Bayesian methods in nuclear effective field theories

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The BUQEYE collaboration

Bayesian uncertainty quantification: errors for your EFT

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BUQ>EYE priorities

Full uncertainty quantification for low-energy nuclear theory (structure/reactions)

Using statistics and machine learning techniques to gain physics insight

Collaboration and coordination with experts in statistics/machine learning

Pushing through computational bottlenecks (mostly from theory calculations)
  - emulation/surrogates (gaussian processes, eigenvector continuation, etc.)
  - simplifications that ease computational burden

Informing experimental design from the theory side
Uncertainty Quantification in Nuclear Physics

To produce meaningful experimental measurements and theoretical predictions, it is essential to quantify uncertainties!

\[ y_{\text{th}} = y_{\text{exp}} + \delta y_{\text{exp}} + \delta y_{\text{th}} \]

Theory discrepancy:

- missing physics
- numerical/method errors
- fitting to uncertain data

Notes

- likely to be "systematic"
- not usually fully quantified
- often assumed to be normal

Experimental discrepancy:

- counting statistics
- background and selection effects
- systematic uncertainties

Notes

- systematic errors may not be well understood or inflated
- often assumed to be normal
Effective field theories are special

EFT convergence properties allow us to model theory discrepancies

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\[ y_{th} = y_{exp} + \delta y_{exp} + \delta y_{th} \]

Theory error consists of several (correlated) contributions

\[ \delta y_{th} = \delta y_k + \delta y_{LECs} + \delta y_{num} \]

Also the possibility of regulator artifacts, alternate power-counting, etc.
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A healthy EFT improves systematically with order

Ignore other uncertainty sources other than EFT truncation uncertainty \( \delta y_k \)

\[ y = y_{\text{ref}} \sum_{n=0}^{k} c_n Q^n + y_{\text{ref}} \sum_{n=k+1}^{\infty} c_n Q^n \]

theory calculation

where \( Q \sim \frac{p}{\Lambda_b} \) and \( c_n \)’s extracted from order-by-order calculations.
Status report 1: parameter estimation

EFTs have unconstrained parameters, the low-energy constants (LECs)

Strategy for nuclear interactions: constrain LECs using data

For an EFT at order $k$, let LECs be given by $\tilde{a}_k$

\[
\text{Interaction}(\tilde{a}_k) \rightarrow \text{ Observable calculation } \rightarrow \text{ Prediction}(\tilde{a}_k)
\]
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$$\text{Interaction}(\tilde{a}_k) \rightarrow \text{Observable calculation} \rightarrow \text{Prediction}(\tilde{a}_k)$$

Then compare the value with data

Adjust parameters $\tilde{a}_k$ according to favorite optimization procedure OR

Use a Bayesian approach and compute a parameter pdf for $\tilde{a}_k$
Status report 1: parameter estimation

nucleon-nucleon sector for chiral effective field theories

e.g. \( ^1S_0 \) channel at N\(^3\)LO (4 parameters)

Estimate LEC probability distribution

Markov Chain Monte Carlo (MCMC)

\[
\text{pr}(\vec{a}_k | D, I) \propto e^{-\chi^2/2}
\]

\[
\chi^2(\vec{a}_k) = \sum_{i=1}^{N} \left( \frac{d_i - y_k(p_i; \vec{a}_k)}{\sigma_i} \right)^2
\]

Bottleneck = theory calculation

This does not include \( \delta y_{th} \)
Status report 1: parameter estimation

Including theory discrepancy in the parameter estimation procedure

SW et al., JPG 46, 045102 (2019)

Use model of EFT truncation error to include $\delta y_{th}$

$$y = y_{ref} \sum_{n=0}^{k} c_n Q^n + y_{ref} \sum_{n=k+1}^{\infty} c_n Q^n$$

theory calculation

Assume a prior pdf on $c_n$s and marginalize to get

$$pr(\vec{a}_k | D, I) \propto e^{-\chi^2(\vec{a}_k)/2} = e^{-\frac{1}{2} (y_{exp} - y_{th}(\vec{a}_k))^T (\Sigma_{exp} + \Sigma_{th})^{-1} (y_{exp} - y_{th}(\vec{a}_k))}$$

Simple modified $\chi^2$ form under certain assumptions
Status report 1: parameter estimation

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SW et al., JPG 46, 045102 (2019)

Accounting for truncation error absorbs higher-order effects

Purple: not accounting for $\delta y_{th}$
Green: stabilizes when including $\delta y_{th}$
Status report 1: parameter estimation

The three-nucleon sector (fitting $C_D$ and $C_E$) [preliminary]

SW, Andreas Ekstrom, et al. 2020 [in preparation]

Data:

- energy/radius of $^4$He
- energy of $^3$H
- $^3$H $\beta$-decay half-life

Fixed NN potential: NNLO$_{sat}$

As before, including estimated $\delta y_{th}$

Not including uncertainty from NN sector
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Made possible by eigenvector continuation Frame et al., PRL 121 032501 (2018)
Status report 1: parameter estimation

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SW, Andreas Ekstrom, et al. 2020 [in preparation]
Status report 2: Truncation error and GPs

Further improve model of truncation error: include correlations

Jordan Melendez, SW, et al. PRC 100 044001 (2019)

Gaussian process model to study EFT truncation errors

For observables that vary over a continuous domain $x$

E.g., NN scattering observables in energy and angle $x = \{ E_{\text{lab}}, \theta \}$

$$y(x) = y_{\text{ref}}(x) \sum_{n=0}^{k} c_n(x)Q(x)^n + y_{\text{ref}}(x) \sum_{n=k+1}^{\infty} c(x)_n Q(x)^n$$

Still using lower-order convergence to inform missing corrections

E.g., truncation error at $E_{\text{lab}} = 50$ MeV won't be too different from 51 MeV
Status report 2: Truncation error and GPs

Good evidence in NN sector that truncation errors are well-modeled by GPs

Differential cross-section of np scattering, $E_{\text{lab}} = 150$ MeV

From order-by-order predictions from LO to N$^4$LO (5 orders)

GPs are random curves with some mean function and covariance kernel

Status report 2: Truncation error and GPs

A correlated vs. pointwise truncation error model
J. Melendez, SW, et al. PRC 100 044001 (2019)

Major feature: can use statistical validation tools to gain physics insight!
Status report 2: Truncation error and GPs

In preparation: Melendez, SW, et al. (2020)

Use GP model with modern NN potentials to diagnose convergence

This figure: toy problem

Estimate correlation length and EFT breakdown scale!

Currently applying diagnostics to modern NN potentials

Package gsum freely available to use: buqeye.github.io/software
More ongoing BUQYEBE projects

- Convergence analysis of infinite matter calculations
  Drischler, Melendez, Furnstahl, Phillips

- Bayesian experimental design for proton Compton scattering experiments
  Melendez, Furnstahl, Griesshammer, McGovern, Phillips

- Ongoing questions about Bayesian model selection in EFTs

See everything at buqeye.github.io
Summary and status

- Bayesian statistics is the ideal tool for effective field theories
- Build and include physics assumptions explicitly through Bayesian priors
- A data-driven study of theory expectations
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Gain physics insight from statistical tools
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Gain physics insight from statistical tools

- Continuing need for expertise in statistics and machine learning
- Model selection for EFTs? Power-counting comparison and diagnosis?
  - major bottleneck is observable computation
- Fully quantify uncertainties on EFT predictions
  - understand full correlation/interplay of all errors
  - easily usable approaches for nuclear structure practitioners