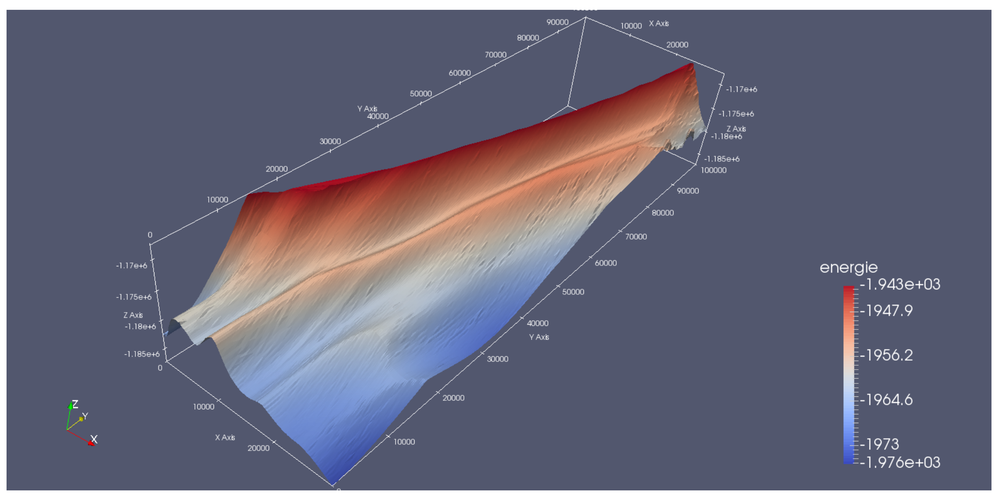

Figure 1: Potential energy surface fission with constraints q_{20}, q_{30} and q_{40}.

Including the additional variable q_{40} would involve roughly 2.106 constrained HFB calculations, imply a numerical cost $\approx$ 1.106 cpu.h for a full 3D PES.

Metrics Evaluation

Summary of the result with the non-parametic regression algorithms for both 1% (3894 data points) and 5% (19 470 data points) of the 389 440 available points.

	1%	
Method	**Average RMSE**	**Standard deviation**
Linear Regression	6.04 MeV	+/- 0.42
Polynomial Regression	1.21 MeV	+/- 0.38
LASSO	6.33 MeV	+/- 0.43
RIDGE	6.04 MeV	+/- 0.42
kNN (k=4)	1.76 MeV	+/- 0.25
SVM	1.46 MeV	+/- 0.22
DecisionTree (CART)	2.56 MeV	+/- 0.21
CART-Bagging (=RF)	1.58 MeV	+/- 0.19
CART-Boosting	1.22 MeV	+/- 0.18
CART-Stacking	0.99 MeV	+/- 0.04
Neural Network	0.77 MeV	+/- 0.02
Gaussian Process	0.47 MeV	+/- 0.03
	5%	
	Average RMSE	**Standard deviation**
Linear Regression	6.04 MeV	+/- 0.34
Polynomial Regression	0.82 MeV	+/- 0.02
LASSO	6.33 MeV	+/- 0.43
RIDGE	6.04 MeV	+/- 0.42
kNN (k=4)	1.05 MeV	+/- 0.09
SVM	1.56 MeV	+/- 0.06
DecisionTree (CART)	1.42 MeV	+/- 0.05
CART-Bagging (=RF)	0.79 MeV	+/- 0.06
CART-Boosting	0.67 MeV	+/- 0.06
CART-Stacking	0.57 MeV	+/- 0.02
Neural Network	0.45 MeV	+/- 0.01
Gaussian Process	0.40 MeV	+/- 0.04

Evolution of the RMSE as the percentage of training data

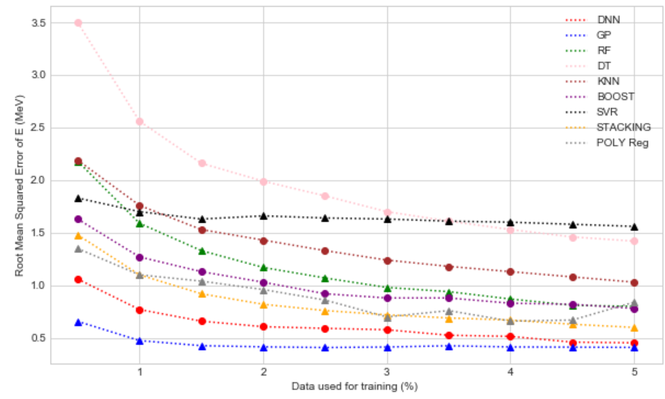

Figure 2: RMSE of the HFB Energy (using cross-validation) as a function of the size of the training set (in percent of PES Database

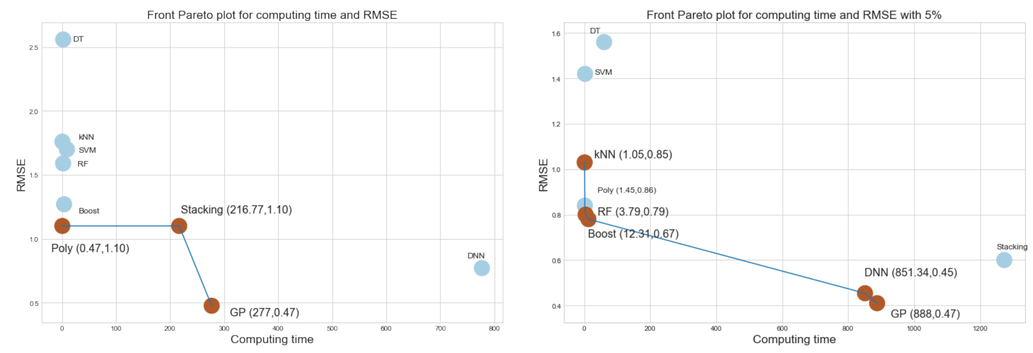

Figure 3: Front pareto for each methods w.r.t to precision and training time (left 3894 points - right 19470 points

