Moving forward with uncertainty quantification in ab-initio calculations using Bayesian methods

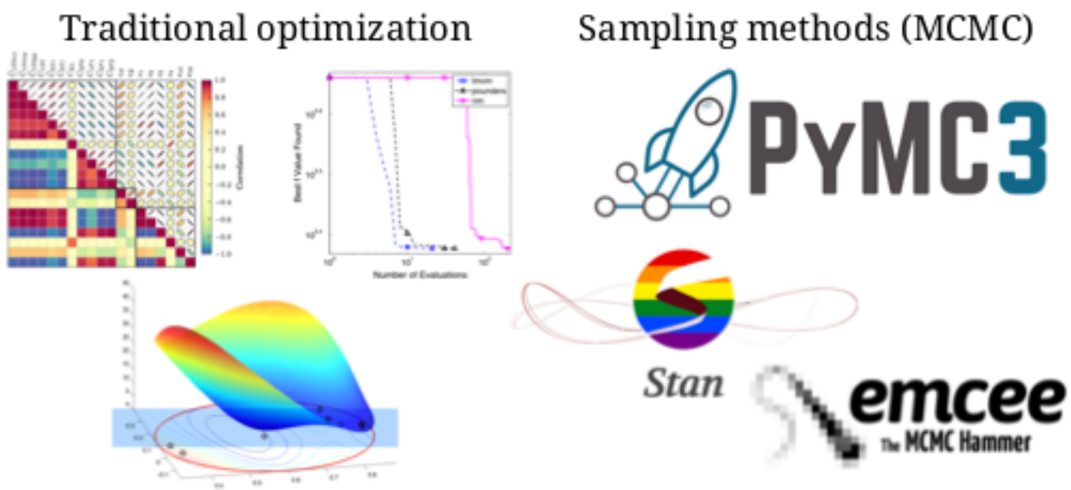
Sarah Wesolowski
Salisbury University

Nuclear Structure at the Crossroads, INT 2019

Salisbury UNIVERSITY

Designer nuclear forces in *ab initio* calculations

Status: Advances in optimization + need for reliable, usable interactions



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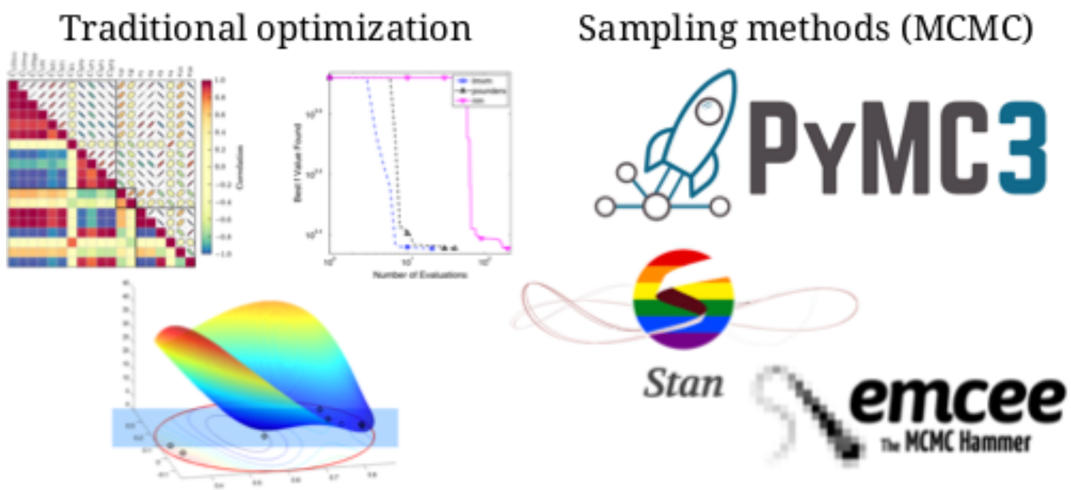


We are in an era of Designer (EFT) Interactions

Need practical, usable interactions for a variety of calculations

Change input data, formulation, regulators (by sector) to suit the calculation

Well-known fact: this is not consistent with a true EFT philosophy

Designer nuclear forces in *ab initio* calculations

Practical structure calculations (chiral EFT)

More traditional fits to few-body data

- Epelbaum, Krebs, Meißser, Reinert (up to 3N)
  (RKE) Reinert et al., EPJ A 54 (2018)
  (EKM) Epelbaum et al., EPJ A 51 (2015)
  Binder et al. PRC **98**, 014002 (2018)
  (+3N) Epelbaum et al., PRC 99, 024313 (2019)
- NNLOsim/sep (up to 3N)
  Carlsson et al., PRX **6** 011019 (2016)
- Entem, Machleidt, and Nosyk (NN)
  Entem et al., PRC 96, 024004 (2017)
- BUQEYE: recent Bayesian exploration (NN)
  Wesolowski et al., JPG 46, 045102 (2019)
- Local interactions (up to 3N + Deltas)
  Piarulli at al., PRC 91, 024003 (2015), Piarulli et al., PRL 120, 052503 (2018)

Useful for medium-mass/nuclear matter

- NNLOsat (up to 3N)
  Ekström et al., PRC 91, 051301 (2015)
- "Hebeler+" for nuclear matter (up to 3N)
  Hebeler et al., PRC 83, 031301(R) (2011)
  Drischler et al, PRL 122 042501 (2019)

But what about... RG invariance??

Explorations of power counting have (mostly) diverged from the many-body calculations

- Kaplan, Savage, and Wise (1998)
  Kaplan et al., Nuc. Phys. B 534 (1998)
- Nogga, Timmermans, Van Kolck (2005)
  Nogga et al., PRC 72 054006 (2005)
- Recent work (not in agreement)
  M. Sánchez Sánchez et al., Phys. Rev. C 97 024001 (2018)
  Epelbaum et al., EPJ A 54 11 (2018)
  S. Wu and B. Long, PRC 99 024003 (2019)

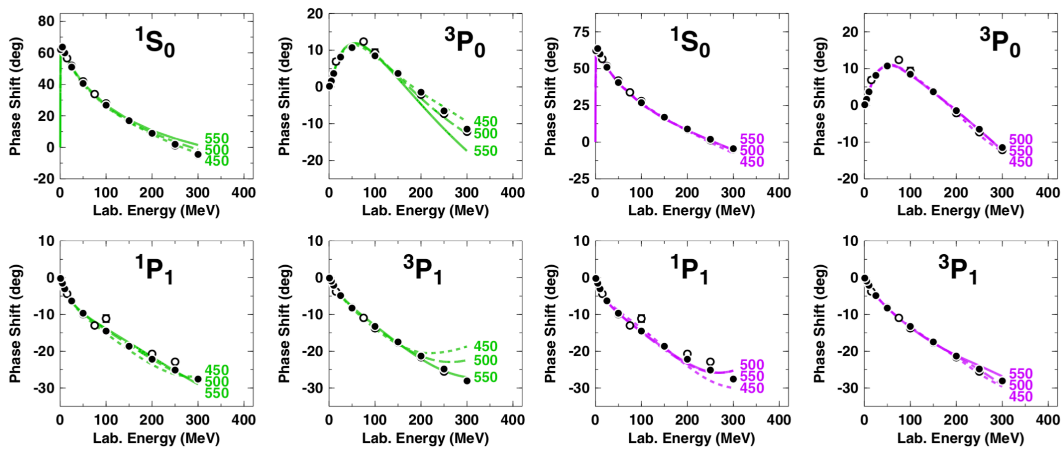
- Recent collaboration for nuclear structure (NCSM) calculations J. Yang + Chalmers

- Practitioners of nuclear structure need matrix elements and the ability to evaluate higher order observables perturbatively

(I tried to make this useful and representative but it is not exhaustive)

Issues with chiral forces currently in use

1. Calculations are not independent of the cutoff. Is this ok?



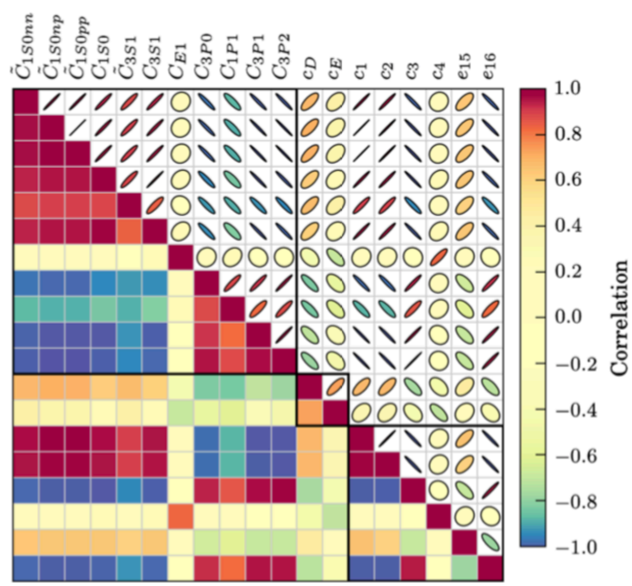
Entem et al., PRC 96 024004 (2017)

- Spread is lower as order is increased. BUT: lots of LECs = overfitting?
- Cutoff variation = lower bound on error
- If NN/NNN sector are overfit: impact on nuclei/ nuclear matter??

Issues with chiral forces currently in use

2. Fitting has advanced, but need more than just the LEC values

Correlations and uncertainty are important for error propagation.

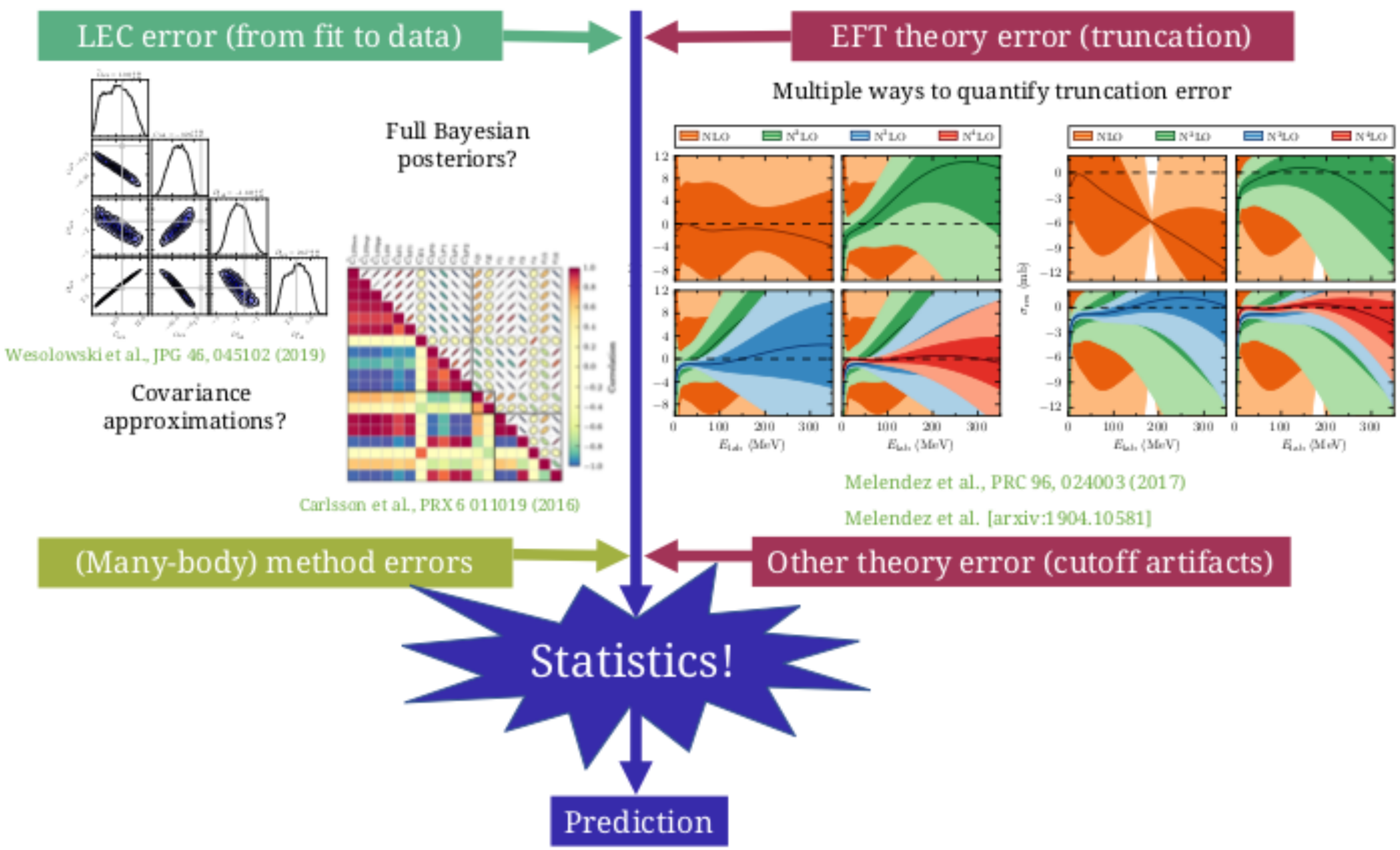


NNLOsim covariance matrix, Carlsson et al., PRX 6 011019 (2016)

Also, what to use in the πN sector?
Roy-Steiner as inputs? Informative priors? Hoferichter at al., PRL 115, 192301 (2015)

Issues with chiral forces currently in use

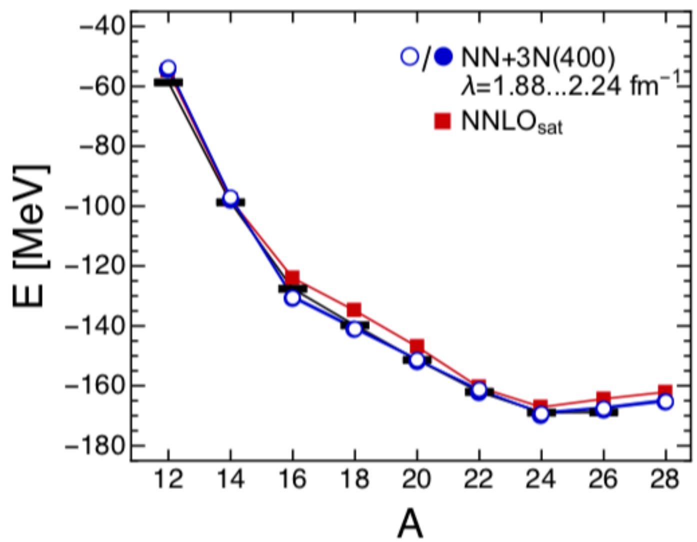
3. Even with LEC uncertainty/correlations, how to combine all errors?

