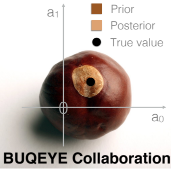
A recipe for EFT uncertainty quantification

Dick Furnstahl

Department of Physics
Ohio State University

RUB Seminar

April 30, 2015



Collaborators: D. Phillips, N. Klco, A. Thapilaya (OU), S. Wesolowski (OSU)

Outline

Theory errors and nuclear EFT

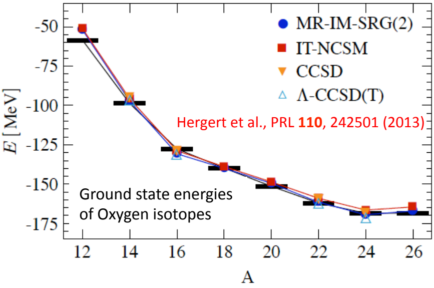
Bayesian methods applied to a model problem

Application to chiral EFT $\Longrightarrow$ building on EKM

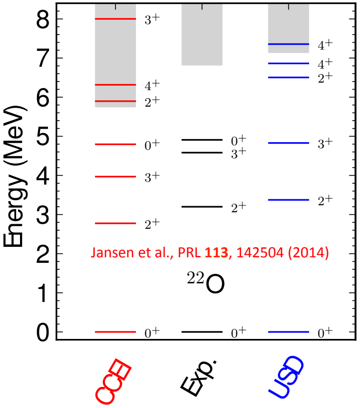
Going forward . . .

Where are the error bars from the chiral EFT Hamiltonian?

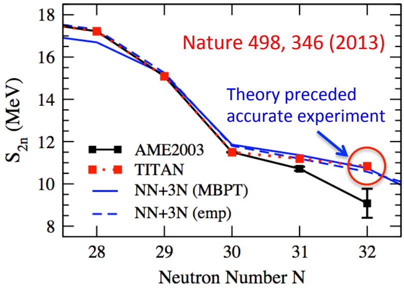
Oxygen isotopes with different methods



^{22}O spectrum with CCEI (also IM-SRG)



S_{2n} for Calcium isotopes (MBPT, also CC)



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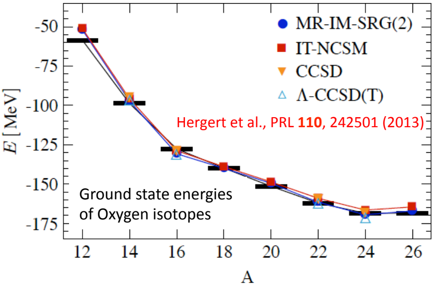

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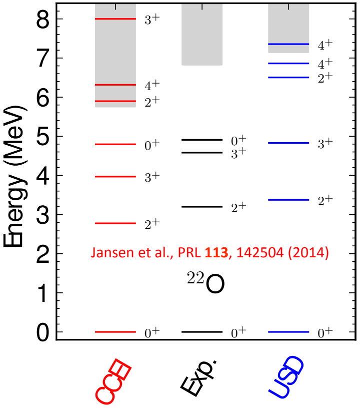

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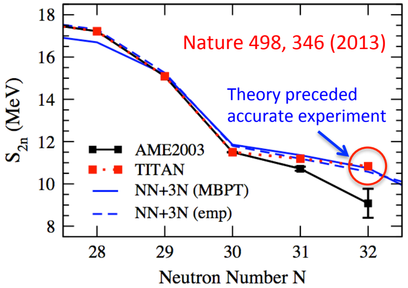

- Benchmarking methods: uncertainty?
- Chiral EFT Hamiltonian UQ
  - errors in input data for fit
  - truncation + regulator artifacts
- We seek UQ of *all* errors

Uncertainty Quantification (UQ) for nuclear *theory*

Physical Review A Editorial, April 2011

The purpose of this Editorial is to discuss the importance of including uncertainty estimates in papers involving theoretical calculations of physical quantities.

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* without a detailed discussion of the uncertainties involved in the measurements….

The question is to what extent can the same high standards be applied to papers reporting the results of theoretical calculations…..There are many cases where it is indeed not practical to give a meaningful error estimate for a theoretical calculation….However, there is a broad class of papers where estimates of theoretical uncertainties can and should be made.

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1. If the authors claim high accuracy, or improvements on the accuracy of previous work.
2. If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.
3. If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

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To truly assess precision and accuracy, we need to know theory error bars.
Much work to be done to establish rigorous UQ. But a lot of activity!

See J. Phys. G special issue: *Enhancing the interaction between nuclear experiment and theory through information and statistics*, eds. D. Ireland and W. Nazarewicz

Types of *systematic* theory errors (not exhaustive)

- Truncation of [harmonic oscillator] model space

- Truncation of [EFT] expansion but unknown higher coefficients

- Incomplete or possibly incorrect model [e.g., energy functional]

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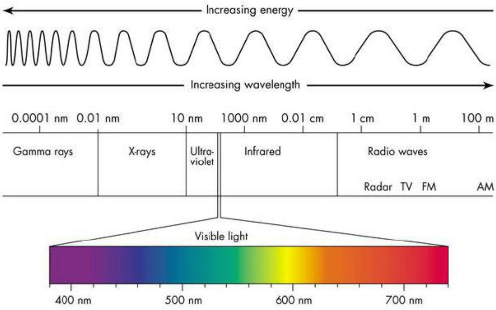
EFT common principle: Draw a line between IR and UV

- In coordinate space, use R to separate short and long distance physics
- In momentum space, use Λ to separate high and low momenta
- Much freedom *how* this is done (e.g., different regulator forms) $\Longrightarrow$ different scales / schemes



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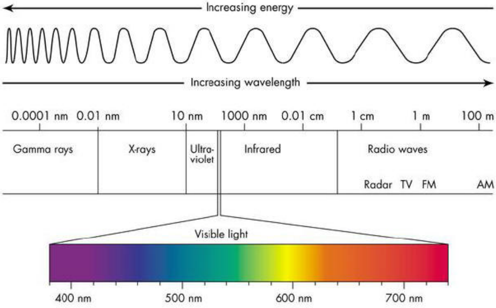
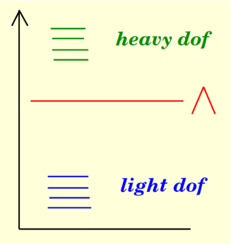


- Long distance solved explicitly (symmetries); short-distance captured in some LECs. Naturalness $\Longrightarrow$ scaled LECs are $\mathcal{O}(1)$
- Power counting $\Longrightarrow$ expansion parameter(s); e.g., ratio of scales: $\{p, m_\pi\}/\Lambda$
- If $\Lambda < \Lambda_{\text{breakdown}} \Longrightarrow$ regulator artifacts (use RG!)
- Model independence comes from completeness of operator basis (use QFT).



Nucleon-nucleon force up to N^{3}LO

Ordonez et al. '94; Friar & Coon '94; Kaiser et al. '97; Epelbaum et al. '98,'03; Kaiser '99-'01; Higa et al. '03; …

Chiral expansion for the 2N force:

$$V_{2N} = V_{2N}^{(0)} + V_{2N}^{(2)} + V_{2N}^{(3)} + V_{2N}^{(4)} + \ldots$$

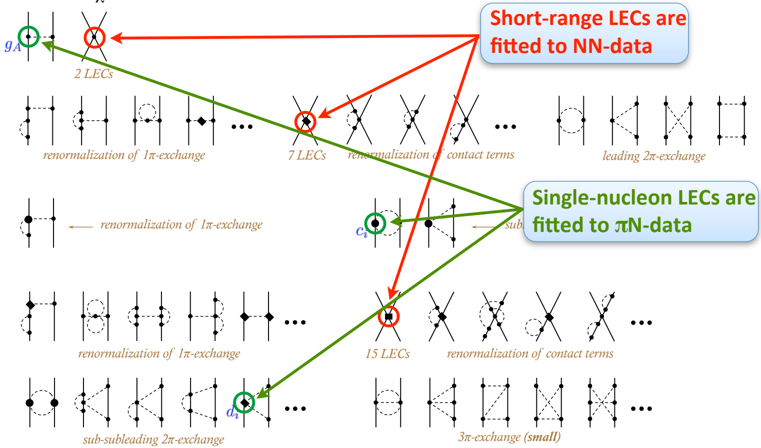
breakdown scale $\Lambda_b = \Lambda_\chi \sim$ 500-1000 MeV

LO: $\mathcal{O}((q/\Lambda_\chi)^0)$

NLO: $\mathcal{O}((q/\Lambda_\chi)^2)$

N^{2}LO: $\mathcal{O}((q/\Lambda_\chi)^3)$

N^{3}LO: $\mathcal{O}((q/\Lambda_\chi)^4)$



+ 1/m and isospin-breaking corrections…

figure from H. Krebs

New alternative approaches to EFT Hamiltonians

NN potentials unchanged for 10 years but now many parallel developments

Different philosophies, regulators (schemes), fitting protocols, ...

