From Deterministic To Stochastic

In a classic approach to ML, the error is known only at the data points. What can we say about the reliability of the fit at a generic location?

Plus … 3 main concerns about the deterministic PIP-NN deterministic approach …

- ✦ The uncertainty on the data points (Schrödinger Eq. solutions) has not been taken into account;
- ✦ Overfitting Risk;
- ✦ Committee of Neural Networks can produce significantly different results:

No. of fit points N_{pts}	NN		GP	
	1 NN	⟨10 NN⟩	1 GP	⟨10 GP⟩
313	198.00/103.93/87.77	119.11/53.97/43.90	29.09	17.18
625	21.12/12.91/12.03	13.36/7.52/6.53	5.98	3.87
1250	9.29/5.74/4.38	5.74/3.36/2.54	2.17	1.13
2500	4.59/2.43/1.12	2.27/1.23/0.86	1.08	0.62

Fig.1: RMSEs for multiple NN configurations. From: “Neural networks vs Gaussian process regression for representing potential energy surfaces: A comparative study of fit quality and vibrational spectrum accuracy”, J. Chem. Phys. 148, March 2018

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We propose the construction of a **stochastic PES**, which condenses the inaccuracy content related to both the grid of atom configuration chosen and the fitting function adopted.

Thus, we extend the ANN to **Bayesian Neural Networks** (BNNs), following the work initiated by R. Neal and recently pursued by C. Blundell *et al*.

Non-Deterministic attribute of BNNs is a consequence of:

- Functional **parameters treated as random variables** (parameter uncertainty):