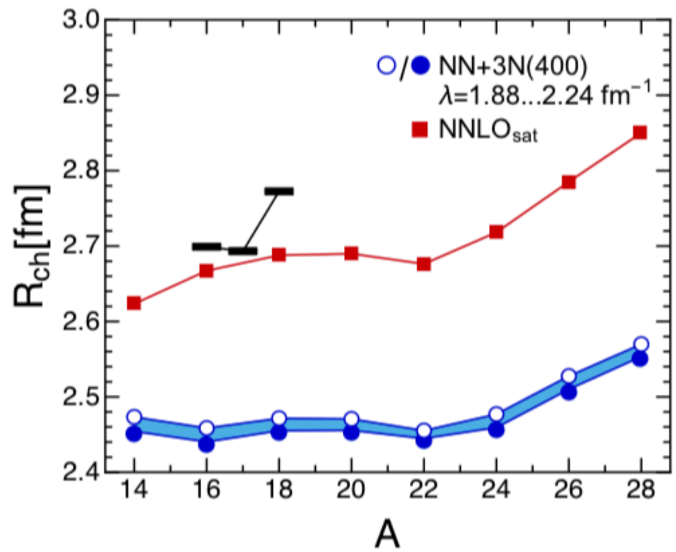


Issues with chiral forces currently in use

4. Are different interactions consistent to within those uncertainties?

Comparing two different input nuclear Hamiltonians
Even oxygen isotope ground states and charge radii





Hergert et al., J. Phys.: Conf. Ser. 1041 012007, (2018)
Comparing NN+3N(400) of Gazit et al., PRL 103, 102502 (2009)
and NNLOsat of Ekstrom et al., PRC 91(5) 051301 (2015)

BUQEYEs at the crossroads?

Stands for: "Bayesian Uncertainty Quantification: Errors in Your EFT"
Current/active members

Dick Furnstahl, Jordan Melendez
Matt Pratola (Statistics)

Daniel Phillips

Sarah Wesolowski

BUQEYEs+friends: N. Klco, C. Drischler, H. Hergert, H. Grießhammer, S. König, A. Ekström, C. Forssén...

Statistical/data-driven approaches are critical tools for theory efforts.

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Most obvious: uncertainty quantification (UQ) for observables

Less obvious: using statistical analysis as a validation tool for theory

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For EFTs, Bayesian approaches are useful due to theory expectations

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For EFTs, Bayesian approaches are useful due to theory expectations

Validate by testing the fulfilment of expectations

(codified in a Bayesian framework)

What is Bayesian statistics?

Basic idea: interpret probability as a state of information

This allows treatment of many types of quantities as random variables

Assumptions can be included explicitly as probability distributions

What I'll highlight here

1. Statistical model for EFT theory (truncation) errors
2. Validation and testing (Being able to tell when are things going wrong!)
3. How can model selection help us moving foward?

Discrepancy model for EFT predictions

Describing observables with theory:

$$\boldsymbol{y}_{\text{exp}} = \boldsymbol{y}_{\text{th}} + \delta\boldsymbol{y}_{\text{th}} + \delta\boldsymbol{y}_{\text{exp}}$$

Totally agnostic to formulation of theory and how the discrepancies behave.

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Totally agnostic to formulation of theory and how the discrepancies behave.

Other sources of error can be included

E.g., numerical errors

$$\boldsymbol{y}_{\text{exp}} = \boldsymbol{y}_{\text{th}} + \delta\boldsymbol{y}_{\text{th}} + \delta\boldsymbol{y}_{\text{num}} + \delta\boldsymbol{y}_{\text{exp}}$$

Discrepancies are random variables (possibly correlated!)

Big question: how to describe discrepancies mathematically?

Discrepancy model for EFT predictions

A properly formulated EFT has systematic theory error

$$\boldsymbol{y}_{\rm exp} = \boldsymbol{y}_{\rm th} + \delta\boldsymbol{y}_{\rm th} + \delta\boldsymbol{y}_{\rm exp}$$

Statistical model for EFTs: predictions/errors at the level of observables

$$y_{\rm th} = y_{\rm ref} \sum_{n=0}^{k} c_n Q^n \qquad \delta y_{\rm th} = y_{\rm ref} \sum_{n=k+1}^{\infty} c_n Q^n$$

(This can also handle subdominant contributions from non-analytic terms.)

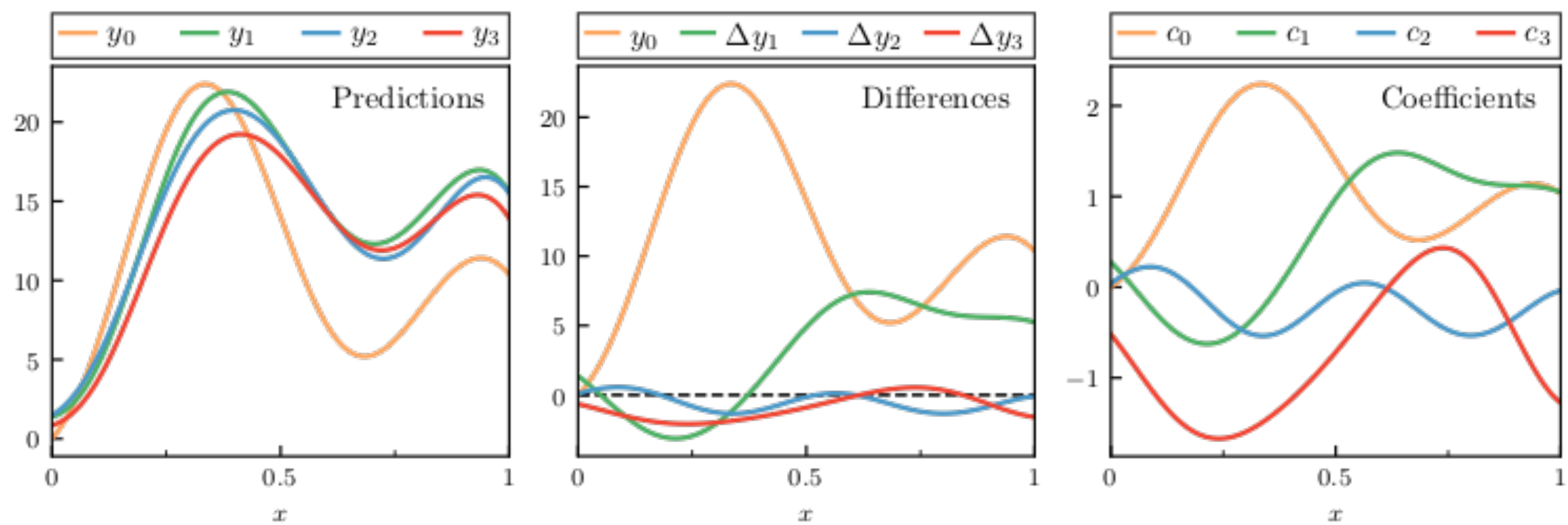
Note: assuming prescription for $Q = \{p, m_\pi\}/\Lambda_b$ and particular values of Λ_b

Does the statistical discrepancy model make sense?

$$y_{\text{th}} = y_{\text{ref}} \sum_{n=0}^{k} c_n Q^n$$

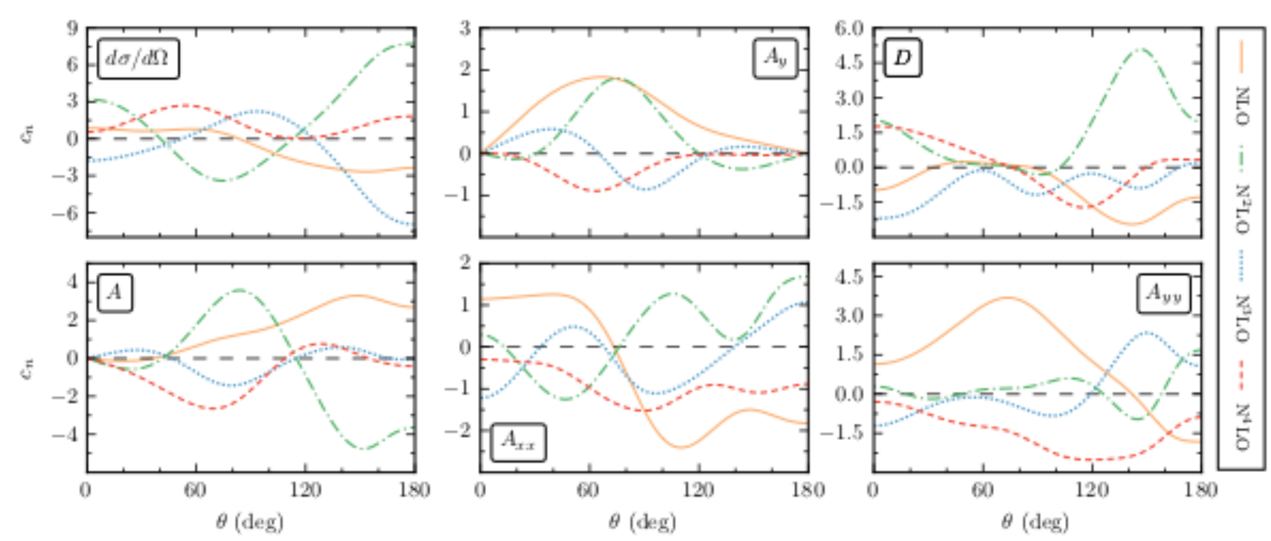
$$\rightarrow y_k(x) = y_{\text{ref}}(x) \sum_{n=0}^{k} c_n(x)\, x^n$$

Order-by-order toy observable as a function of a kinematic parameter x



Do real EFT predictions behave like this?

np scattering observables at $E_{\rm lab} = 96\,{\rm MeV}$, extracted coefficients



computed using SCS interaction of Epelbaum, Krebs, Meißner with $R = 0.9\,{\rm fm}$ and $\Lambda_b = 600\,{\rm MeV}$; Epelbaum et al., EPJ A 51 (2015), Epelbaum et al., PRL 115 122301 (2015)

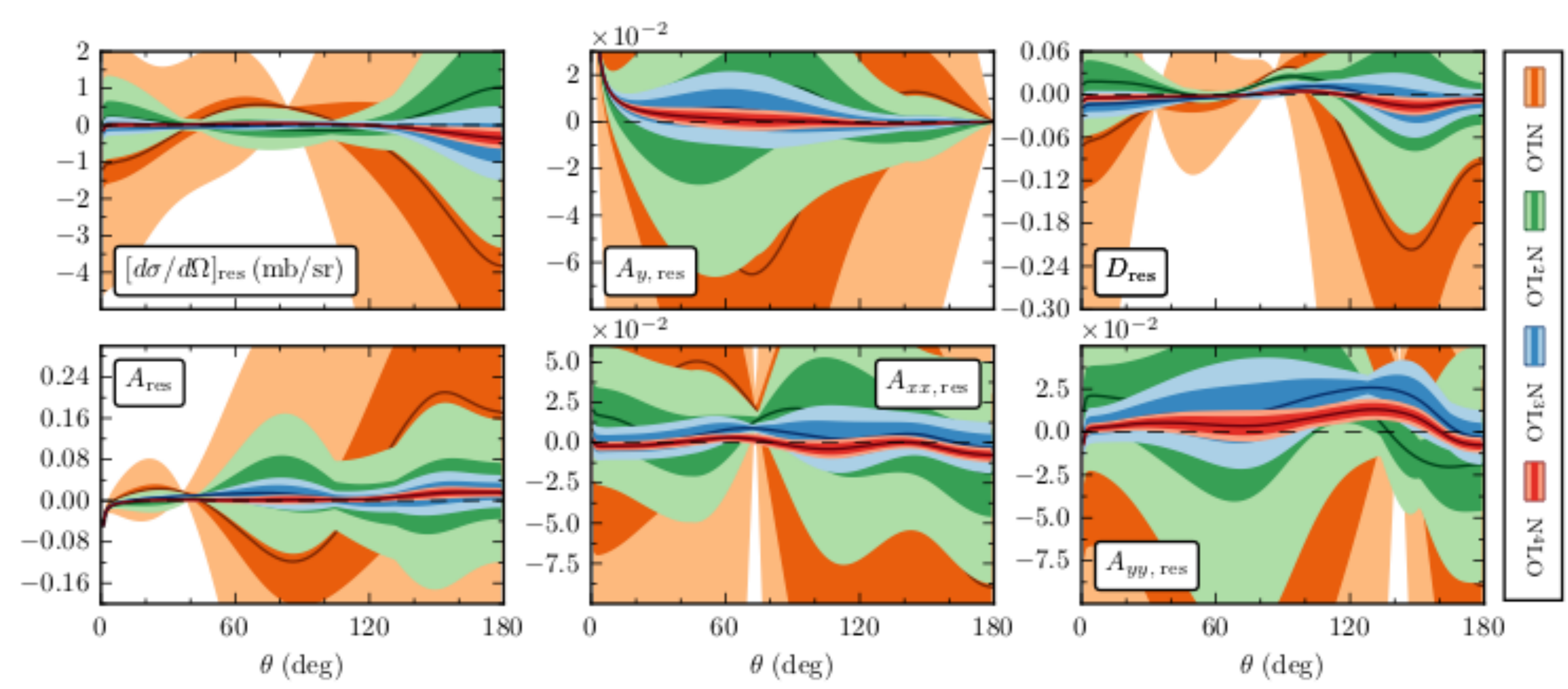
Figures courtesy of Jordan Melendez, OSU, See arxiv:1904.10581 by Melendez, SW et al. and Melendez, SW et al., PRC 96, 024003 (2017) [Editor's suggestion]

Use the natural behavior of these coefficients to predict missing higher orders.

Assigning truncation error

Using prescriptions detailed in Melendez, SW et al., PRC 96, 024003 (2017) [Editor's suggestion]

Plot of residuals: theory - NPWA value, Dark band: 68%, Light band: 95%



Predictions converge how we would expect in an EFT...

Is the EFT really well-behaved?

If the EFT itself has issues, the statistical model of truncation error is invalid

How can we tell when things are going wrong?

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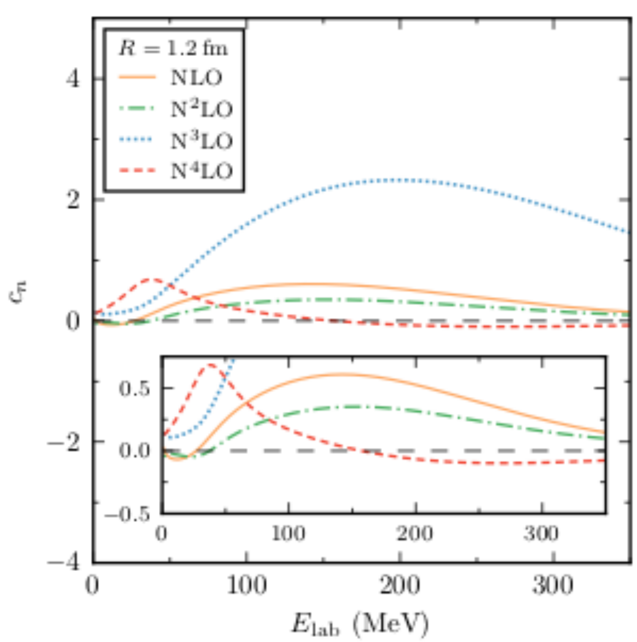
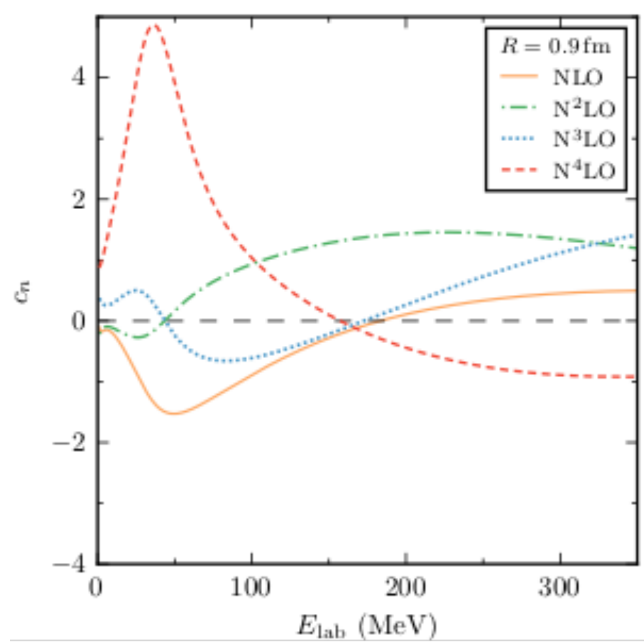
How can we tell when things are going wrong?