- If not strictly renormalizable (regulator dependence completely removed at each order), then not EFT $\Longrightarrow$ new power counting
- Weinberg power counting with strict adherence to EFT principles (e.g., fix c_i's in πN to isolate physics; order-by-order predictions)
- High-accuracy, sophisticated fitting protocol, covariance analysis
- Simultaneous sophisticated fit of πN, NN, NNN LECs
- Broaden range of fit beyond few-body systems to improve many-body accuracy (e.g., energies and radii)

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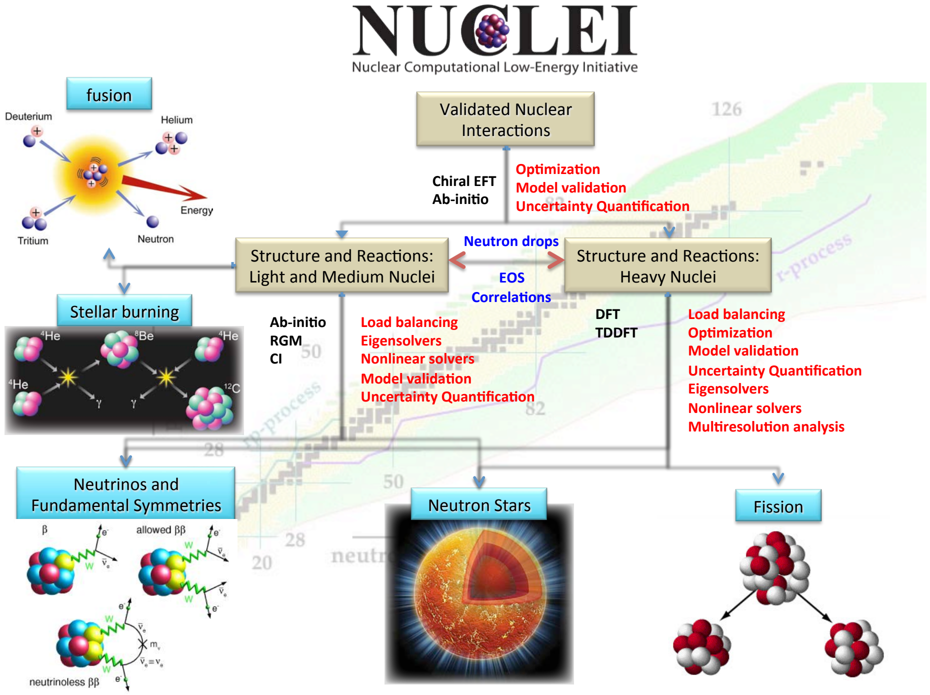
How do we reconcile? Different approaches for different problems?
What can each approach tell about the others?

What about EFT truncation and fitting errors?


NUCLEI
Nuclear Computational Low-Energy Initiative
Validated Nuclear Interactions
Chiral EFT
Ab-initio
Optimization
Model validation
Uncertainty Quantification
Structure and Reactions: Light and Medium Nuclei
Neutron drops
EOS
Correlations
Structure and Reactions: Heavy Nuclei
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Nonlinear solvers
Multiresolution analysis
fusion
Deuterium
Helium
Energy
Tritium
Neutron
Stellar burning
^{4}He
^{8}Be
^{4}He
^{4}He
^{12}C
γ
γ
Neutrinos and Fundamental Symmetries
β
allowed ββ
neutrinoless ββ
Neutron Stars
Fission
126
82
50
82
28
50
28
20
r-process
rp-process

Goal: order-by-order chiral calculations with better UQ

LENPIC

Low Energy Nuclear Physics International Collaboration

TECHNISCHE UNIVERSITÄT DARMSTADT — Sven Binder, Angelo Calci, Kai Hebeler, Joachim Langhammer, Robert Roth

IOWA STATE UNIVERSITY — Pieter Maris, Hugh Potter, James Vary

THE OHIO STATE UNIVERSITY — Richard J. Furnstahl

RUB — Evgeny Epelbaum, Hermann Krebs

universitätbonn — Ulf-G. Meißner

IPN INSTITUT DE PHYSIQUE NUCLÉAIRE ORSAY — Veronique Bernard

JÜLICH FORSCHUNGSZENTRUM — Andreas Nogga

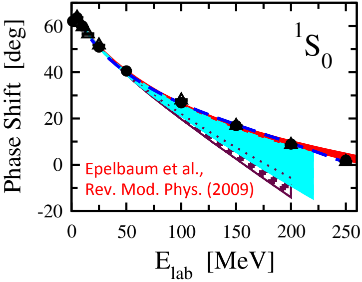
JAGIELLONIAN UNIVERSITY IN KRAKOW — Jacek Golak, Roman Skibinski, Kacper Topolniki, Henryk Witala

Kyutech Kyushu Institute of Technology — Hiroyuki Kamada

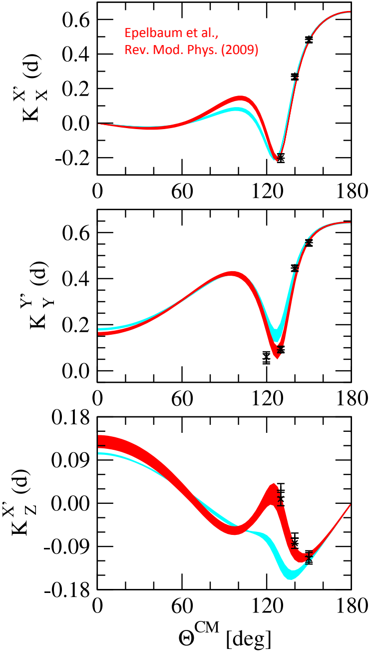
LENPIC

Previous UQ: Error bands in chiral EFT

- Bands from EFT cutoff variation
- below: neutron-proton $^1S_0$ phase shift at NLO, N^2LO, and N^3LO



- right: chiral EFT predictions for *p–d* spin observables



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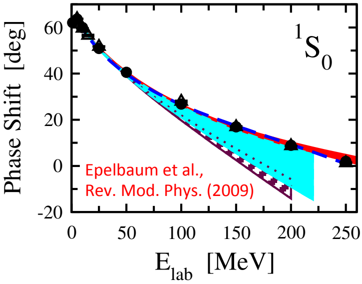

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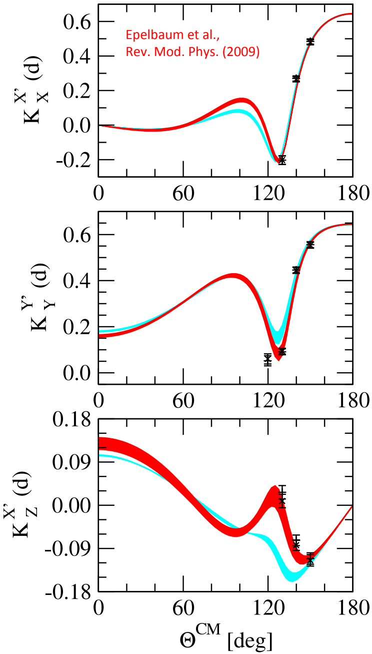
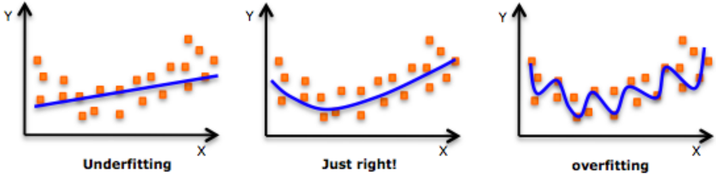


Problems with this as UQ:

- Unpleasing systematics of bands
- Often underestimates uncertainty
- Statistical interpretation???