Gaussian Process and Neural Network

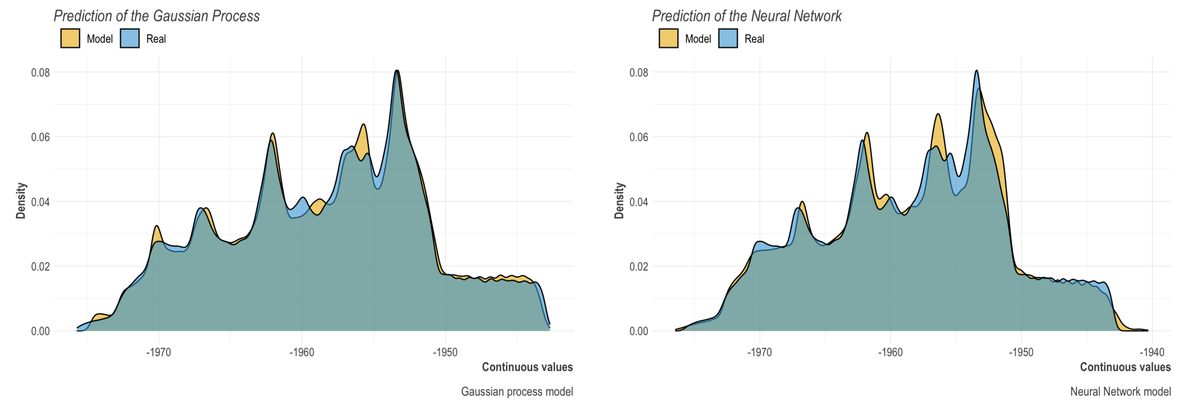

Figure 4: Density comparisons of predicted value vs real value. Left Gaussian Process, right Neural Network.

Physical usability of such methods

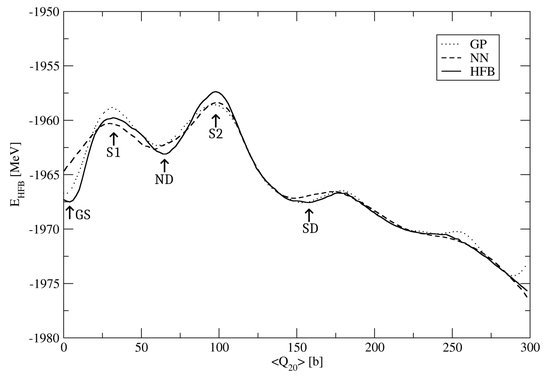

Figure 5: Comparison of the symmetric ($q_{30} = 0$) minimum binding energy along q_{20} with different interpolations. GP stands for Gaussian Process, NN for Neural Network, and HFB for the original HFB solutions.

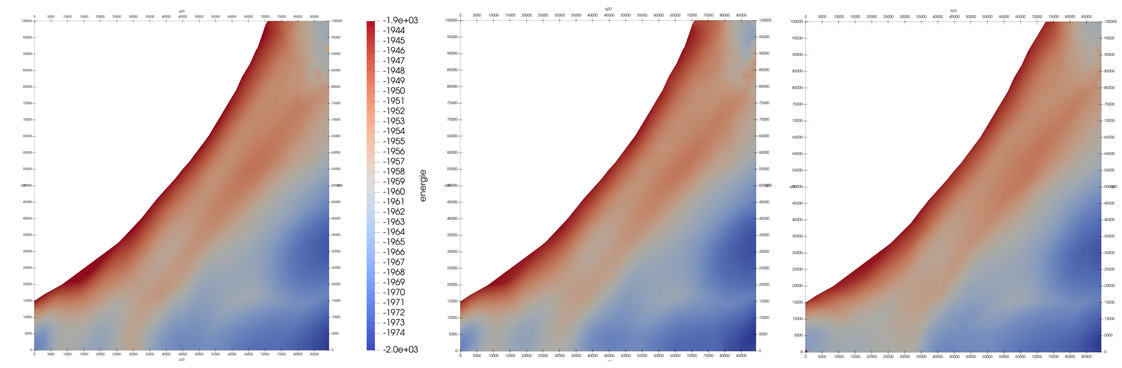

Figure 6: From left to right, PES of the nucleus, prediction of the PES using Neural Network and prediction of the PES using Gaussian Process.

Conclusion

In this work we build a new way to speed up microscopic evaluation of a Potential Energy Surface using cutting edge methods in the field of machine learning. We reached impressive performances a RMSE of ~ 500 keV with only ~ 4000 inputs on a map of more than 380000 data points.

- Rasmussen C. E., William C. K., Gaussian Processes for Machine Learning, 2005, The MIT Press.
- Bishop C. M., Neural Networks for Pattern Recognition, 1995, Oxford University Press, Inc.