Total np cross section coefficients using SCS interactions from LO to N4LO



$R = 1.2$ fm, $\Lambda_b = 400\,\mathrm{MeV}$



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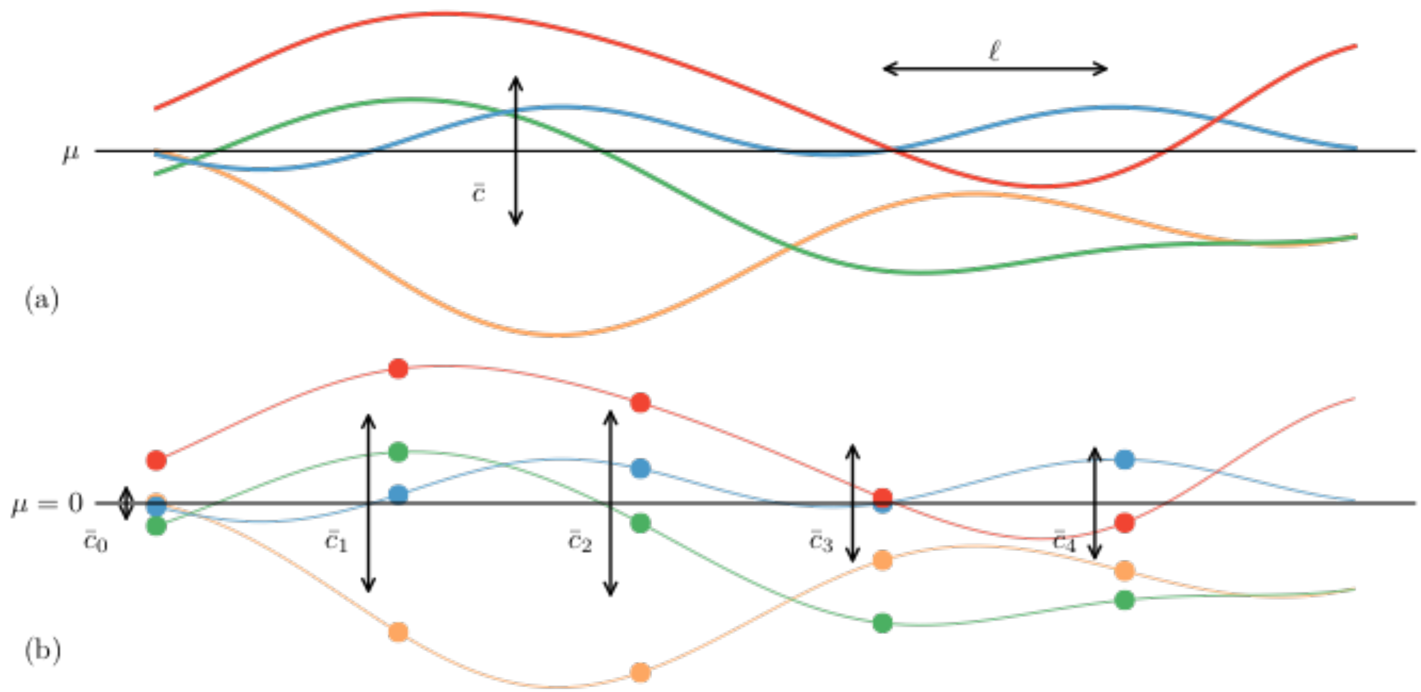
Additional complication: Correlations are important

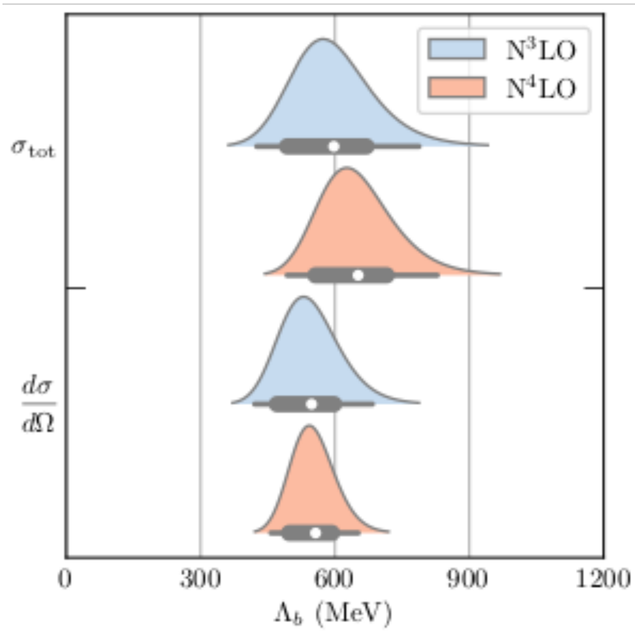
In general, we need to consider finite correlation length for truncation errors

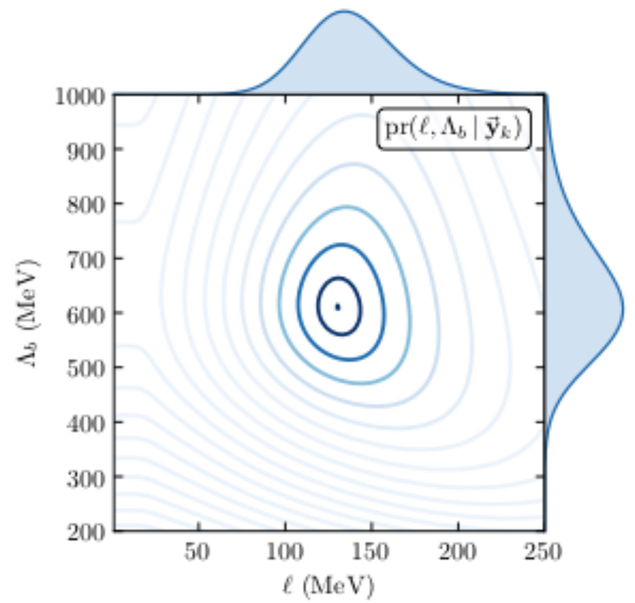
Use Gaussian processes, a non-parametric tool, to model truncation error



Posteriors for the chiral EFT breakdown scale

Using the expected EFT convergence pattern, use order-by-order calculations to estimate the pdf of the breakdown scale and correlation length





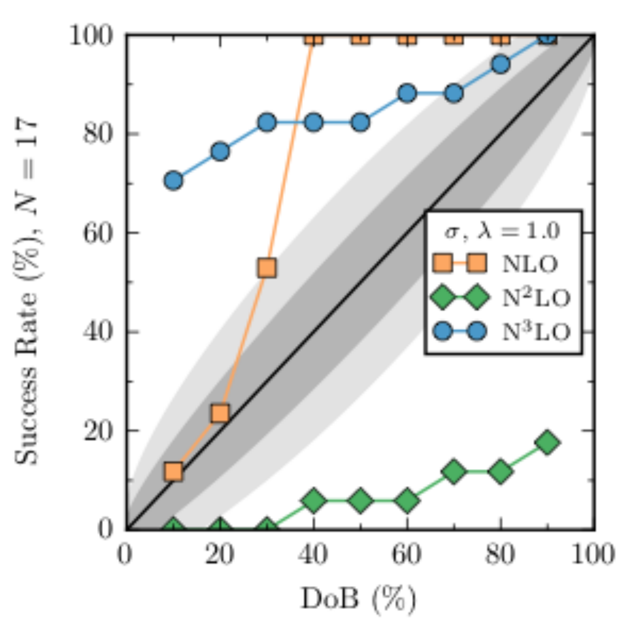
For all this and more: arxiv:1904.10581 by Melendez, SW et al.
See also the gsum package: https://github.com/buqeye

Validation: determining when something is wrong

Validation example: Empirical coverage plots

A p% error band should cover the true value about p% of the time

We should neither under- or over-estimate error bands



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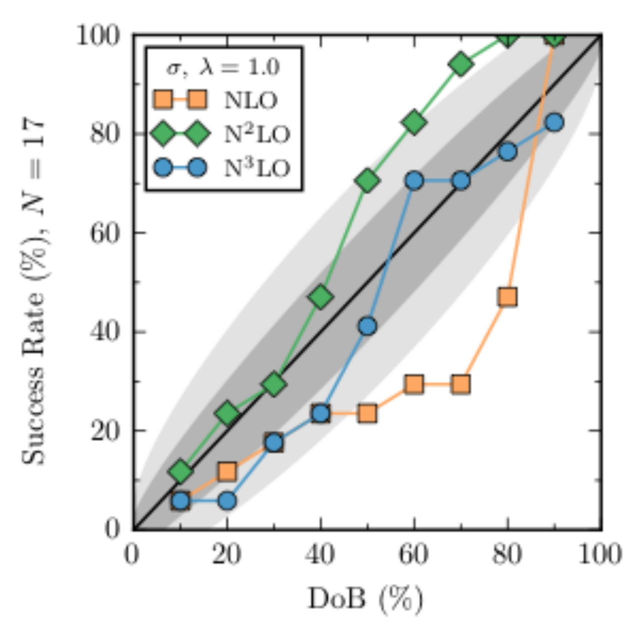

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More with Bayes

A theoretical calculation involves a vector of parameters $\vec{a}$
Estimate them using some experimental data D
Information I contains all background, e.g., EFT regularization scheme used

1. Parameter estimation: calculate *posterior* probability distribution (pdf)

$$\mathrm{pr}(\vec{a}|D, I) = \frac{\mathrm{pr}(D|\vec{a}, I)\,\mathrm{pr}(\vec{a}|I)}{\mathrm{pr}(D|I)}$$

2. Model selection: can it help us in EFTs?

Evidence ratio: two competing (statistical) models

$$\frac{\mathrm{pr}(M_1|D, I)}{\mathrm{pr}(M_2|D, I)} = \frac{\int d\vec{a}_1\, \mathrm{pr}(D|\vec{a}_1, I)\,\mathrm{pr}(\vec{a}_1|I)}{\int d\vec{a}_2\, \mathrm{pr}(D|\vec{a}_2, I)\,\mathrm{pr}(\vec{a}_2|I)}$$

(Assuming both "models" are *a priori* equally probable)

Depending on the case, these integrals can be very hard to evaluate.

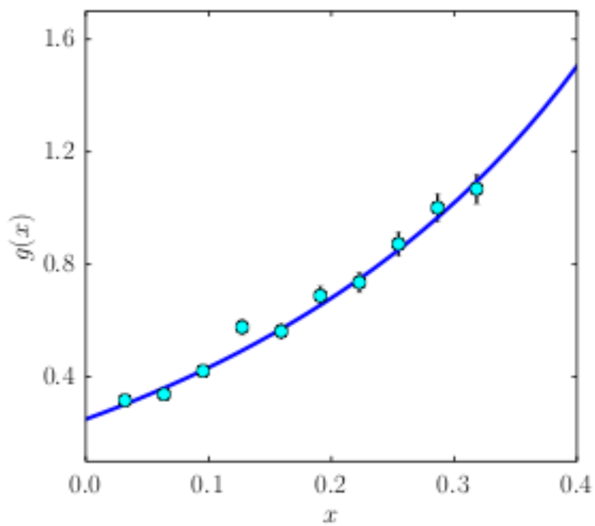
Model selection

Promising application for EFT model problem

fitting a Taylor series expansion with natural coefficients to synthetic data

Question: how many coefficients can be estimated from a given dataset?

Toy example: a Taylor series in x for a function g that converges for $x \leq 1$



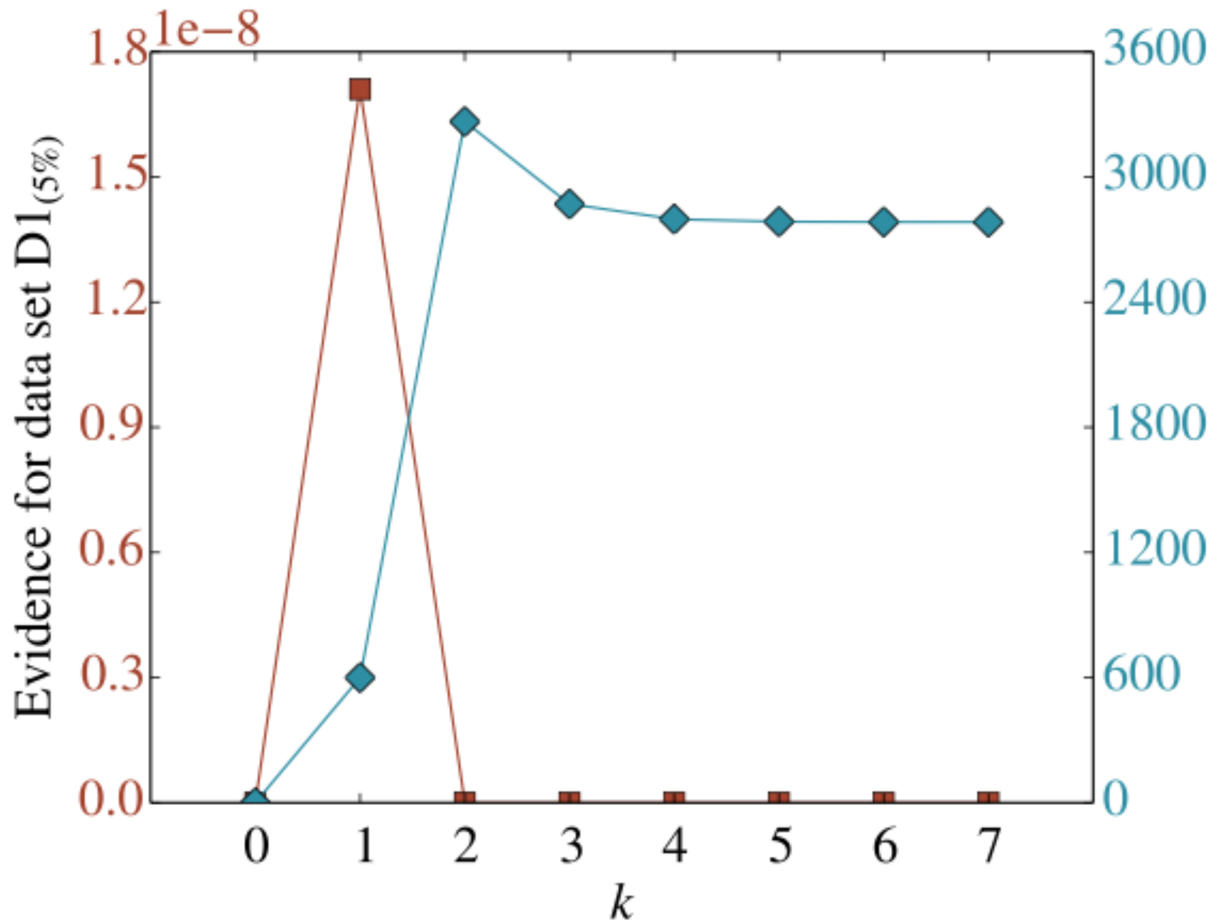
$$g_{\mathrm{th}}(x) = \sum_{n=0}^{k} a_n x^n$$

How many a_ns can be extracted?