What can go wrong in an EFT fit?



[from pingax.com/regulatization-implementation-r]

- Overfitting (high variance) or underfitting (high bias) or misfitting?
- Well-defined for statistical fits how to check
  - If underfit, then chi-squared fails (if theory were correct, then you wouldn't get that data)
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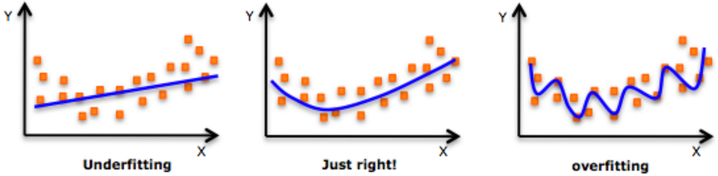

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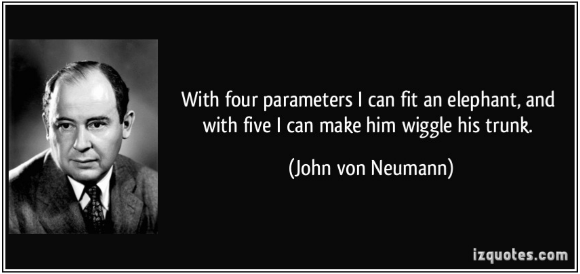
  - Validate with subset: if overtrained then fail on additional set (overfit); but how to avoid?
- What can happen in an EFT fit? What are the complications?
  - More statistical power if larger energy range included, but EFT is less accurate approaching breakdown scale $\Longrightarrow$ Where to fit?
  - How do we combine data and theory uncertainties?
  - Is the EFT working? Or just a lot of parameters?

Famous von Neumann quote



Attributed to John von Neumann by Enrico Fermi, as quoted by Freeman Dyson in “A meeting with Enrico Fermi” in Nature **427** (22 January 2004).

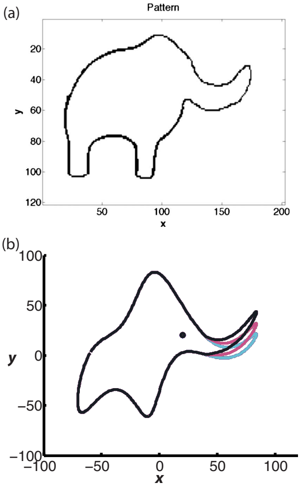


Fig. 1. (a) Outline of an elephant. (b) Three snapshots of the wiggling trunk.

“Drawing an elephant with four *complex* parameters,” J. Mayer, K. Khairy, and J. Howard, Am. J. Phys. **78**, 648 (2010).

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Going forward . . .

Why is a Bayesian framework well suited to EFT errors?

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  - Outcomes of experiments treated as random variables
  - Predict probabilities of observing various outcomes
  - Well adapted to quantities that fluctuate randomly
  - But systematic errors can be problematic

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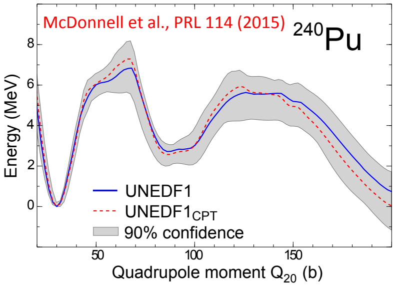
  - But systematic errors can be problematic
- Bayesian probabilities: pdf is a measure of state of our knowledge
  - Ideal for treating systematic errors (such as theory errors!)
  - Assumptions (or expectations) about EFT encoded in prior pdfs
  - Can predict values of observables with credibility intervals (errors)
  - Incorporates usual statistical tools (e.g., covariance analysis)
- For EFT, makes explicit what is usually implicit, allowing assumptions to be applied consistently, tested, and modified given new information

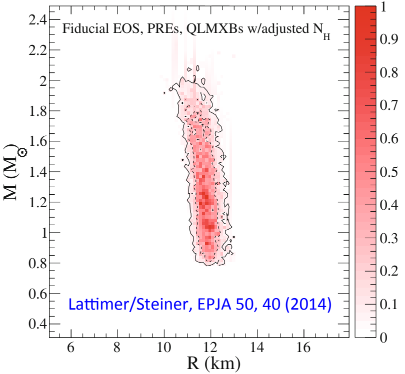
Why is a Bayesian framework well suited to EFT errors?

- Widespread application of Bayesian approaches in theoretical physics
  - Interpretation of dark-matter searches; structure determination in condensed-matter physics; constrained curve-fitting in lattice QCD
  - Is supersymmetry a “natural” approach to the hierarchy problem?
  - Estimating uncertainties in perturbative QCD (e.g., parton distributions)

- Nuclear EDFs [Schunck et al.]



- Neutron stars [Steiner et al.]



Advertisement: INT Program in 2016

Bayesian Methods in Nuclear Physics (INT-16-2a)

June 13 to July 8, 2016

R.J. Furnstahl, D. Higdon, N. Schunck, A.W. Steiner

A four-week program to explore how Bayesian inference can enable progress on the frontiers of nuclear physics and open up new directions for the field. Among our goals are to

- facilitate cross communication, fertilization, and collaboration on Bayesian applications among the nuclear sub-fields;
- provide the opportunity for nuclear physicists who are unfamiliar with Bayesian methods to start applying them to new problems;
- learn from the experts about innovative and advanced uses of Bayesian statistics, and best practices in applying them;
- learn about advanced computational tools and methods;
- critically examine the application of Bayesian methods to particular physics problems in the various subfields.

Existing efforts using Bayesian statistics will continue to develop over the coming months, but Summer 2016 will be an opportune time to bring the statisticians and nuclear practitioners together.

Bayesian rules of probability as principles of logic

Notation: $\mathrm{pr}(x|I)$ is the probability (or pdf) of x being true given information I

1. **Sum rule:** If set $\{x_i\}$ is exhaustive and exclusive,

$$\sum_i \mathrm{pr}(x_i|I) = 1 \quad \longrightarrow \quad \int dx\, \mathrm{pr}(x|I) = 1$$

   - cf. complete and orthonormal
   - implies *marginalization* (cf. inserting complete set of states)

$$\mathrm{pr}(x|I) = \sum_j \mathrm{pr}(x, y_j|I) \quad \longrightarrow \quad \mathrm{pr}(x|I) = \int dy\, \mathrm{pr}(x, y|I)$$

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2. **Product rule:** expanding a joint probability of x and y

$$\mathrm{pr}(x, y|I) = \mathrm{pr}(x|y, I)\,\mathrm{pr}(y|I) = \mathrm{pr}(y|x, I)\,\mathrm{pr}(x|I)$$

   - If x and y are mutually independent: $\mathrm{pr}(x|y, I) = \mathrm{pr}(x|I)$, then

$$\mathrm{pr}(x, y|I) \longrightarrow \mathrm{pr}(x|I)\,\mathrm{pr}(y|I)$$

   - Rearranging the second equality yields Bayes' theorem

$$\mathrm{pr}(x|y, I) = \frac{\mathrm{pr}(y|x, I)\,\mathrm{pr}(x|I)}{\mathrm{pr}(y|I)}$$

Applying Bayesian methods to LEC estimation

Definitions:

- $\mathbf{a} \equiv$ vector of LECs $\Longrightarrow$ coefficients of an expansion $(a_0, a_1, \ldots)$
- $D \equiv$ measured data (e.g., cross sections)
- $I \equiv$ all background information (e.g., data errors, EFT details)

Bayes theorem: How knowledge of $\mathbf{a}$ is updated

$$\underbrace{\mathrm{pr}(\mathbf{a}|D,I)}_{\text{posterior}} = \underbrace{\mathrm{pr}(D|\mathbf{a},I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\mathbf{a}|I)}_{\text{prior}} \,/\, \underbrace{\mathrm{pr}(D|I)}_{\text{evidence}}$$

- Posterior: probability distribution for LECs given the data
- Likelihood: probability to get data D given a set of LECs
- Prior: What we know about the LECs *a priori*
- Evidence: Just a normalization factor here
  [Note: The evidence is important in model selection]

