Bayesian uncertainty analysis of the elastic nucleon-deuteron scattering observables

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Outline

- We want to study the nuclear force by examining its ability to predict neutron-deuteron scattering.
- Various observables have been measured for both the elastic reaction and the breakup reaction $\mathrm{nd} \rightarrow \mathrm{nnp}$.
- The Faddeev approach can solve this quantum three-body problems.
- But it is computationally expensive in both time & memory: running one set of parameters takes on average 4-5 hrs to evaluate neutron-deuteron elastic & inelastic scattering observables.
- Here we develop a Gaussian Process (GP) "emulator' that is trained at a small number of points in parameter space but can predict elsewhere.
- Such emulators make Uncertainty Quantification for this reaction feasible.

- Starting point is Lagrangian for nucleonic and pionic fields with broken chiral symmetry like in QCD.
- Effective Hamiltonian for nucleons and pions.
- Power counting – perturbative ordering $((Q/\Lambda)^{\nu})$ of various contributions to two- and many-body forces. Finite number of diagrams at given order.
- Short range interactions are included to the contact terms.

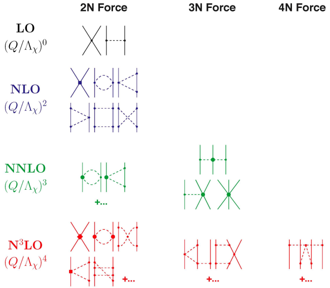


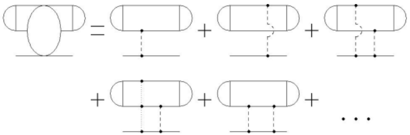
Figure is taken from R. Machleidt Nuclear Forces

- Three-nucleon forces (3NFs) play a small but critical role in nuclear structure and reactions.

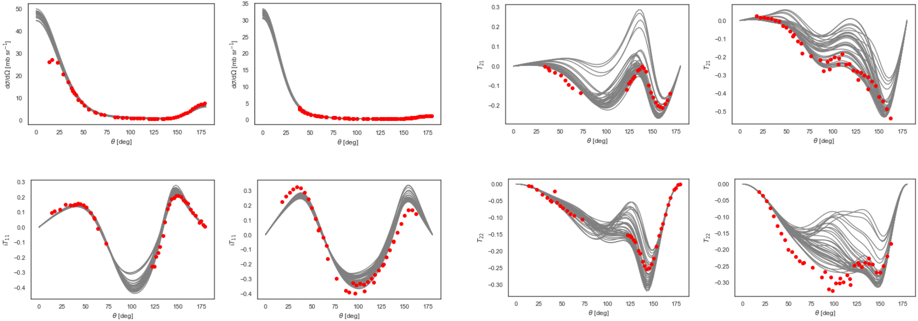
Using `surmise`'s tools to do uncertainty quantification:

- We use 37 training points of NN and 3N LECs (for a total of 12 dimensions). For the 3NF LEC's, we simply use a Latin hypercube design in the range $[-2, 2]$ (20 points) and $[-5, 5]$ (17 points). For the 10 NN LEC's, we start with a Latin hypercube design in the range $[-1, 1]$.
- Use Principal Components to select more suitable values of parameters & observables.
- Bayesian calibration of the c_D and c_E parameters based on experimental data and the 3N scattering observables through their posterior distribution function (PDF) allows us to estimate the uncertainty range of 3N observables.

- 2N bound state: Schrödinger equation.
- 2N scattering state: Lippmann-Schwinger equation for the t-matrix (interaction + free propagation): $t(E) = V + VG_0(E)V + VG_0(E)VG_0(E)V + \dots$
  $G_0(E) \equiv \lim_{\varepsilon \to 0^+} \frac{1}{E - H_0 + i\varepsilon}$
- 3N: Faddeev equation:
  $T = tP\phi + (1 + tG_0)V_{123}^{(1)}(1 + P)\phi + tPG_0T + (1 + tG_0)V_{123}^{(1)}(1 + P)G_0T$
- Transition amplitudes
  $U = PG_0^{-1} + V_{123}^{(1)}(1 + P)\phi + PT + PT + V_{123}^{(1)}(1 + P)G_0T$ (for elastic scattering) and $U_0 = (1 + P)T$ (for breakup) can be represented by the following diagram



- Dominant piece of 3NF depends on two parameters: c_D and c_E.
- Want to constrain them from nd scattering data.
- Curves below shows predictions for various 37 sets of (c_D, c_E) values, together with experimental data (Sekiguchi2001):



$E_{\rm lab} = 70$ MeV　$E_{\rm lab} = 135$ MeV　$E_{\rm lab} = 70$ MeV　$E_{\rm lab} = 135$ MeV `surmise`'s work is categorized into three routines:

- `emulation`: carries out Bayesian emulation of the 3N scattering Fadeev calculations using the chiral NN+3NF forces and generates inputs for calibration.

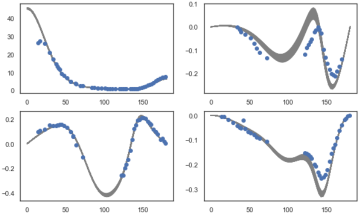
  1. Emulation via PC's

$$O(\theta; c_D, c_E) = \sum_{i=1}^{q} \mathbf{k}_i w_i(\theta : c_D, c_E) + \epsilon \ .$$

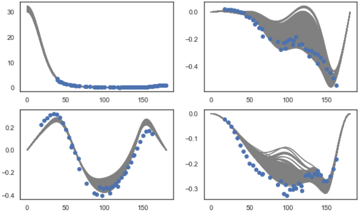
  2. 10 PC's are enough.
  3. Employ surmise to link emulation and calibration and run `emcee` sampler: preliminary calibration of c_D and c_E to nd data at 70 and 135 MeV.

- `calibration`: generates estimates of the calibration parameters based on field observations of the real process and an output from emulation

- "`utilities`": performs different utility tasks such as a sampler (e.g., Metropolis-Hastings) to generate posterior draws of calibration parameter



$E_{\mathrm{lab}} = 70$ MeV, with ^{3}H



$E_{\mathrm{lab}} = 135$ MeV, with ^{3}H

- We applied the SMS chiral NN potentials of Ref. Reinert 2018, along with the consistently regularized 3NF, both up to N^{2}LO in chiral EFT, to study selected observables in nd elastic scattering.
- Following the approach of Ref. BAND Github Repository, we have explored the use of a basic GP toolset for reducing the scattering observables predictive uncertainty by calibrating parameters, i.e.c_D and c_E potential parameters directly to the data and ^{3}H binding energy.
- We have found the impact of including NN LEC uncertainties on the c_D and c_E posterior is small.
- We have shown that the `surmise` library as part of the BAND framework allows to use Bayesian parameter estimation and propagation of uncertainties, for example, to draw error bands for the elastic neuron-deuteron predictions using chiral SMS NN+3NF at N^{2}LO order.