Use Bayesian evidence ratio to test this...

Model selection

Including naturalness prior on LECs vs not including one



Summary and looking forward

- Bayesian statistics allows inclusion and testing of physics expectations
- Not just uncertainty quantification, but also validation
- We have implemented and tested a statistical model for truncation errors
  - Application to NN in Melendez et al., PRC 96, 024003 (2017)
  - Latest!! Gaussian processes arxiv:1904.10581
- Statistical exploration of 3NFs fit to few-body data with consistent inclusion of truncation error

Christian Forssén
Andreas Ekström

CHALMERS
UNIVERSITY OF TECHNOLOGY

- Model selection: lots of possible avenues to explore in power counting, Deltas, pionless, ...
- Quantifying uncertainties in MR IMSRG calculations

Heiko Hergert

MICHIGAN STATE
UNIVERSITY

Example: parameter estimation

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Often can't be calculated directly: use Bayes theorem to rearrange

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$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{evidence}}$$

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Example: parameter estimation

Relationship to standard least-squares

$$\mathrm{pr}(\vec{a}|D, I) = \frac{\mathrm{pr}(D|\vec{a}, I)\,\mathrm{pr}(\vec{a}|I)}{\mathrm{pr}(D|I)} \propto \mathrm{pr}(D|\vec{a}, I)\,\mathrm{pr}(\vec{a}|I)$$

$$\mathrm{pr}(\vec{a}|D, I) \propto e^{-\chi^2/2}\,\mathrm{pr}(\vec{a}|I)$$

If the prior is uniform (i.e. flat) in $\vec{a}$ space

$$\mathrm{pr}(\vec{a}|D, I) \propto e^{-\chi^2/2}$$

Minimizing χ^2 corresponds to maximizing the probability (likelihood)

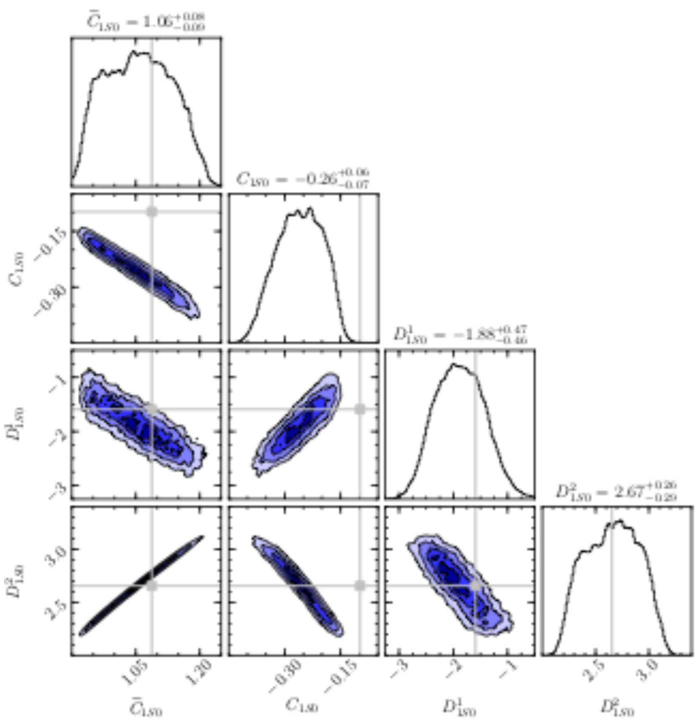
$$\chi^2(\vec{a}) = \sum_{i=1}^{N_d} \frac{r_i(\vec{a})^2}{\sigma^2_{\mathrm{exp},i}}$$

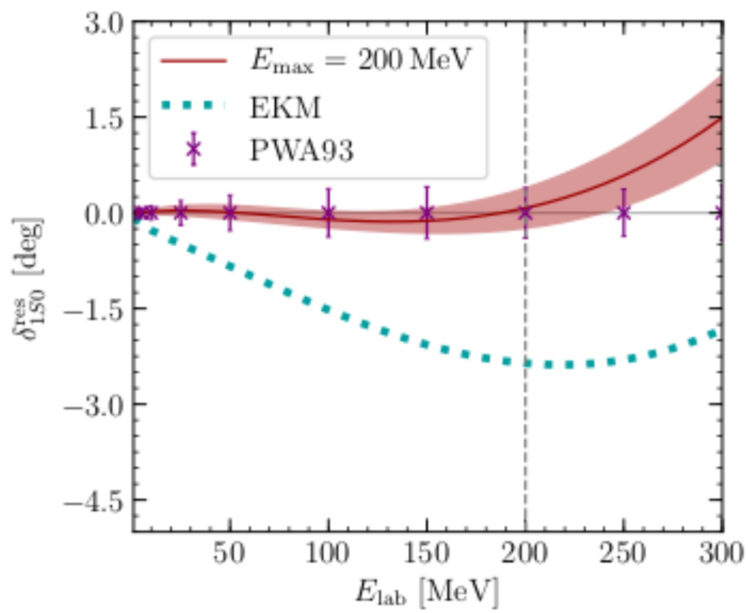
where $\mathbf{r}(\vec{a}) = \boldsymbol{y}_{\mathrm{exp}} - \boldsymbol{y}_{\mathrm{th}}(\vec{a})$ (difference between expt. and theory)

But the prior and likelihood can be more complicated!

An operator redundancy uncovered

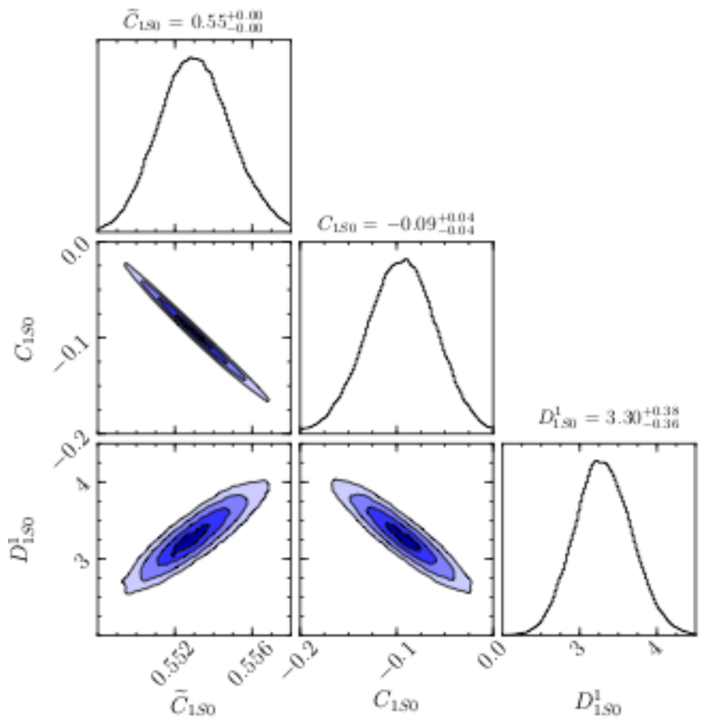
$$\mathrm{pr}(\vec{a}_k \,|\, \boldsymbol{y}_{\mathrm{exp}}, \Sigma_{\mathrm{exp}}) \propto \exp\left[-\frac{1}{2}\sum_{i=1}^{N_d} \frac{r_i^2}{\sigma_i^2}\right] \times e^{-(\vec{a}_k)^2/2\bar{a}^2}$$

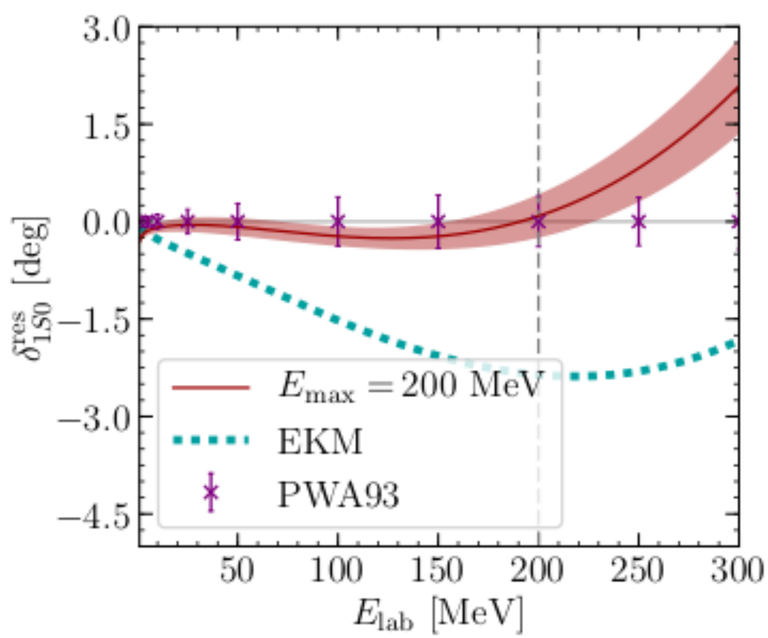




Wesolowski et al., JPG 46, 045102 (2019)

An operator redundancy uncovered





The $^1S_0$ channel at fourth order (N^3 LO), (also applies for $^3S_1$, $^3S_1 - {}^3D_1$)

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

An operator redundancy uncovered

At fourth order in the expansion, this term vanishes on-shell

$$\begin{aligned}\langle {}^1S_0|V_{NN}|{}^1S_0\rangle &= D^1_{1S0}p^2p'^{\,2} + D^2_{1S0}\,(p^4 + p'^{\,4}) \\ &= \frac{1}{4}(D^1_{1S0} + 2D^2_{1S0})(p^2 + p'^{\,2})^2 - \frac{1}{4}(D^1_{1S0} - 2D^2_{1S0})(p^2 - p'^{\,2})^2\end{aligned}$$

Non-perturbative calculation, not as clear that this does not contribute to two-body observables in χEFT (vs. e.g., pionless)

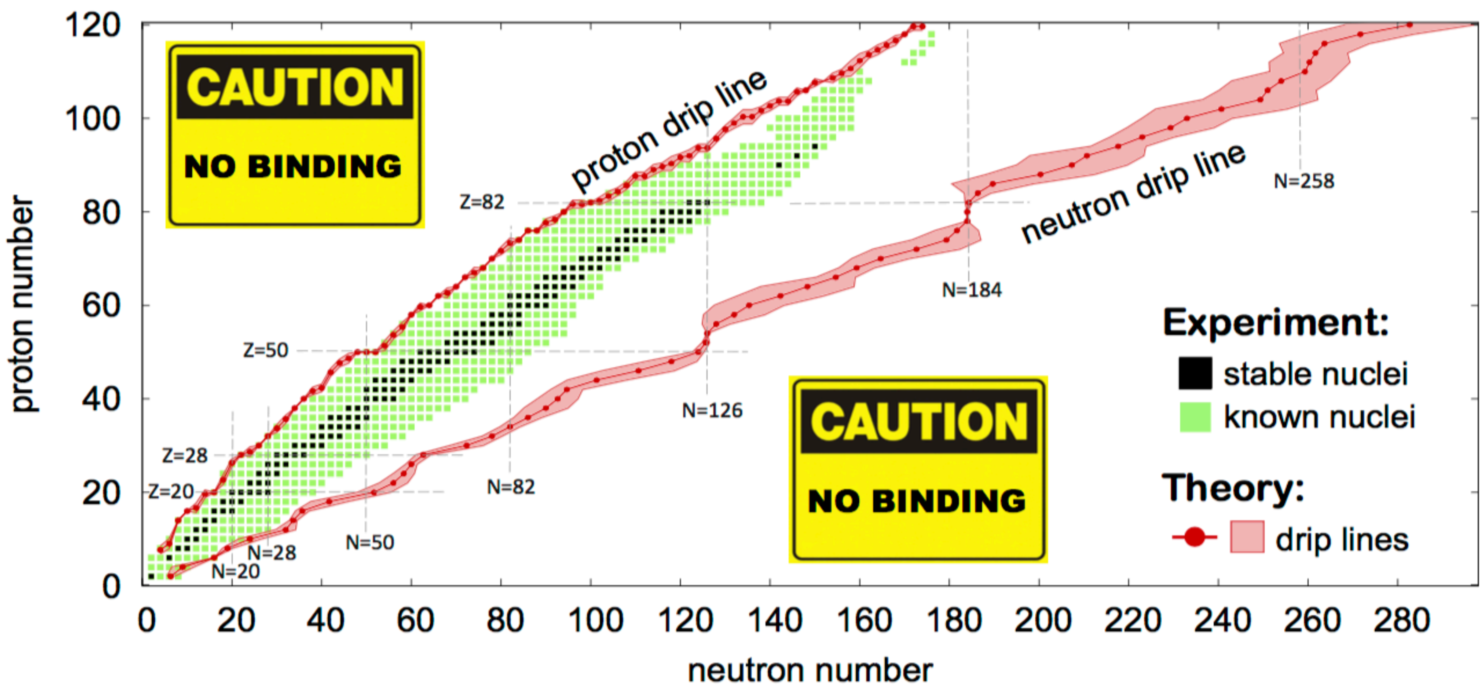
Removing a linear combination of D^1_{1S0}, D^2_{1S0} should remove the redundancy

We choose to set $D^2_{1S0} = 0$, last slide confirmed results not sensitive

Further confirmed by Reinert et al. using unitary transformations

First-principles calculations of nuclei

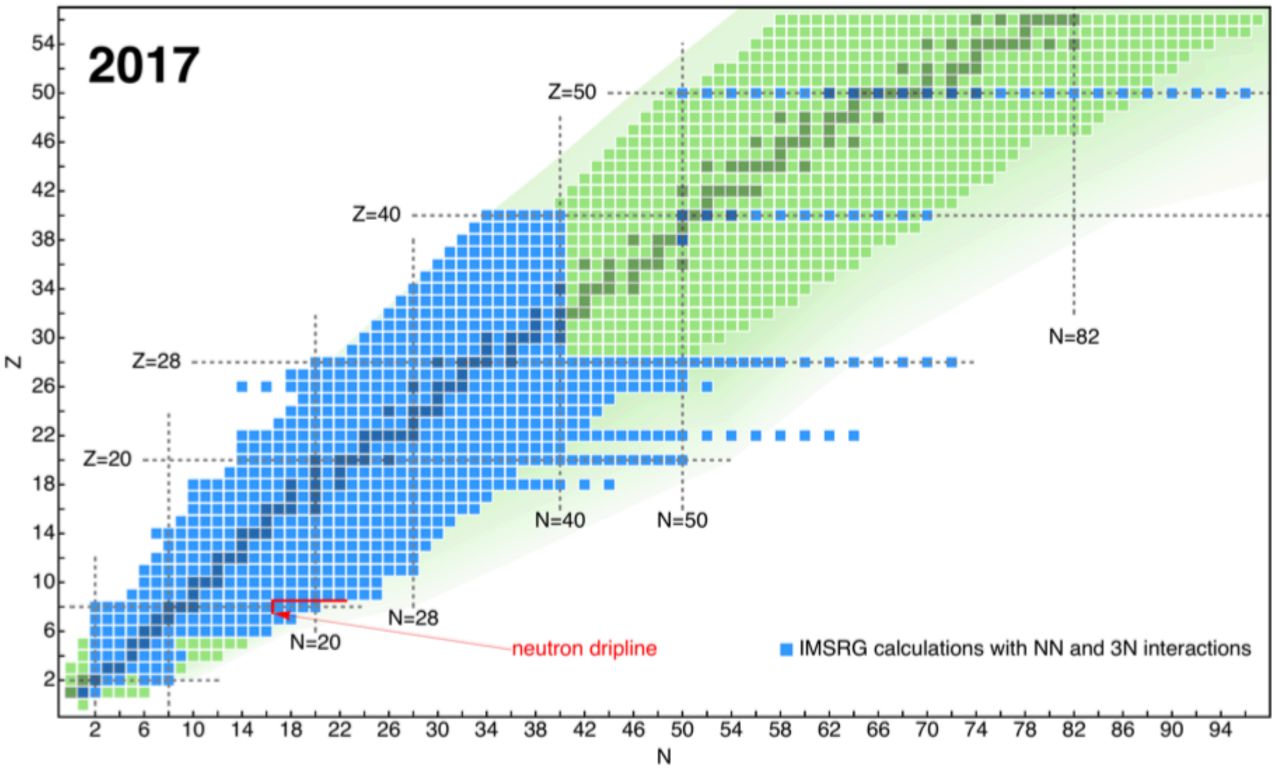
Pushing the frontiers of precision *ab initio* calculations