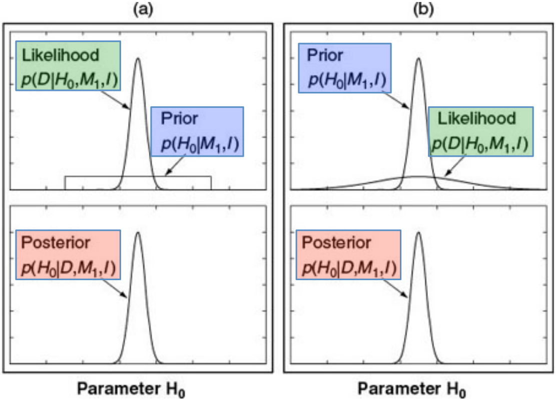
The posterior lets us find the most probable values of parameters or the probability they fall in a specified range ("credibility interval")

Limiting cases in applying Bayes' theorem

Suppose we are fitting a parameter H_0 to some data D given a model M_1 and some information (e.g., about the data or the parameter)

Bayes' theorem tells us how to find the posterior distribution of H_0:

$$\mathrm{pr}(H_0|D,M_1,I) = \frac{\mathrm{pr}(D|H_0,M_1,I)\times \mathrm{pr}(H_0|M_1,I)}{\mathrm{pr}(D|I)}$$



[From P. Gregory, "Bayesian Logical Data Analysis for the Physical Sciences"]

Special cases:

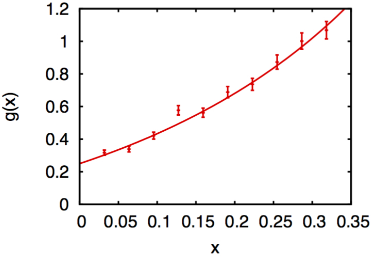
(a) If the data is overwhelming, the prior has no effect on the posterior

(b) If the likelihood is unrestrictive, the posterior returns the prior

Toy model for natural EFT [Schindler/Phillips, Ann. Phys. 324, 682 (2009)]

"Real world": $g(x) = (1/2 + \tan(\pi x/2))^2$

"Model" $\approx 0.25 + 1.57x + 2.47x^2 + \mathcal{O}(x^3)$



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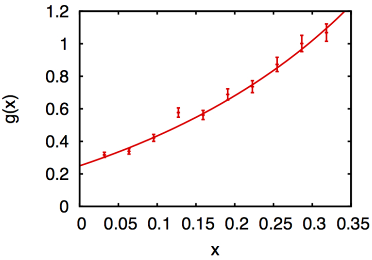
$$\mathbf{a}_{\text{true}} = \{0.25, 1.57, 2.47, 1.29, \ldots\}$$



Generate synthetic data D with noise with 5% relative error:

$$D: \; d_j = g_j \times (1 + 0.05\eta_j) \quad \text{where} \quad g_j \equiv g(x_j)$$

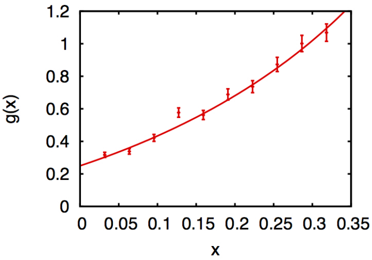
η is normally distributed random noise $\rightarrow \sigma_j = 0.05\, g_j\, \eta_j$

Toy model for natural EFT [Schindler/Phillips, Ann. Phys. 324, 682 (2009)]

"Real world": $g(x) = (1/2 + \tan(\pi x/2))^2$

"Model" $\approx 0.25 + 1.57x + 2.47x^2 + \mathcal{O}(x^3)$

$$\mathbf{a}_{\text{true}} = \{0.25, 1.57, 2.47, 1.29, \ldots\}$$



Generate synthetic data D with noise with 5% relative error:

$$D: \; d_j = g_j \times (1 + 0.05\eta_j) \quad \text{where} \quad g_j \equiv g(x_j)$$

η is normally distributed random noise $\rightarrow \sigma_j = 0.05\, g_j\, \eta_j$

Pass 1: $\mathrm{pr}(\mathbf{a}|D, I) \propto \mathrm{pr}(D|\mathbf{a}, I)\,\mathrm{pr}(\mathbf{a}|I)$ with $\mathrm{pr}(\mathbf{a}|I) \propto$ constant

$$\Longrightarrow \; \mathrm{pr}(\mathbf{a}|D, I) \propto e^{-\chi^2/2} \text{ where } \chi^2 = \sum_{j=1}^{N} \frac{1}{\sigma_j^2} \left(d_j - \sum_{i=0}^{M} a_i x^i \right)^2$$

That is, if we assume no prior information about the LECs (uniform prior), the fitting *procedure* is the same as least squares!

Toy model Pass 1: Uniform prior

Find the maximum of the posterior distribution; this is the same as fitting the coefficients with conventional χ^2 minimization.
Pseudo-data: $0.03 < x < 0.32$.

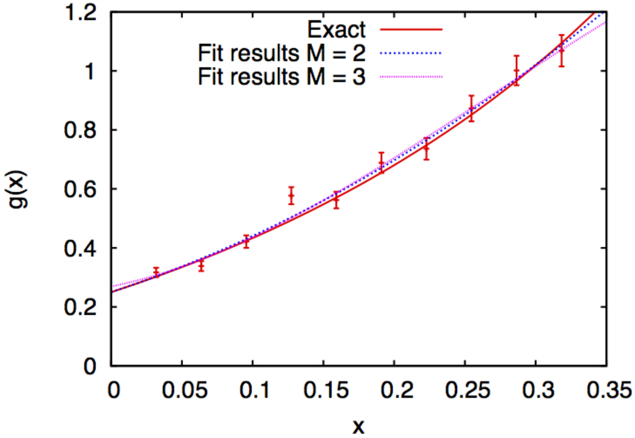
M	χ^2/dof	a_0	a_1	a_2
true		0.25	1.57	2.47
1	2.24	0.203±0.01	2.55±0.11	
2	1.64	0.25±0.02	1.6±0.4	3.33±1.3
3	1.85	0.27±0.04	0.95±1.1	8.16±8.1
4	1.96	0.33±0.07	−1.9±2.7	44.7±32.6
5	1.39	0.57±0.3	−14.8±6.9	276±117

Pass 1 results

- Results highly unstable with changing order M (e.g., see a_1)
- The errors become large and also unstable
- But χ^2/dof is not bad! Check the plot . . .

Toy model Pass 1: Uniform prior

Would we know the results were unstable if we didn't know the underlying model? Maybe some unusual structure at $M = 3 \ldots$



- Insufficient data $\Longrightarrow$ not high or low enough in x, or not enough points, or available data not precise (entangled!)
- Determining parameters at finite order in x from data with contributions from all orders

Toy model Pass 2: A prior for naturalness

Now, add in our knowledge of the coefficients in the form of a *prior*

$$\mathrm{pr}(\mathbf{a}|D) = \left(\prod_{i=0}^{M} \frac{1}{\sqrt{2\pi}R}\right) \exp\left(-\frac{\mathbf{a}^2}{2R^2}\right)$$

R encodes "naturalness" assumption, and M is order of expansion.
Same procedure: find the maximum of the posterior . . .

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R encodes "naturalness" assumption, and M is order of expansion.
Same procedure: find the maximum of the posterior . . .

Results for $R = 5$: *Much* more stable!

