ML for PESs: Introduction

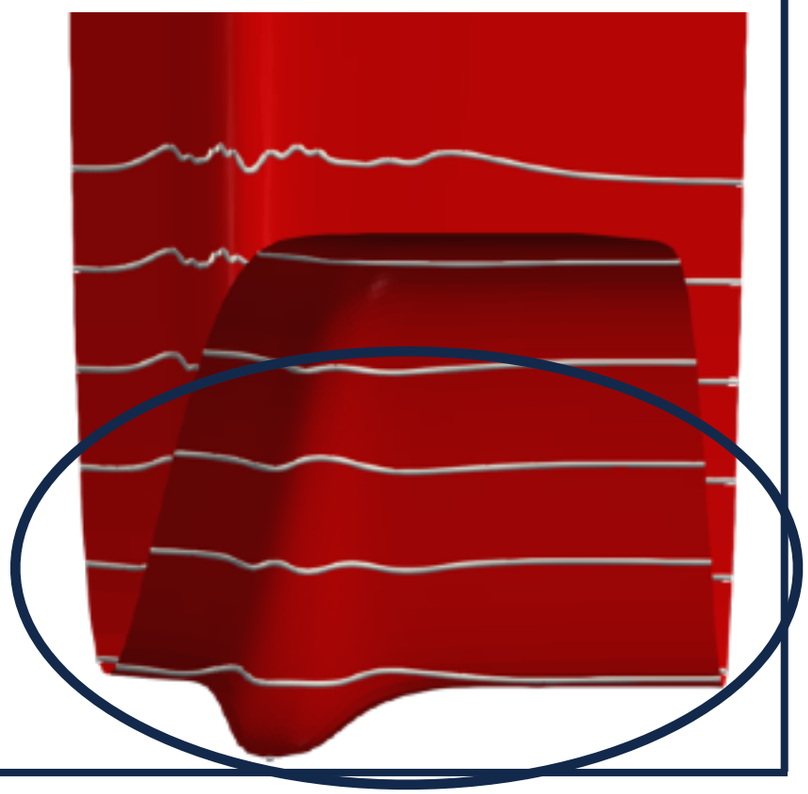
In the last decade there has been an increasing effort in taking advantage of Machine Learning for constructing Potential Energy Surfaces. In particular, using:

- ✦ **Gaussian Processes**
- ✦ **Neural Network**

- ✦ "*Representing Global Reactive Potential Energy Surfaces Using Gaussian Processes*", *J. Phys. Chem. A 2017*;
- ✦ "Comparison of permutationally invariant polynomials, neural networks, and Gaussianapproximation potentials in representingwater interactions through many-bodyexpansions", J. Chem. Phys. 2018;
- ✦ "Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces", Phys. Rev. Lett. 2007;
- ✦ "Permutation invariant potential energy surfaces for polyatomic reactions using atomistic neural networks", J. Chem. Phys. 2016;
- ✦ …

However, almost the entire literature focuses on the relatively low energy part of the PES.

Through this work, we want to assess if the ML reconstruction can achieve reasonable accuracy for the region of the surface of Hypersonic interest.



ANN for PESs: Methodology

Multi-layer feed-forward Neural Networks (NN) have been adopted **as fitting functional**:

- ✦ Easy to implement;
- ✦ Easy to train;
- ✦ Easy to generalize to new systems;
- ✦ Easy to differentiate in **R**;
- ✦ Cost effective;
- ✦ Easy to be refined;
- ✦ Widely tested;
- ✦ Easy to be extended to the stochastic case.

Permutation Invariant Polynomials Neural Networks (PIP-NN):

theano

Lasagne

1. A **Symmetrized Polynomial Vector** (**G**) is constructed, in order to account for the permutation symmetries; for example, for a A3-type system:

$$G_1 = p_1 + p_2 + p_3$$
$$G_2 = p_1p_2 + p_2p_3 + p_1p_3$$
$$G_3 = p_1p_2p_3$$

where $p_i = \exp(-\lambda_i(R_i - r_{e_i}))$, being λ_i and r_{e_i} tunable parameters.