Nuclear landscape figure from the 2015 NSAC Long Range Plan

First-principles calculations of nuclei

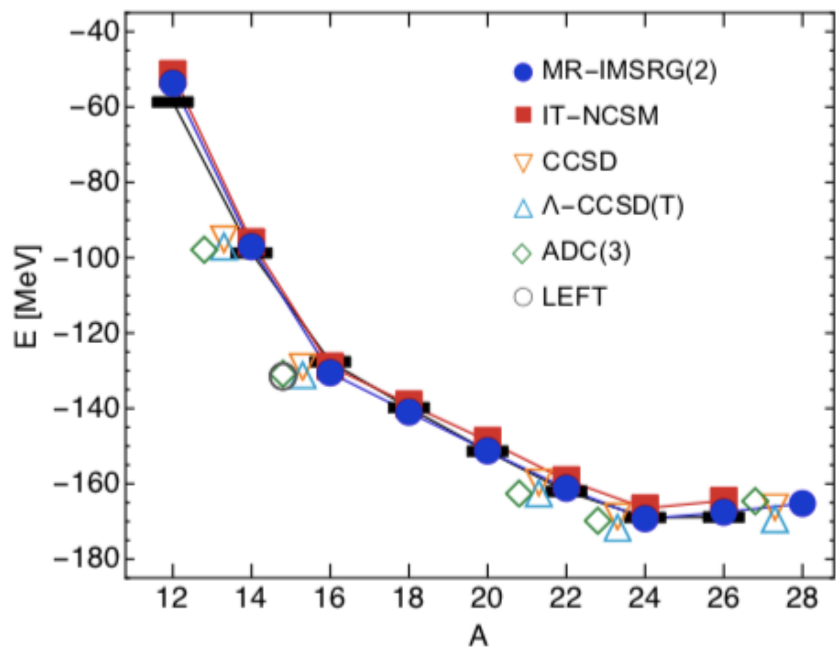
Limits of nuclear predictions with the In-medium Similarity Renormalization Group (IMSRG) as an example



Hergert et al., J. Phys.: Conf. Ser. 1041 012007, (2018)

First-principles calculations of nuclei

Different *ab initio* calculations of even oxygen isotope ground states



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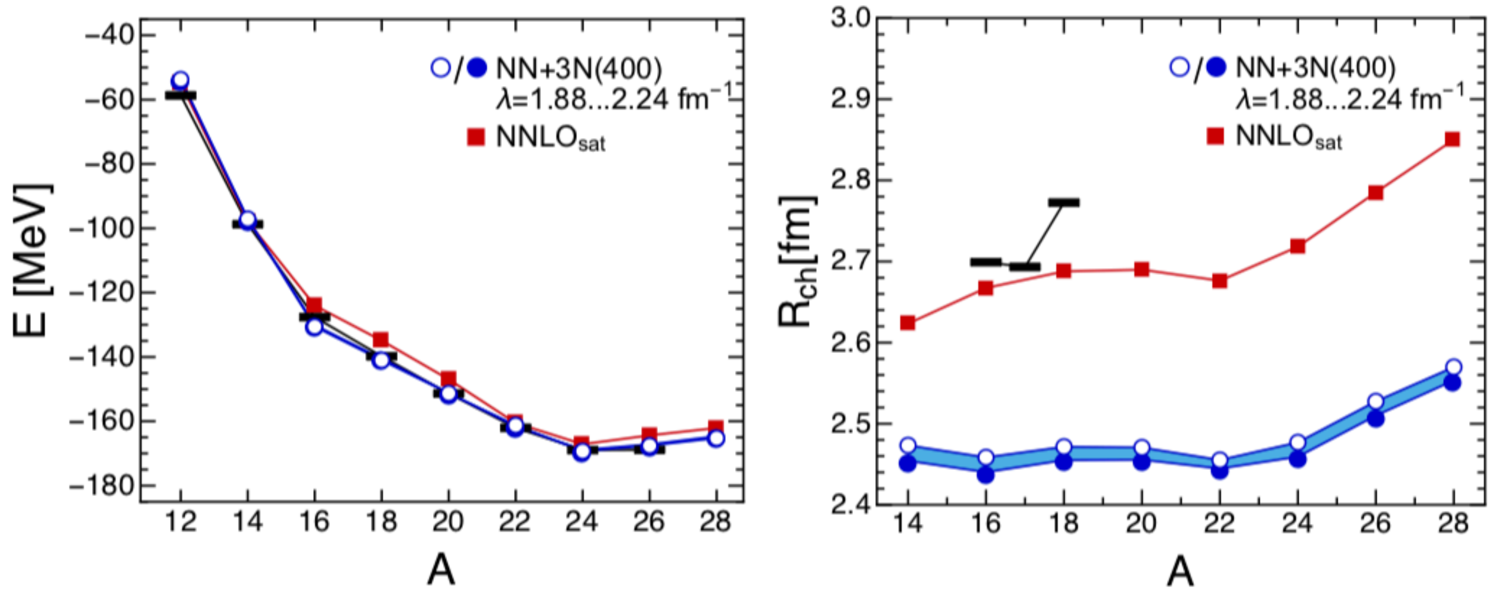
First-principles calculations of nuclei

Comparing two different input nuclear Hamiltonians

Even oxygen isotope ground states and charge radii



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Comparing theory and experiment

- Predictions need uncertainty estimates
- Comparison is unclear without them
- Statistical interpretation? When do we decide something is inconsistent?
- Is it acceptable to provide theory calculations without uncertainty estimates for nuclear calculations?

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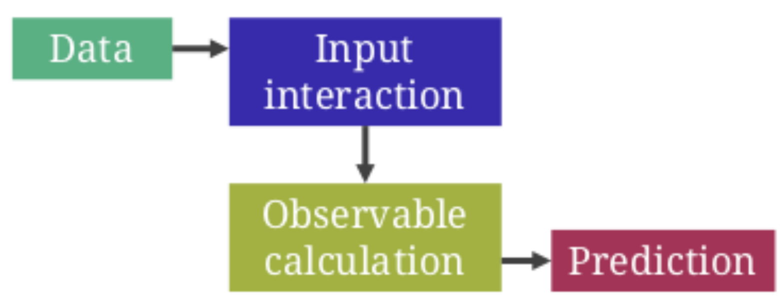
PRA Editorial from 2011:

> It is not unusual for manuscripts on theoretical work to be submitted without uncertainty estimates for numerical results. In contrast, papers presenting the results of laboratory measurements would usually not be considered acceptable for publication in Physical Review A... graphical presentation of data is always accompanied by error bars for the data points. The determination of these error bars is often the most difficult part of the measurement. Without them, it is impossible to tell whether or not bumps and irregularities in the data are real physical effects, or artifacts of the measurement.

First-principles calculations of nuclei



- The major limitation is the input interaction
- What is the flow from data to prediction?
- Strategy: focus on light nuclei to make progress and understand input nuclear interactions
- This talk: nucleon-nucleon (NN) force, two-body problem
- Ongoing work: looking at few-body bound states

Consistent treatment of theory uncertainties

Major goals

1. Understand and quantify all sources of uncertainty in a theory prediction. "Uncertainty quantification" (UQ)

2. Use statistics to validate theory

   - appropriate agreement of theory with experiment
   - validate theory expectations, recognize issues with the theory

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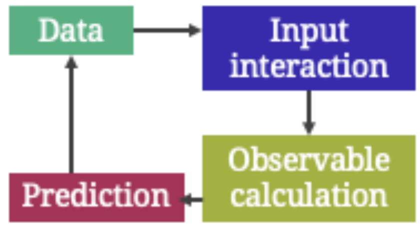
Need to understand interplay of calculation and inputs

1. Uncertainty in data used to constrain interactions
2. Limitations of interaction (theory uncertainty)
3. Limitations of quantum many-body method
4. ...Anything else!

These are often correlated!

Procedure of constraining a theory



- Errors in theory and calculation enter when constraining the theory

$$y_{\text{exp}} = y_{\text{th}} + \delta y_{\text{th}} + \delta y_{\text{exp}} + \delta y_{\text{num.}}$$

- Standard least-squares for theory parameters $\vec{a}$ (assume $\delta y_{\text{th}}, \delta y_{\text{num.}} = 0$)

$$\chi^2(\vec{a}) = \sum_{i=1}^{N_d} \frac{r_i(\vec{a})^2}{\sigma^2_{\text{exp},i}}$$

where $\mathbf{r}(\vec{a}) = y_{\text{exp}} - y_{\text{th}}(\vec{a})$

- But where do you put the theory error? Add (in quadrature) to the experimental error? *Ad hoc* weighting?

Statistical analysis the Bayes way

$$\mathrm{pr}(A|B,I) = \frac{\mathrm{pr}(B|A,I)\mathrm{pr}(A|I)}{\mathrm{pr}(B|I)} \Longrightarrow \underbrace{\mathrm{pr}(x|\mathrm{data},I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(\mathrm{data}|x,I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(x|I)}_{\text{prior}}$$

Why use Bayesian statistics?

- Fitting: conventional optimization recovered as special case
- Update expectations using Bayes' theorem when have more information
- Assumptions are made explicit (e.g. naturalness of LECs)
- Clear prescriptions for combining errors
- Statistics as diagnostics for physics
- Model checking: we can test if our UQ model works and study sensitivities
- Model selection: Is the Delta needed? Pionless vs. pionful formulations, ...
- Particularly well suited for (any) EFT, generally suited for theory errors

Interlude: Effective field theory

Effective field theory (EFT), implemented correctly, is model independent

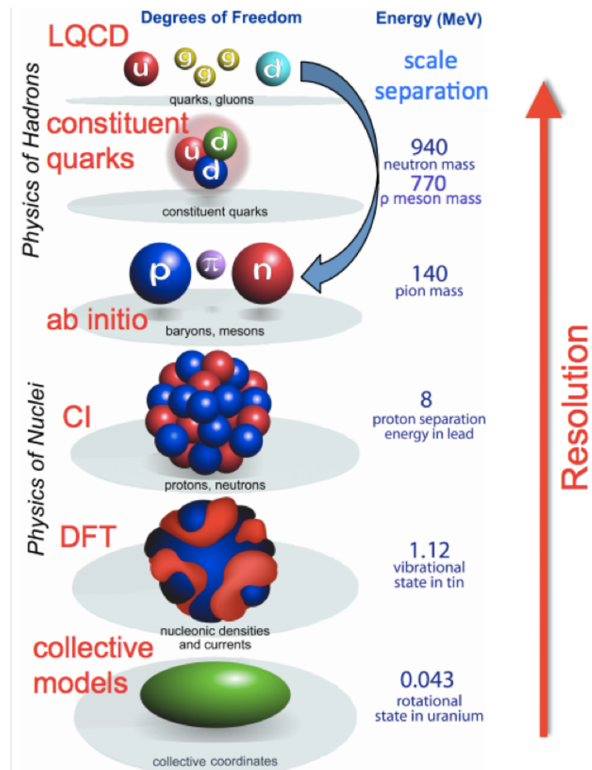
Approximate high-resolution details in terms of low-resolution degrees of freedom

Infinite series of operators, organized by the power counting

Price: infinite, natural-sized parameters, called "low-energy constants" (LECs)

Use nucleon (and pion) degrees of freedom: χPT (one baryon) $\rightarrow$ χEFT (> one baryon)

χEFT implemented in practice as a (non-relativistic) potential



Interlude: Effective field theory

Model of a properly constructed, well-behaved EFT, truncated at order k:

$$y_{\rm th} = y_{\rm ref} \sum_{n=0}^{k} c_n Q^n$$

where the expansion parameter $Q = \{p, m_\pi\}/\Lambda_b$ (for χEFT)

Error from truncation is then

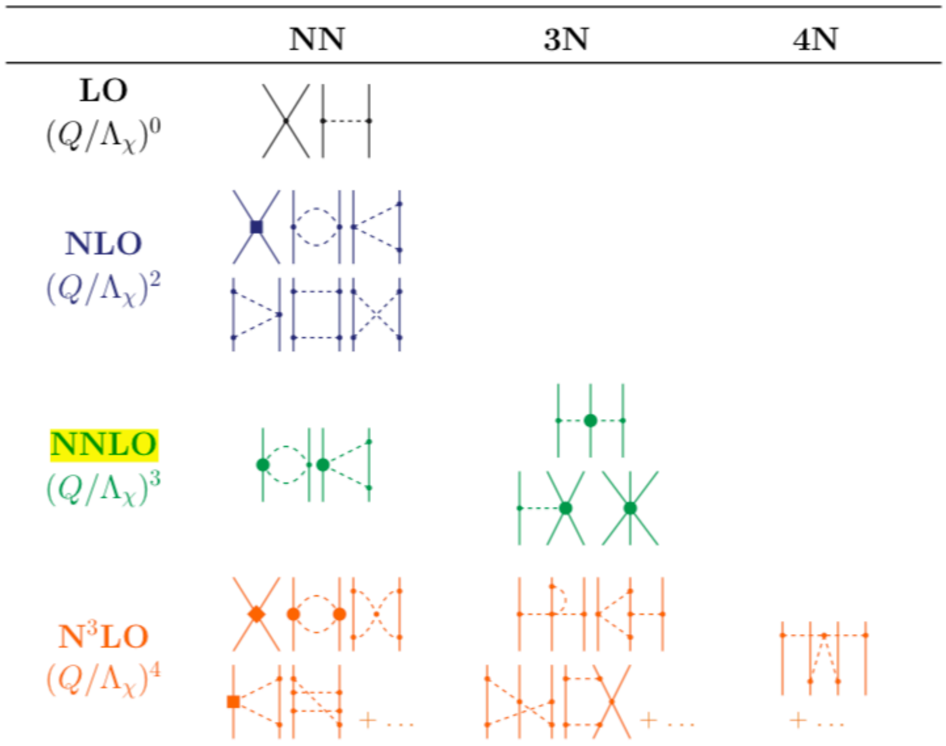
$$\delta y_{\rm th} = y_{\rm ref} \sum_{n=k+1}^{\infty} c_n Q^n$$

If we can treat this appropriately, can incorporate into our statistical analysis

EFTs (or any systematic calculation) are special!