M	a_0	a_1	a_2
true	0.25	1.57	2.47
2	0.25±0.02	1.63±0.4	3.2±1.3
3	0.25±0.02	1.65±0.5	3±2.3
4	0.25±0.02	1.64±0.5	3±2.4
5	0.25±0.02	1.64±0.5	3±2.4

- What to choose for R? $\Longrightarrow$ *marginalize* over R (integrate).
- We used a Gaussian prior; where did this come from?
  $\Longrightarrow$ Maximum entropy distribution for $\langle \sum_i a_i^2 \rangle = (M+1)R^2$

Aside: Maximum entropy to determine prior pdfs

- Basic idea: least biased $\mathrm{pr}(x)$ from maximizing entropy

$$S[\mathrm{pr}(x)] = -\int dx\, \mathrm{pr}(x) \log\left[\frac{\mathrm{pr}(x)}{m(x)}\right]$$

  subject to constraints from the prior information

  - $m(x)$ is an appropriate measure (often uniform)

- One constraint is normalization: $\int dx\, \mathrm{pr}(x) = 1$
  $\Longrightarrow$ alone it leads to uniform $\mathrm{pr}(x)$

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  - $m(x)$ is an appropriate measure (often uniform)
- One constraint is normalization: $\int dx\, \mathrm{pr}(x) = 1$
  $\Longrightarrow$ alone it leads to uniform $\mathrm{pr}(x)$
- If the average variance is assumed to be: $\langle \sum_i a_i^2 \rangle = (M+1)R^2$, for fixed M and R ("ensemble naturalness") maximize

$$Q[\mathrm{pr}(\mathbf{a}|M,R)] = -\int d\mathbf{a}\, \mathrm{pr}(\mathbf{a}|M,R) \log\left[\frac{\mathrm{pr}(\mathbf{a}|M,R)}{m(x)}\right] + \lambda_0\left[1 - \int d\mathbf{a}\, \mathrm{pr}(\mathbf{a}|M,R)\right]$$
$$+ \lambda_1\left[(M+1)R^2 - \int d\mathbf{a}\, \mathbf{a}^2 \mathrm{pr}(\mathbf{a}|M,R)]\right]$$

  Then

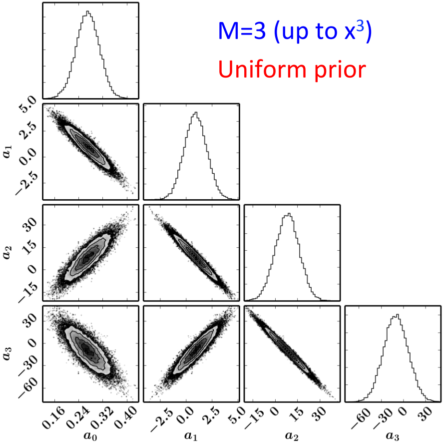
$$\frac{\delta Q}{\delta \mathrm{pr}(\mathbf{a}|M,R)} = 0 \text{ and } m(\mathbf{a}) = \text{const.} \Longrightarrow \mathrm{pr}(\mathbf{a}|M,R) = \left(\prod_{i=0}^{M} \frac{1}{\sqrt{2\pi}R}\right) \exp\left(-\frac{\mathbf{a}^2}{2R^2}\right)$$

Diagnostic tools 1: Triangle plots of posteriors from MCMC

Sample the posterior with an implementation of Markov Chain Monte Carlo (MCMC) [note: MCMC not actually needed for this example!]

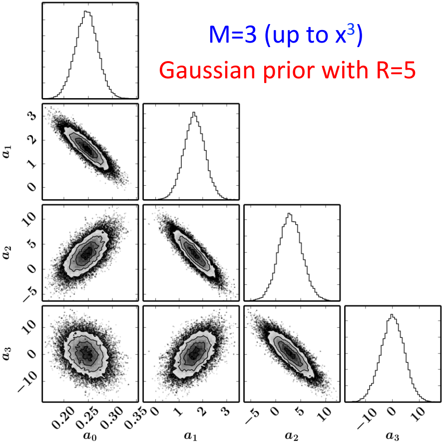
M=3 (up to x^3)

Uniform prior



M=3 (up to x^3)

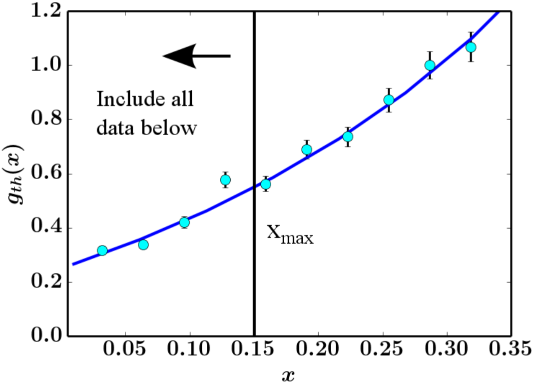
Gaussian prior with R=5



- With uniform prior, parameters play off each other
- With naturalness prior, much less correlation; note that a_2 and a_3 return prior $\Longrightarrow$ no information from data (but marginalized)

Diagnostic tools 2: Variable $x_{\max}$ plots $\Longrightarrow$ change fit range

Plot a_i with $M = 0, 1, 2, 3, 4, 5$ as a function of endpoint of fit data ($x_{\max}$)



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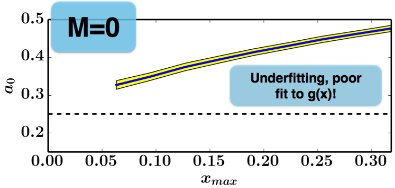
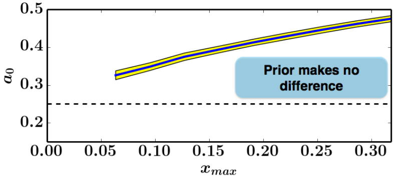


Naturalness prior ($R = 5$)



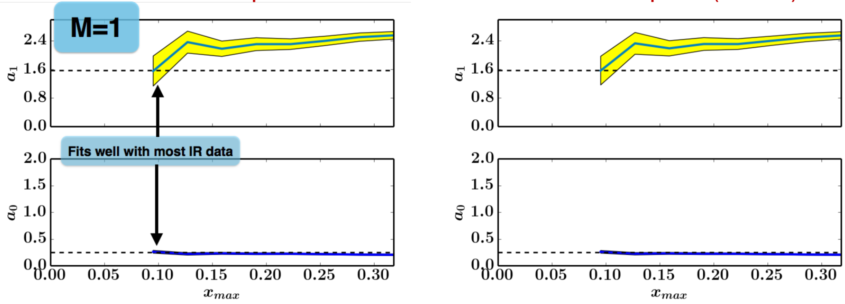
- For $M = 0$, $g(x) = a_0$ works only at lowest x (otherwise range too large)
- Very small error (sharp posterior), but wrong!
- Prior is irrelevant given a_0 values; we need to account for higher orders
- Bayesian solution: marginalize over higher M

Diagnostic tools 2: Variable $x_{\max}$ plots $\Longrightarrow$ change fit range

Plot a_i with $M = 0, 1, 2, 3, 4, 5$ as a function of endpoint of fit data ($x_{\max}$)

Uniform prior

Naturalness prior ($R = 5$)

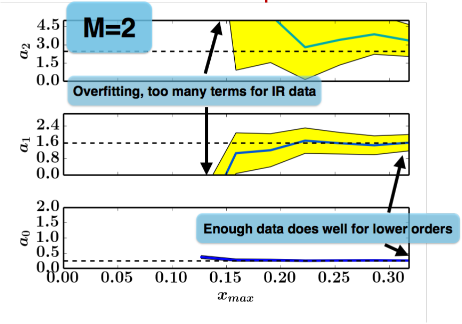


- For $M = 1$, $g(x) = a_0 + a_1 x$ works with smallest $x_{\max}$ only
- Errors (yellow band) from sampling posterior
- Prior is irrelevant given a_i values; we need to account for higher orders
- Bayesian solution: marginalize over higher M

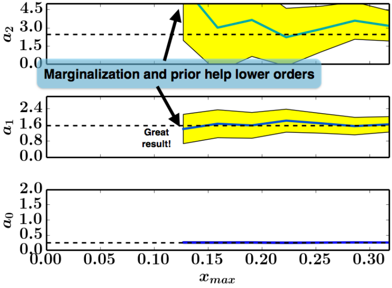
Diagnostic tools 2: Variable $x_{\max}$ plots $\Longrightarrow$ change fit range

Plot a_i with $M = 0, 1, 2, 3, 4, 5$ as a function of endpoint of fit data ($x_{\max}$)

Uniform prior



Naturalness prior ($R = 5$)

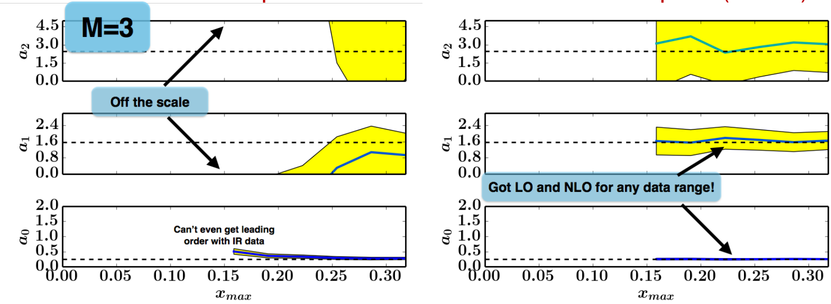


- For $M = 2$, entire fit range is usable
- Priors on a_1, a_2 important for a_1 stability with $x_{\max}$
- For this problem, using higher M is the *same* as marginalization

Diagnostic tools 2: Variable $x_{\max}$ plots $\Longrightarrow$ change fit range

Plot a_i with $M = 0, 1, 2, 3, 4, 5$ as a function of endpoint of fit data ($x_{\max}$)

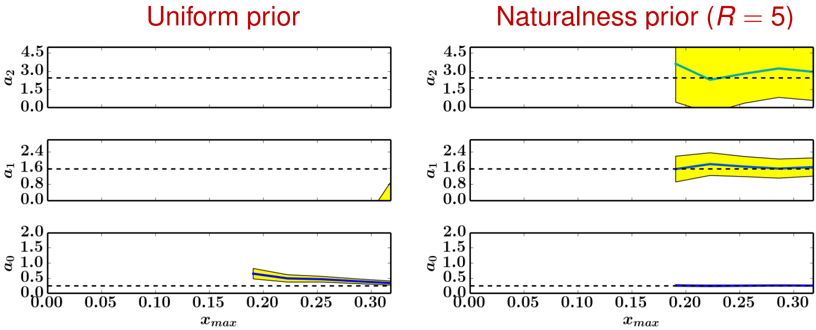
Uniform prior | Naturalness prior ($R = 5$)



- For $M = 3$, uniform prior is off the screen at lower $x_{\max}$
- Prior gives a_i stability with $x_{\max}$ $\Longrightarrow$ accounts for higher orders not in model
- For this problem, higher M is the *same* as marginalization

Diagnostic tools 2: Variable $x_{\max}$ plots $\Longrightarrow$ change fit range

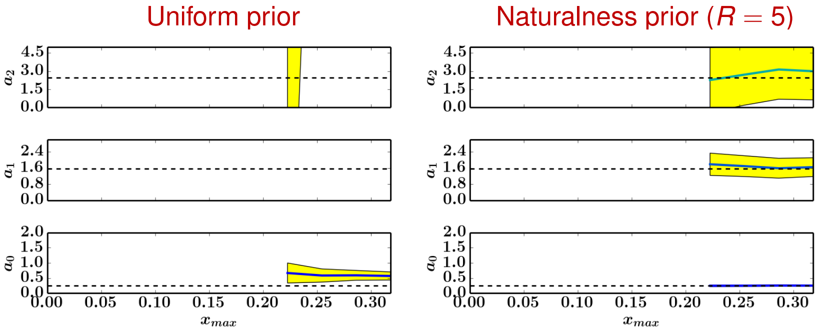
Plot a_i with $M = 0, 1, 2, 3, 4, 5$ as a function of endpoint of fit data ($x_{\max}$)



- For $M = 4$, uniform prior has lost a_0 as well
- Prior gives a_i stability with $x_{\max}$
- For this problem, higher M is the *same* as marginalization

Diagnostic tools 2: Variable $x_{\max}$ plots $\Longrightarrow$ change fit range

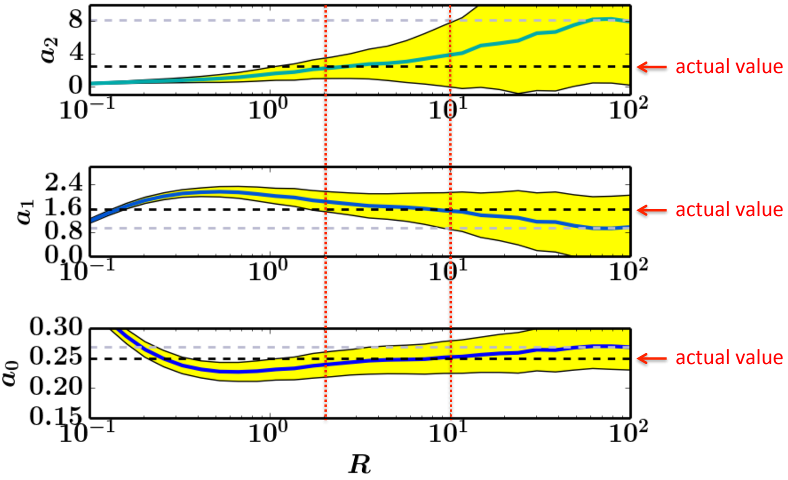
Plot a_i with $M = 0, 1, 2, 3, 4, 5$ as a function of endpoint of fit data ($x_{\max}$)



- For $M = 5$, $g(x) = a_0$ uniform prior has lost a_0 as well (range too large)
- Prior gives a_i stability with $x_{\max}$
- For this problem, higher M is the *same* as marginalization

Diagnostic tools 3: How do you know what R to use?

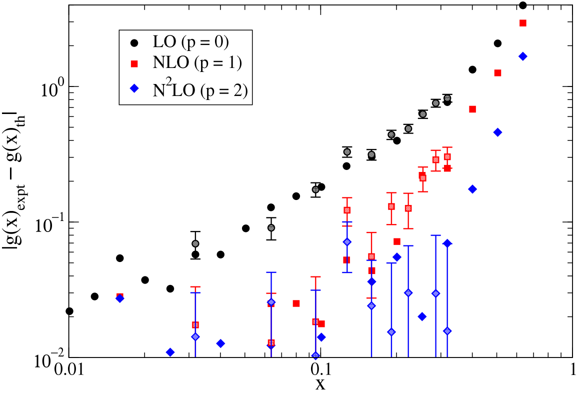
Gaussian naturalness prior but let R vary over a large range



- Error bands from posteriors (integrating over other variables)
- Light dashed lines are maximum likelihood (uniform prior) results
- Each a_i has a reasonable plateau from about 2 to 10 $\Longrightarrow$ marginalize!

Diagnostic tools 4: error plots (à la Lepage)

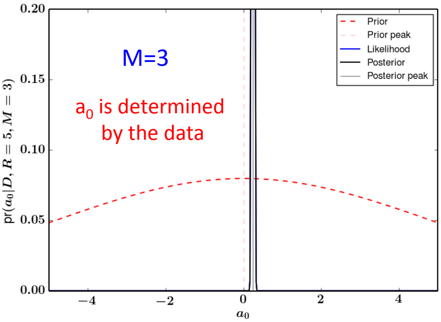
Plot residuals (data − predicted) from truncated expansion

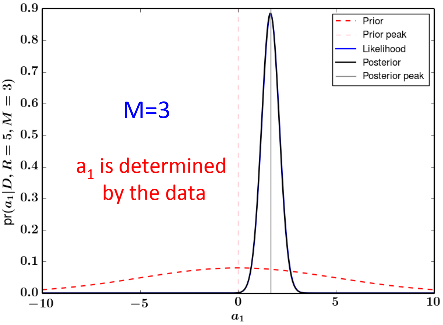


- 5% relative data error shown by bars on selected points
- Theory error dominates data error for residual over 0.05 or so
- Slope increase order $\Longrightarrow$ reflects truncation $\Longrightarrow$ “EFT” works!
- Intersection of different orders at breakdown scale

How the Bayes way fixes issues in the model problem

- By marginalizing over higher-order terms, we are able to use all the data, without deciding where to break; we find stability with respect to expansion order and amount of data
- Prior on naturalness suppresses overfitting by limiting how much different orders can play off each other
- Statistical and systematic uncertainties are naturally combined
- Diagnostic tools identify sensitivity to prior, whether the EFT is working, breakdown scale, theory vs. data error dominance, . . .





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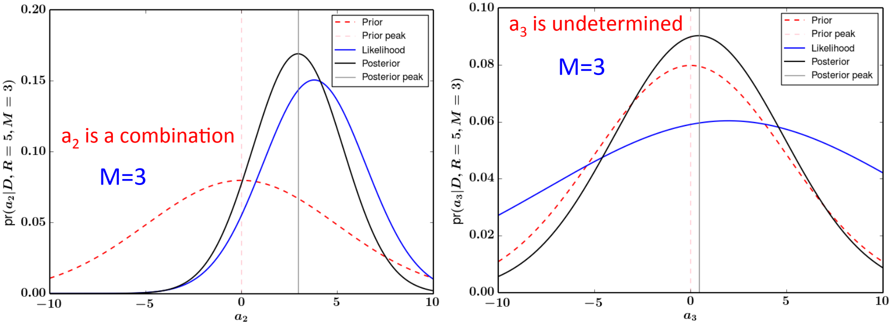

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Could we have done all this just adding a “theory error” to our χ^2 likelihood function (e.g., a penalty for unnatural LECs)?