Chiral effective field theory

Weinberg power-counting prescription, calculated *non-perturbatively*



(Up to N3LO, no diagrams for explicit Deltas shown.)
Hergert et al., J. Phys.: Conf. Ser. 1041 012007, (2018)

Current state of chiral interactions

Two-body: nucleon-nucleon (NN) sector and πN sector

- LENPIC few/many-body NN calculations
  Binder et al. PRC 98, 014002 (2018)
- Ongoing work at Chalmers group beyond N2LO sim/sep
  Carlsson et al., PRX 6 011019 (2016)
- Local chiral potentials with explicit Deltas
  Piarulli at al., PRC 91, 024003 (2015)
- BUQEYE: recent Bayesian exploration (in partial waves)
  SW et al., JPG 46, 045102 (2019)
- coefficients from Roy-Steiner analysis Hoferichter at al., Phys. Rev. Lett. 115, 192301 (2015)

NNN

- LENPIC fits of cD and cE + few/many-body calculations
  Epelbaum et al., arxiv:1807.02848
- More work with light nuclei in QMC
  Baroni et al., PRC 98 (2018) no.4, 044003, Piarulli et al., PRL 120 (2018) no.5, 052503, etc.
- BUQEYE+Chalmers to constrain cD and cE (Bayesian methods)

Two main projects

1. Parameter estimation: LEC fittings for EFTs

   Use data to maximum impact
   Understand how uncertainty propagates through the calculation

Two main projects

1. Parameter estimation: LEC fittings for EFTs

   Use data to maximum impact
   Understand how uncertainty propagates through the calculation

2. Truncation errors in EFTs

   Understand correlations to avoid using redundant information
   Validation tools for testing EFT convergence properties
   Predictions with quantified uncertainty!

Parameter estimation for EFT LECs

Object of interest to calculate:

$$\mathrm{pr}(\vec{a}_k \mid \boldsymbol{y}_{\mathrm{exp}}, \Sigma_{\mathrm{exp}}, \Sigma_{\mathrm{th}}, I)$$

- $\vec{a}_k$: EFT low-energy constants at order k in the theory
- $\boldsymbol{y}_{\mathrm{exp}}, \Sigma_{\mathrm{exp}}$: Experimental values and uncertainties
- Σ_{th} : Theory covariance matrix
- I : Any other background e.g., EFT naturalness

Posterior pdf with naturalness and truncation error:

$$\mathrm{pr}(\vec{a}_k \mid \boldsymbol{y}_{\mathrm{exp}}, \Sigma_{\mathrm{exp}}, \Sigma_{\mathrm{th}}) \propto \mathrm{pr}(\boldsymbol{y}_{\mathrm{exp}} \mid \boldsymbol{y}_{\mathrm{th}}, \Sigma_{\mathrm{exp}}, \Sigma_{\mathrm{th}})\, \mathrm{pr}(\vec{a}_k \mid \bar{a})$$

LEC naturalness: encoded by the “hyperparameter” $\bar{a}$

Truncation error: Σ_{th} , includes theory error assumptions

Exploring projected posteriors for LECs

Starting slow:

$$\boldsymbol{y}_{\rm exp} = \boldsymbol{y}_{\rm th} + \underbrace{\delta \boldsymbol{y}_{\rm th}}_{\to 0} + \delta \boldsymbol{y}_{\rm exp}$$

Work in a regime where theory error is very small: high enough EFT order

Posterior reduces to regular least-squares likelihood augmented by Gaussian prior

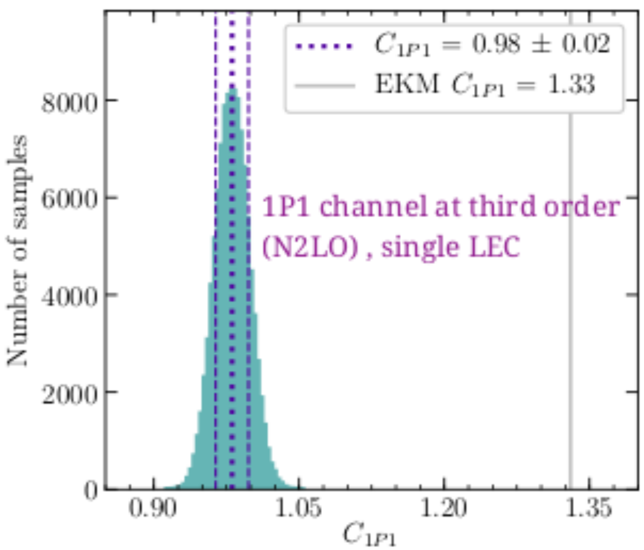
$$\mathrm{pr}(\vec{a}_k | \boldsymbol{y}_{\rm exp}, \Sigma_{\rm exp}) \propto \mathrm{pr}(\boldsymbol{y}_{\rm exp} | \vec{a}_k, \Sigma_{\rm exp})\ \ \mathrm{pr}(\vec{a}_k) \propto e^{-\frac{1}{2}\boldsymbol{r}^T \Sigma_{\rm exp}^{-1} \boldsymbol{r}} \times e^{-(\vec{a}_k)^2/2\bar{a}^2}$$

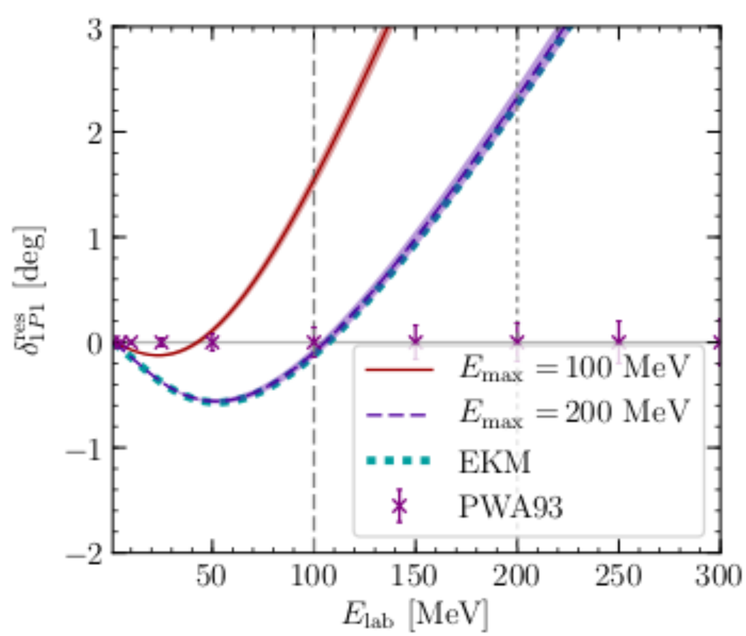
where

$$\boldsymbol{r} = \boldsymbol{y}_{\rm exp} - \boldsymbol{y}_{\rm th}$$

Exploring projected posteriors for LECs

$$\mathrm{pr}(\vec{a}_k | \boldsymbol{y}_{\exp}, \Sigma_{\exp}) \propto \exp\left[-\frac{1}{2}\sum_{i=1}^{N_d} \frac{r_i^2}{\sigma_i^2}\right] \times e^{-(\vec{a}_k)^2/2\bar{a}^2}$$

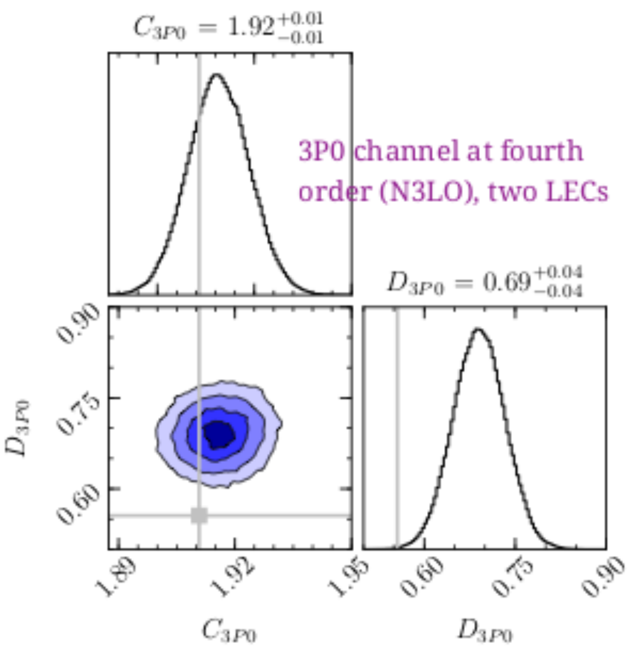


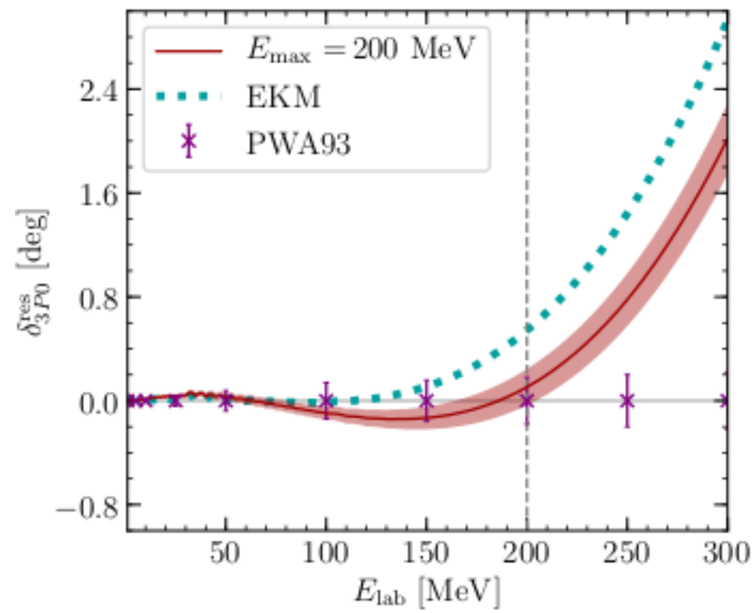


Wesolowski et al., JPG 46, 045102 (2019)

Exploring projected posteriors for LECs

$$\mathrm{pr}(\vec{a}_k|\boldsymbol{y}_{\mathrm{exp}},\Sigma_{\mathrm{exp}}) \propto \exp\left[-\frac{1}{2}\sum_{i=1}^{N_d}\frac{r_i^2}{\sigma_i^2}\right] \times e^{-(\vec{a}_k)^2/2\bar{a}^2}$$

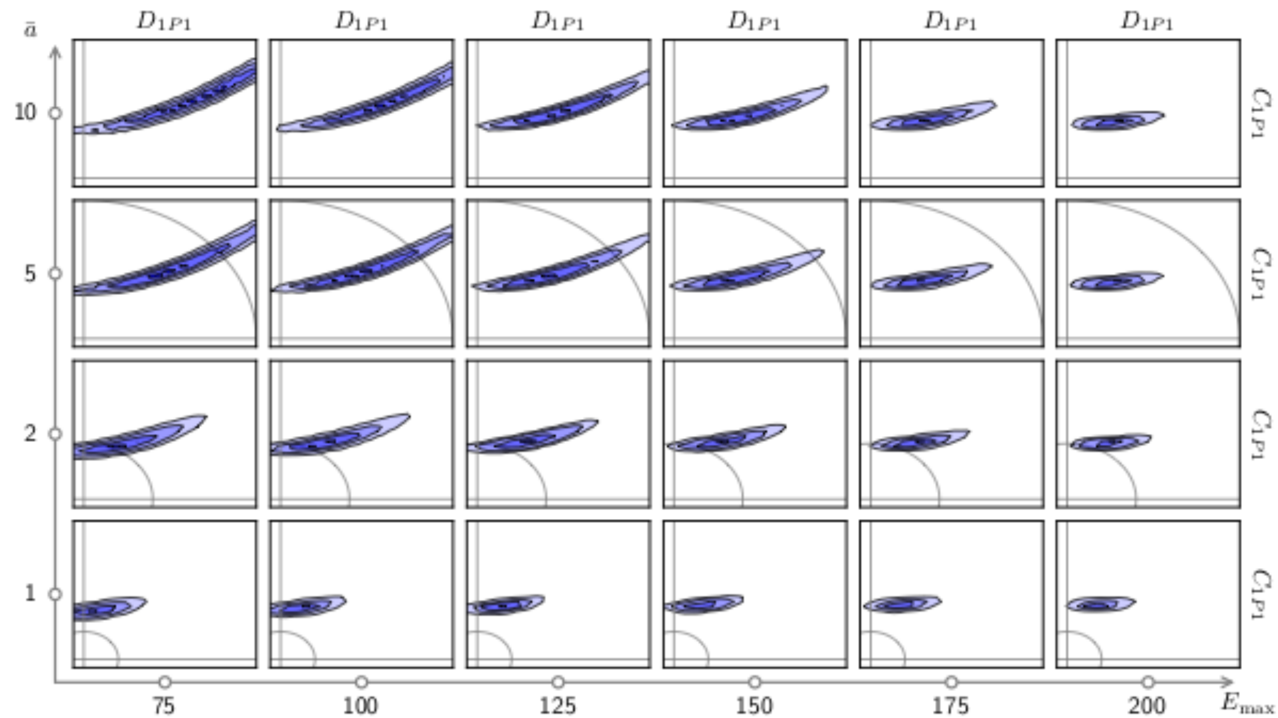




Wesolowski et al., JPG 46, 045102 (2019)

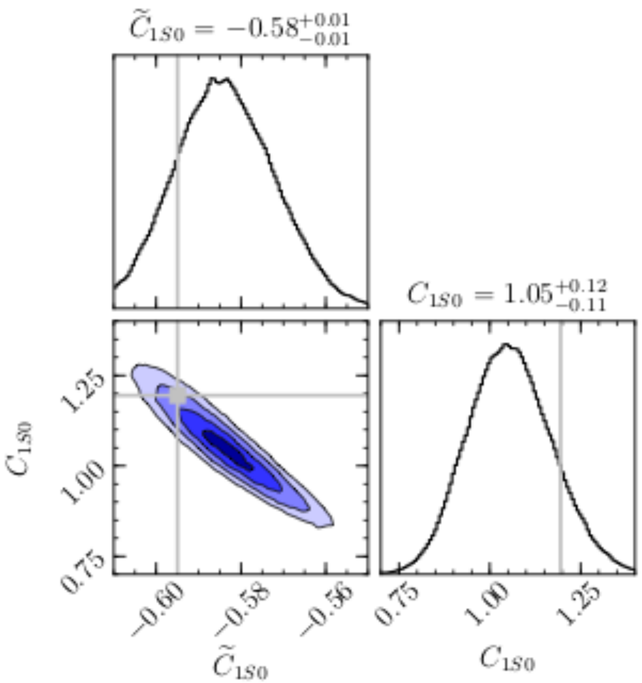
Effect of the prior

Choose one partial wave, repeat problem and vary prior and data
x-axis: increase E_{max}, highest energy datum
y-axis: value of $\bar{a}$ in the prior

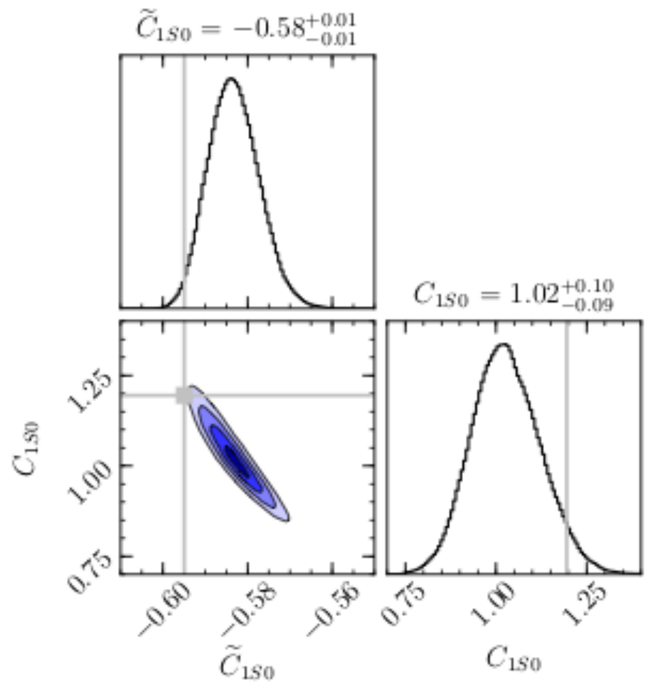


$^1P_1$ channel at N^{3}LO

Including truncation error



Truncation is not correlated
"Zero correlation length"