- When everything is a gaussian, we can combine the prior and likelihood into an “augmented χ^2”. But in general, no.
- Even so, it *doesn’t* take the form of a simple extra weighting for theory error added in quadrature

Many other tests with model problems . . .

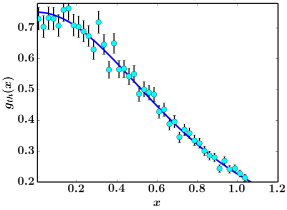
- Alternative functions (including non-linear) to test robustness, e.g.,

$$g_\alpha(x) = \frac{\alpha}{(x^2+\alpha^2)^2}$$

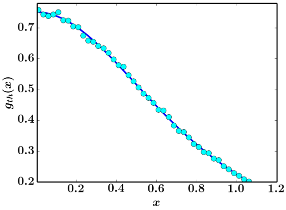
  - For $\alpha = 1.1$, Taylor series is

$$g_{\text{th}}(x) = 0.751 - 1.242x^2 + 1.540x^4 - 1.700x^6 + \mathcal{O}(x^8)$$

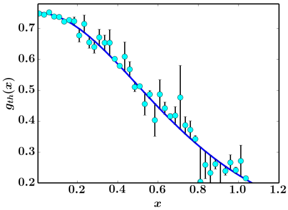
- Different kinds of error on data from $g_{\alpha=1.1}(x)$



5% relative error



1% relative error



High in UV, low in IR

- Alternative priors, error propagation to non-fit observables
- Blind tests of fitting protocols $\Longrightarrow$ shows that unnatural LECs identified

Nucleon mass and sigma term in χPT [in progress]

The chiral expansion of the nucleon mass $M_{\chi\text{PT}}$ in SU(2) χPT as a function of the lowest-order pion mass m is (with renormalization scale μ):

$$M_{\chi\text{PT}}(m) = M_0 + k_1 m^2 + k_2 m^3 + k_3 m^4 \log\left(\frac{m}{\mu}\right) + k_4 m^4 + k_5 m^5 \log\left(\frac{m}{\mu}\right) + k_6 m^5 + k_7 m^6 \log\left(\frac{m}{\mu}\right)^2 + k_8 m^6 \log\left(\frac{m}{\mu}\right) + k_9 m^6 + \mathcal{O}(m^7)$$

- Goal: fit to lattice data and extract sigma term, etc.

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$$\frac{M_{\chi\text{PT}}(m)}{\Lambda} = \frac{M_0}{\Lambda} + \frac{\tilde{k}_1}{\Lambda^2} m^2 + \frac{\tilde{k}_2}{\Lambda^3} m^3 + \frac{\tilde{k}_3}{\Lambda^4} m^4 \log\left(\frac{m}{\mu}\right) + \frac{\tilde{k}_4}{\Lambda^4} m^4 + \frac{\tilde{k}_5}{\Lambda^5} m^5 \log\left(\frac{m}{\mu}\right) + \frac{\tilde{k}_6}{\Lambda^5} m^5$$
$$+ \frac{\tilde{k}_7}{\Lambda^6} m^6 \log\left(\frac{m}{\mu}\right)^2 + \frac{\tilde{k}_8}{\Lambda^6} m^6 \log\left(\frac{m}{\mu}\right) + \frac{\tilde{k}_9}{\Lambda^6} m^6 + \mathcal{O}(m^7)$$

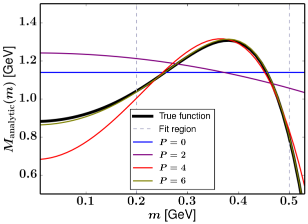
- Goal: fit to lattice data and extract sigma term, etc.
- When scaled to $\Lambda = 0.5\,\text{GeV}$, phenomenological $\tilde{k}_i$'s are natural:

$$\widetilde{M}_0 = 1.76, \quad \tilde{k}_1 = 1.92, \quad \tilde{k}_2 = -1.41, \quad \tilde{k}_3 = 0.81\,, \quad \tilde{k}_4 = 1.03,$$
$$\tilde{k}_5 = 2.97, \quad \tilde{k}_6 = 4.41, \quad \tilde{k}_7 = 0.4, \quad \tilde{k}_8 = 0.31, \quad \tilde{k}_9 = -3.12,$$

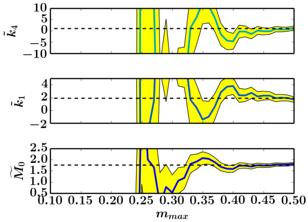
- If non-analytic terms are given, then this looks like our toy models!
- Plan: use pseudo-data to test fitting robustness based on including a naturalness prior, fit range, lattice error, etc.
  - Can we fit the non-analytic terms as well?

Nucleon mass and sigma term in χPT [in progress]

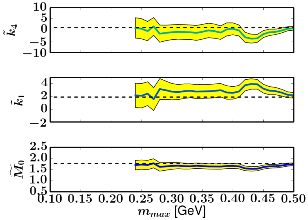
- Fitting window is limited by available lattice data
- Proof-of-principle tests with pseudo-data
- Fits at different orders in χPT expansion



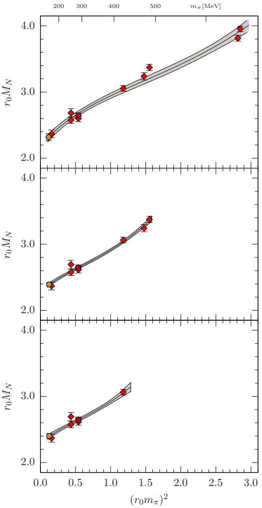
with uniform prior



with naturalness prior



Lattice $n_f = 2$ data, fits



Goal: Use Bayesian framework with naturalness prior plus diagnostic tools to improve stability and robustness of fits. Status: much like toy problems!

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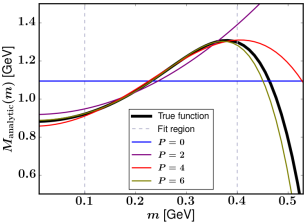
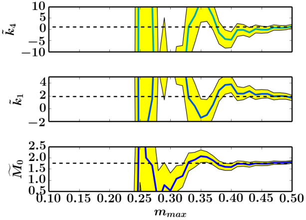
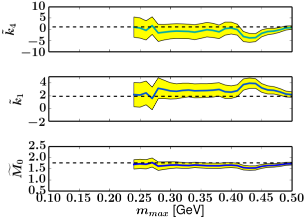


with uniform prior



with naturalness prior



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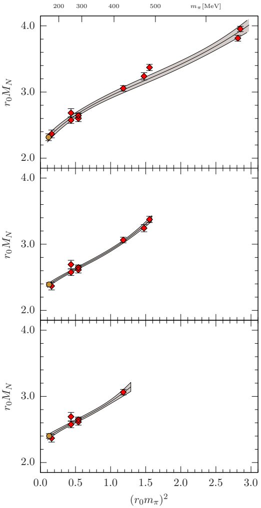

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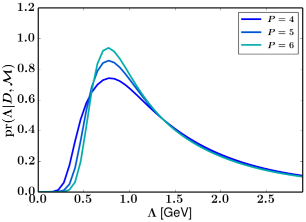
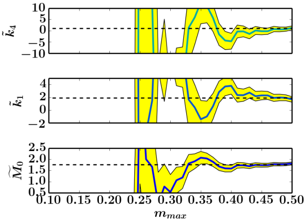
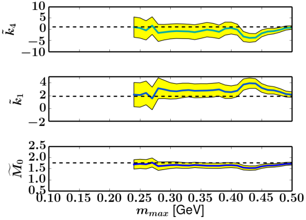


with uniform prior



with naturalness prior



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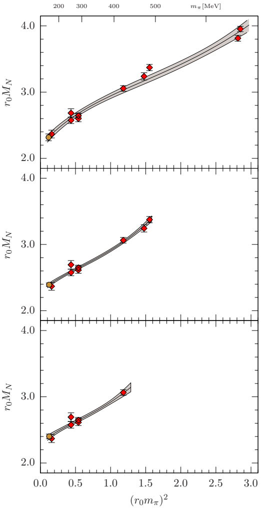