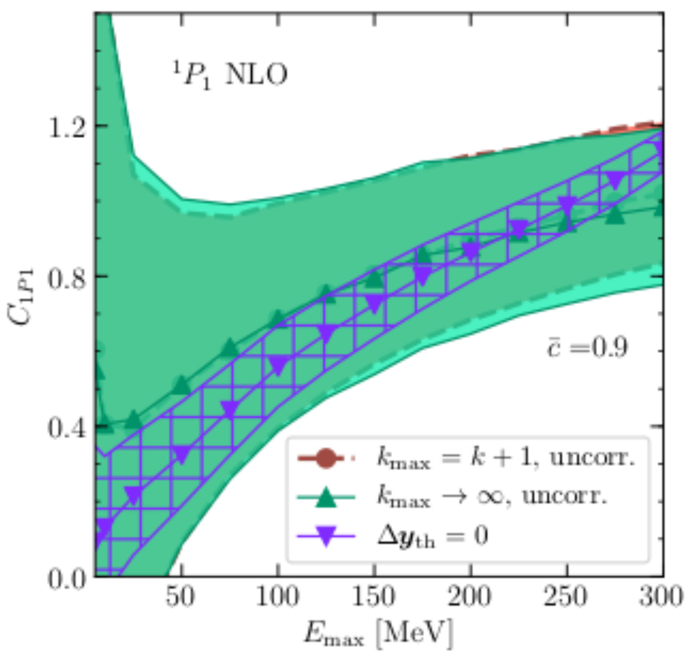
Truncation is fully correlated
"Infinite correlation length"

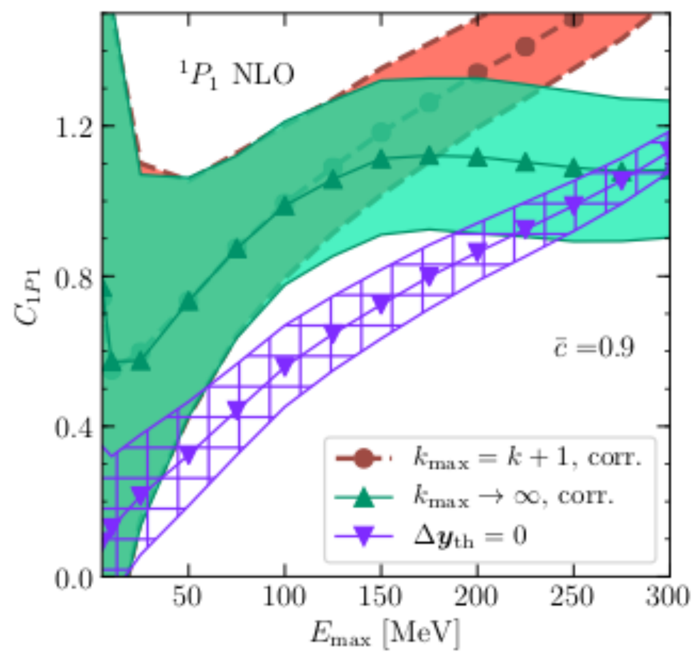
Including $\delta y_{\rm th} = y_{\rm ref} \sum_{n=k+1}^{\infty} c_n Q^n$ and comparing two extreme assumptions

Including truncation error

Strategy: plot extracted coefficients as a function of E_{max}

Note the large error bands when including truncation error in estimates.



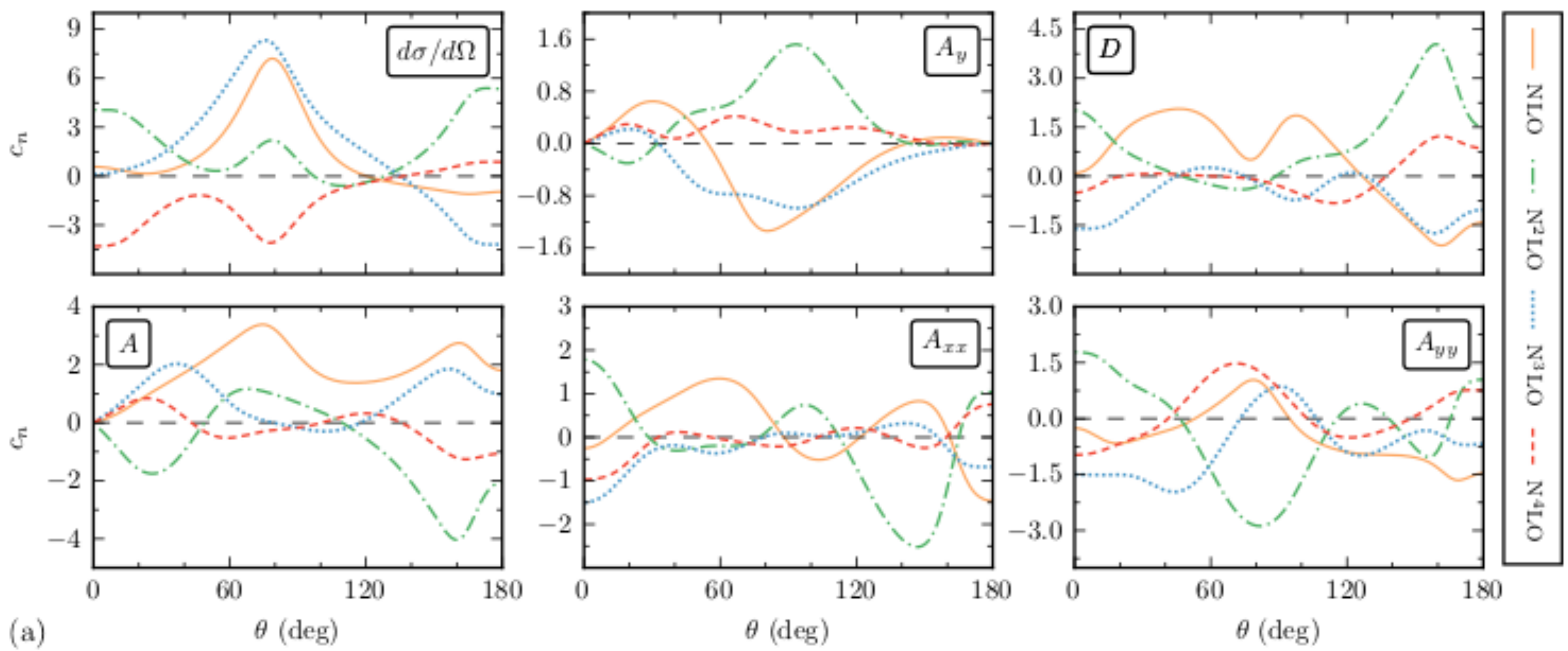


Successful inclusion of theory error: LEC estimates independent of E_{max}

NN observable coefficients

np scattering coefficients for various observables at $E_{\rm lab} = 250$ MeV

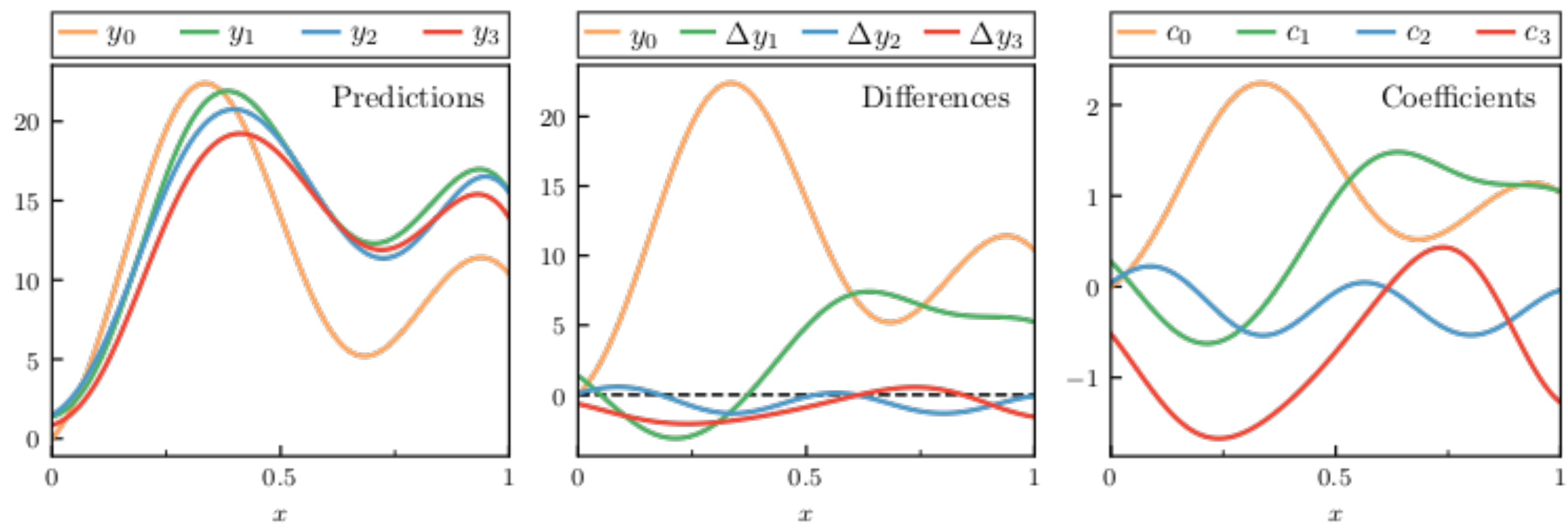
Melendez, SW et al., PRC 96, 024003 (2017) [Editor's suggestion]



$$y_{\rm th}(x) = y_k(x) = y_{\rm ref}(x) \sum_{n=0}^{k} c_n(x) Q^n(x)$$

Correlated truncation errors

Road map from predictions to coefficients of observable expansion

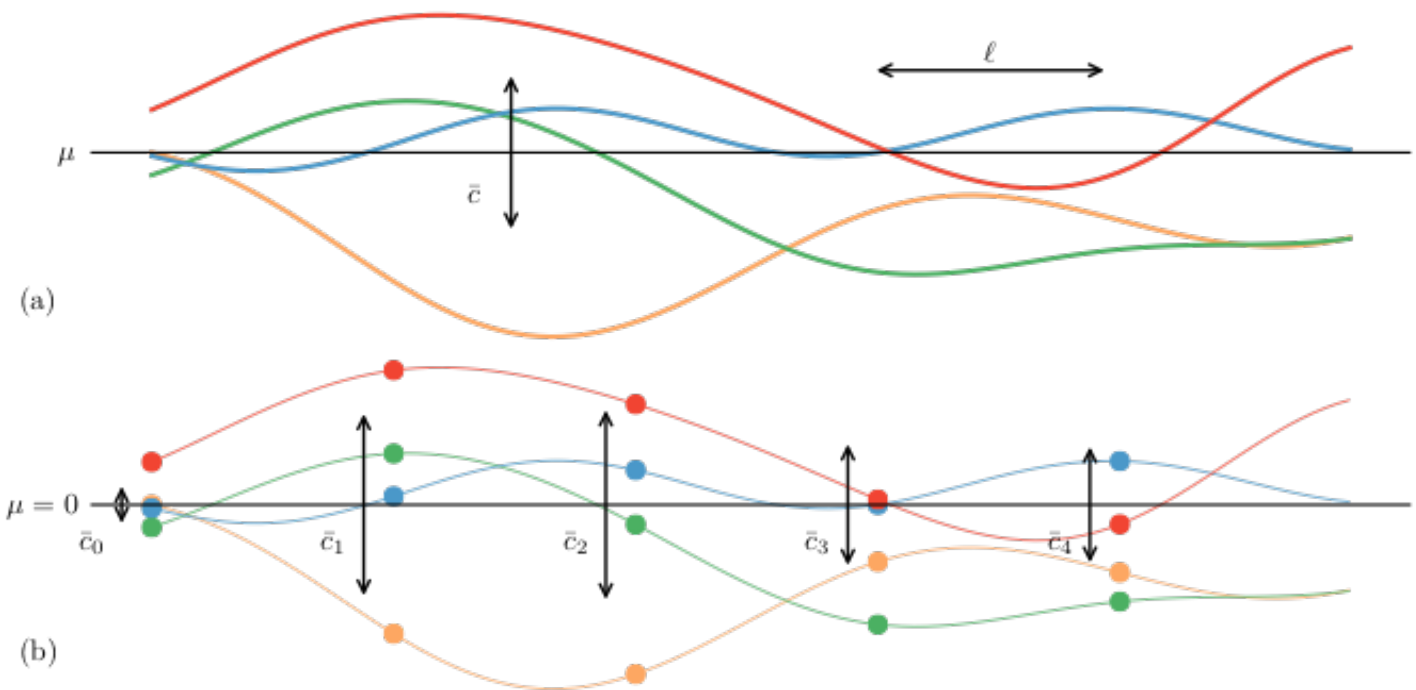


$$y_{\text{th}}(x) = y_k(x) = y_{\text{ref}}(x) \sum_{n=0}^{k} c_n(x) Q^n(x)$$

Correlated truncation errors

In general, we need to consider finite correlation length for truncation errors

Use Gaussian processes, a non-parametric tool, to model truncation error

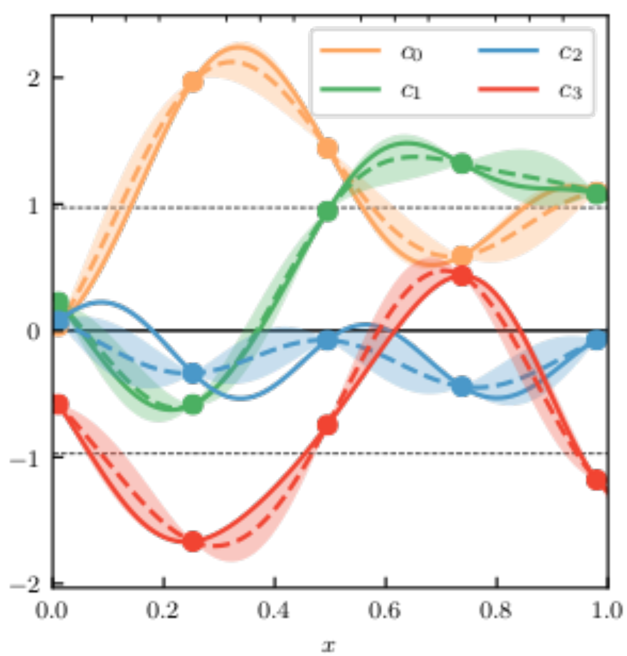


Figures courtesy of Jordan Melendez, OSU,
See arxiv:1904.10581 by Melendez, SW et al.

Gaussian processes for truncation error

Gaussian processes are usually used for interpolation of expensive simulators

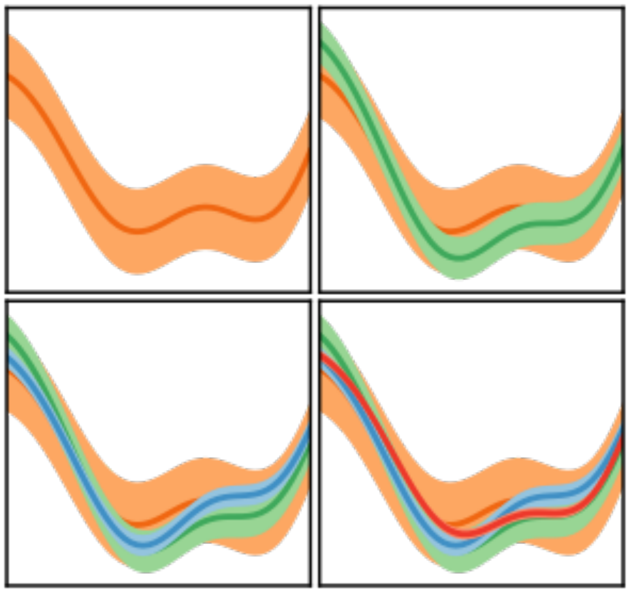
GP is treated as an emulator



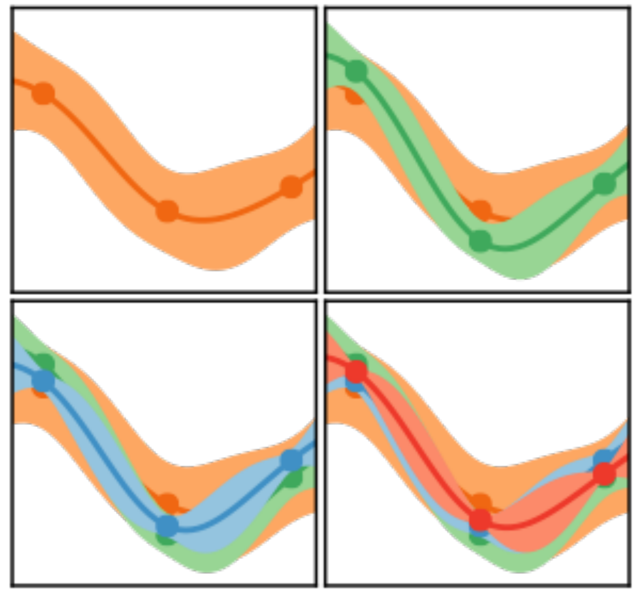
Treat observable coefficients as all arising from a single, underlying GP

Gaussian processes for truncation error

Can use in combination: interpolate and estimate truncation error!

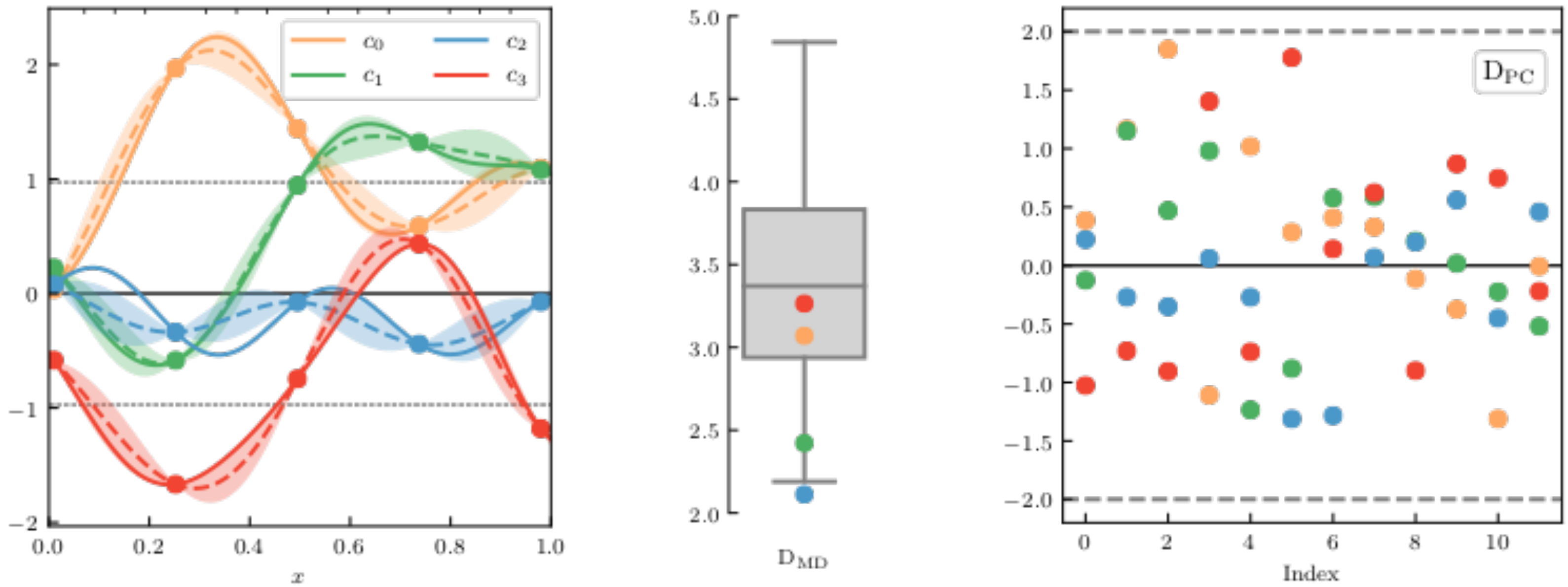


Inexpensive prediction



Expensive predition

Validation tools for Gaussian processes

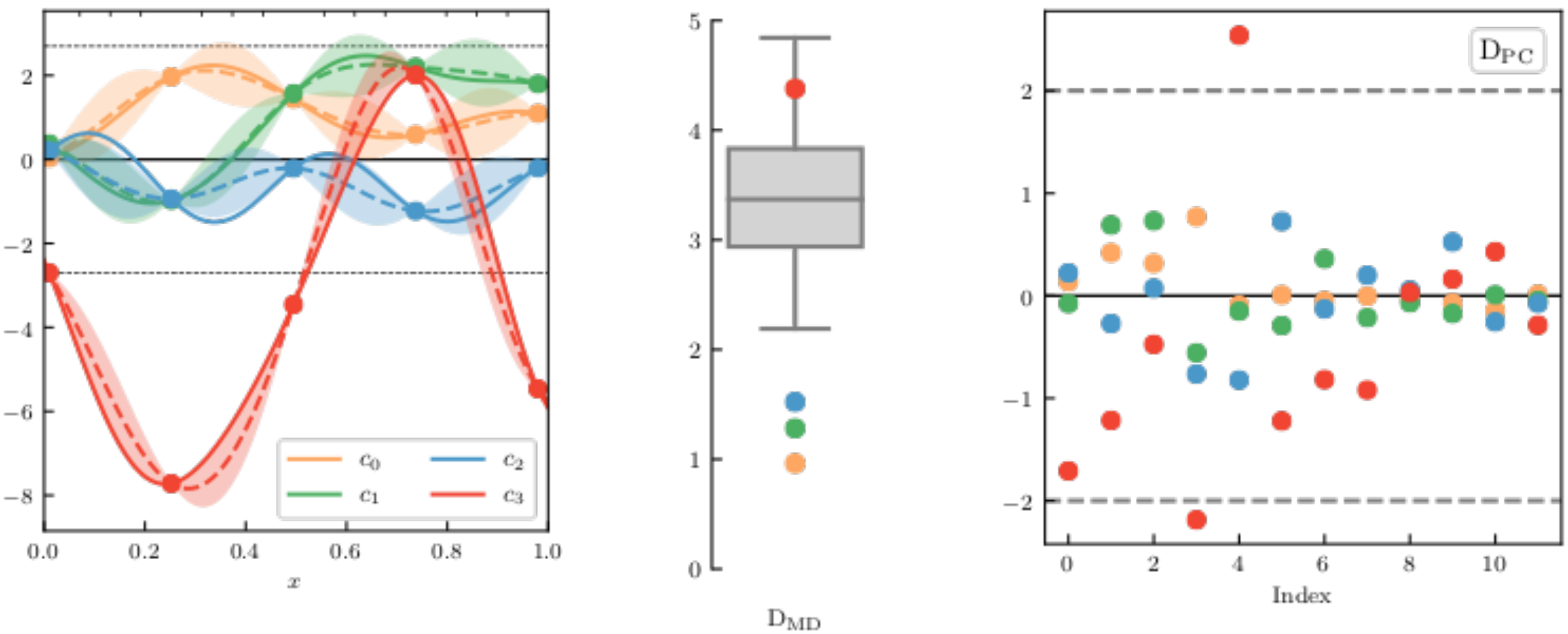


Mahalanobis distance
Pivoted Cholesky decomposition of errors

Inspired by Bastos and O'Hagan

Validation tools for Gaussian processes

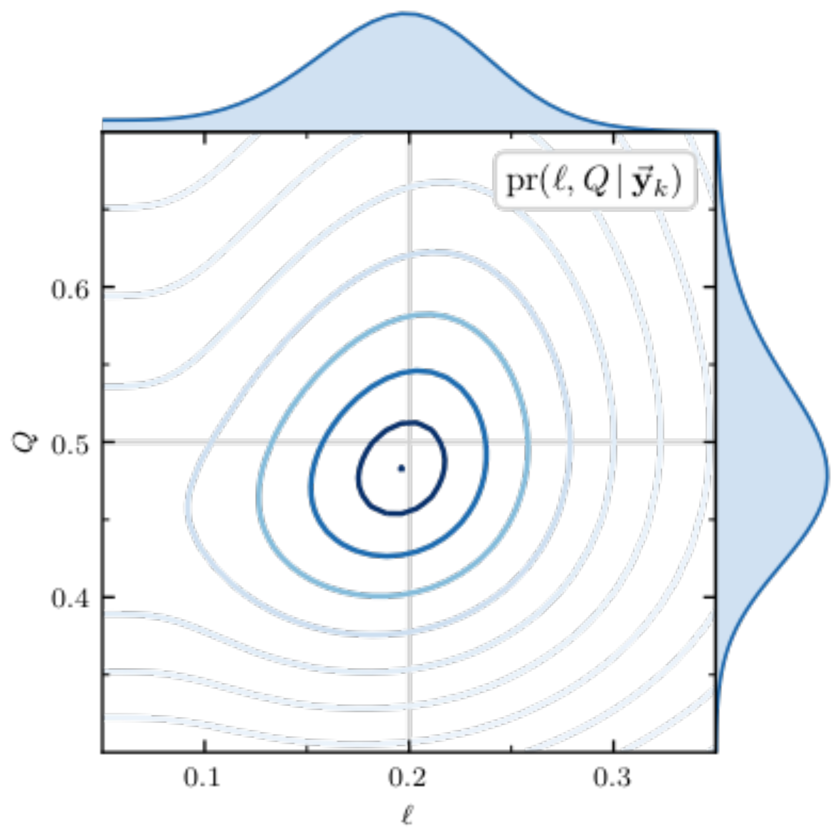
What does it look like when it's not working?



Purposefully underestimate expansion parameter Q

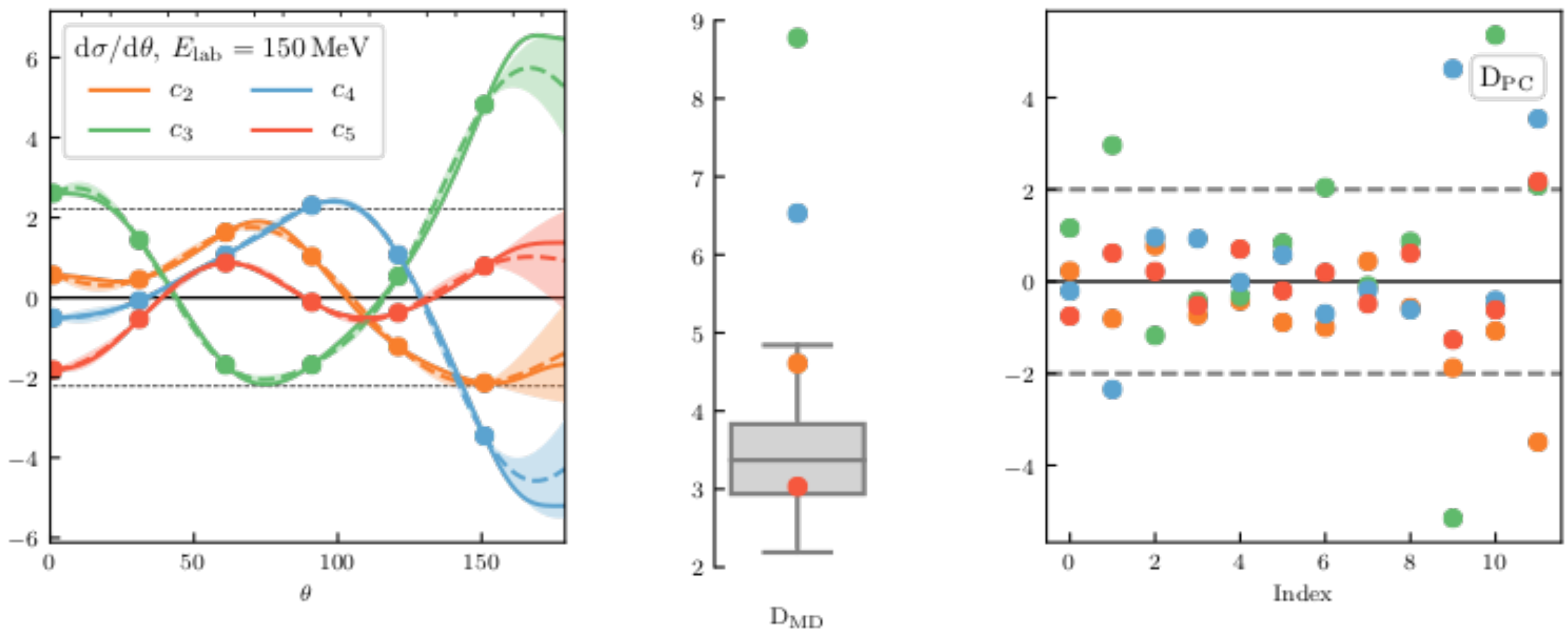
Extracting physical scales using GPs

Posterior pdf for the expansion parameter and correlation length



A real example in NN scattering

np differential cross section coefficients evaluated at $E_{\mathrm{lab}} = 150$ MeV.



Clear issues at large scattering angle

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- [*PRC editor's suggestion*] Melendez et al., PRC 96, 024003 (2017): "Bayesian truncation errors in chiral effective field theory: Nucleon-nucleon observables"
- Wesolowski et al., JPG 46, 045102 (2019): "Exploring Bayesian parameter estimation for chiral effective field theory using nucleon–nucleon phase shifts"
- Melendez et al., Quantifying Correlated Truncation Errors in Effective Field Theory, 2019, pre-print available at arxiv:1904.10581

General Bayes/Machine Learning references

Bayesian statistics

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- Gelman et al., "Bayesian Data Analysis" (3rd edition)
- R. Trotta, "Bayes in the sky: Bayesian inference and model selection in cosmology"

Other stuff (like Gaussian processes)

- Rasmussen and Williams, "Gaussian processes for machine learning"
- D. J.C. MacKay, "Introduction to Gaussian processes"
- D. J.C. MacKay, "Information Theory, Inference, and Learning Algorithms"