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Outline

Theory errors and nuclear EFT

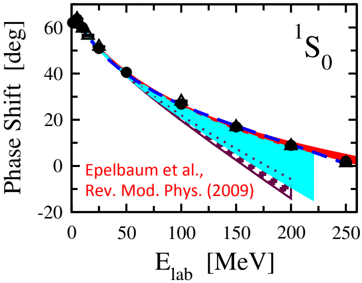
Bayesian methods applied to a model problem

Application to chiral EFT $\Longrightarrow$ building on EKM

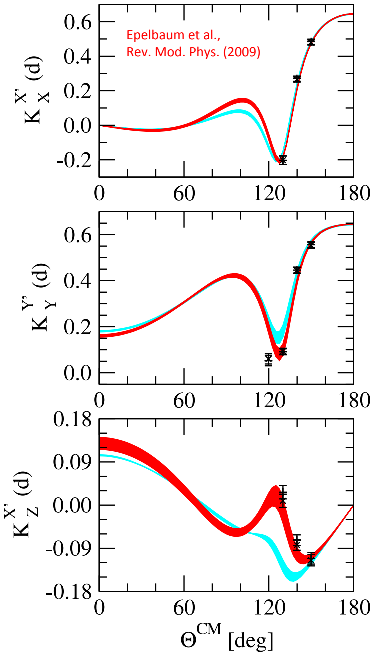
Going forward . . .

Previous UQ: Error bands in chiral EFT

- Bands from EFT cutoff variation
- below: neutron-proton $^1S_0$ phase shift at NLO, N^2LO, and N^3LO



- right: chiral EFT predictions for *p*–*d* spin observables



Problems with this as UQ:

- Unpleasing systematics of bands
- Often underestimates uncertainty
- Statistical interpretation???

New NN potential and theory errors: EKM scheme

"Improved chiral nucleon-nucleon potential up to next-to-next-to-next-to-leading [i.e., fourth] *order"* by E. Epelbaum, H. Krebs, and U.-G. Meißner, arXiv:1412.0142

New choices of regulators to minimize cutoff artifacts

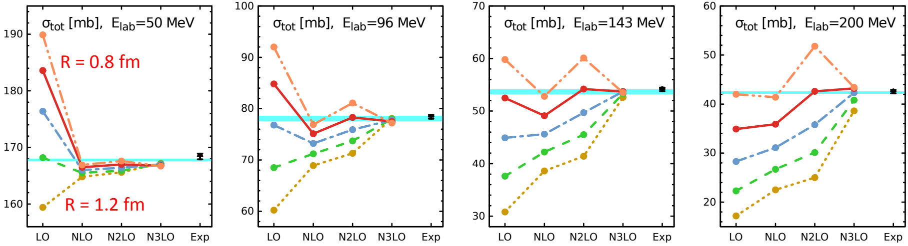
- Local regulator for long-distance parts (pion exchange):

$$V_{\text{long-range}}(\mathbf{r})f(r/R) \quad \text{with} \quad f(x) = [1 - e^{-x^2}]^n \; (n \geq 4)$$

- Non-local regulator for contact interactions:

$$V_{\text{contact}}(\mathbf{p}, \mathbf{p}')e^{-((p^2+p'^2)/\Lambda^2)^{m/2}} \quad (m = 2 \text{ and } \Lambda = 2/R)$$

Order-by-order convergence of total np cross section for $R = 0.8$ to $1.2\,\text{fm}$



Note that R dependence only decreases with new NN LECs

New NN potential and theory errors

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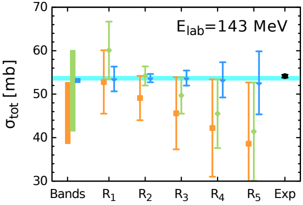
- Local regulator with cutoff R for long-distance parts
- Non-local regulator with cutoff $\Lambda = 2/R$ for contacts



- NLO (orange), N2LO (green), N3LO (blue)

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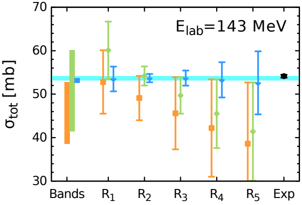
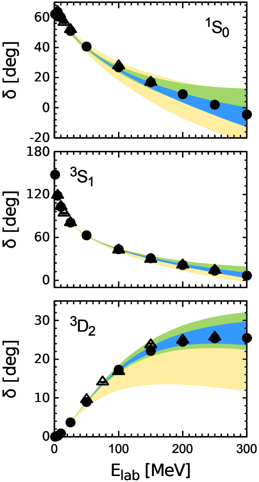
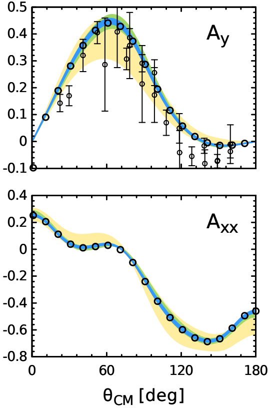


- NLO (orange), N2LO (green), N3LO (blue)
- Right: error bands at fixed $R_2 = 0.9\,\mathrm{fm}$





Old way: "Bands" show range of central results for R_1–R_5

New way: Estimate error range at each R_i by comparison to lower orders

Fitting protocol

1. Restrict the range in energy to fit NPWA phase shifts at each order;
2. Check that LECs from the fit are natural;
3. Add a data point with assumed error for the D-state probability of the deuteron ($P_D = 5\% \pm 1\%$);
4. Use an augmented χ^2 to penalize deviations from Wigner SU(4) symmetry (which implies $\tilde{C}_{1S0} \approx \tilde{C}_{3S1}$); [?]
5. Assumption for the error of the phase shifts from Nijmegen 1993 PWA. Uncertainty for calculating χ^2/datum combining statistical plus systematic errors in phase shifts by ("X" is the channel):

$$\Delta_X = \max\left(\Delta_X^{\mathrm{NPWA}}, |\delta_X^{\mathrm{Nijm\,I}} - \delta_X^{\mathrm{NPWA}}|, |\delta_X^{\mathrm{Nijm\,II}} - \delta_X^{\mathrm{NPWA}}|, |\delta_X^{\mathrm{Reid93}} - \delta_X^{\mathrm{NPWA}}|\right)$$

The determination of errors from omitted higher-order is calculated separately.

Fitting protocol with proposed Bayesian upgrades

1. Restrict the range in energy to fit NPWA phase shifts at each order;
   $\Longrightarrow$ use *all* data and marginalize over missing orders
2. Check that LECs from the fit are natural;
   $\Longrightarrow$ include a naturalness prior on LECs
3. Add a data point with assumed error for the D-state probability of the deuteron ($P_D = 5\% \pm 1\%$);
   $\Longrightarrow$ add a prior on P_D
4. Use an augmented χ^2 to penalize deviations from Wigner SU(4) symmetry (which implies $\tilde{C}_{1S0} \approx \tilde{C}_{3S1}$); [?]
   $\Longrightarrow$ add as a prior on these LECs
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   $\Longrightarrow$ all combined in the posterior PDF

The determination of errors from omitted higher-order is calculated separately.
$\Longrightarrow$ What is a Bayesian alternative?

New NN potential and theory errors: $\mathrm{N^4LO}$

"Precision nucleon-nucleon potential at fifth order in the chiral expansion"
by E. Epelbaum, H. Krebs, and U.-G. Meißner, arXiv:1412.4623

- Identify the expansion parameter Q by

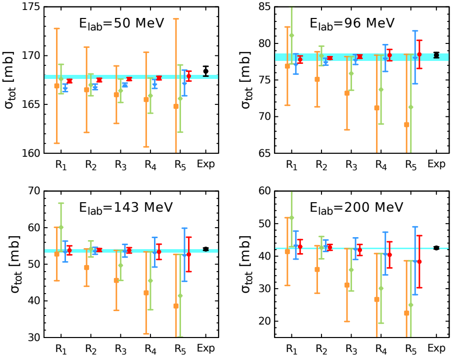
$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right)$$

which entails identifying Λ_b, the breakdown scale of the EFT.

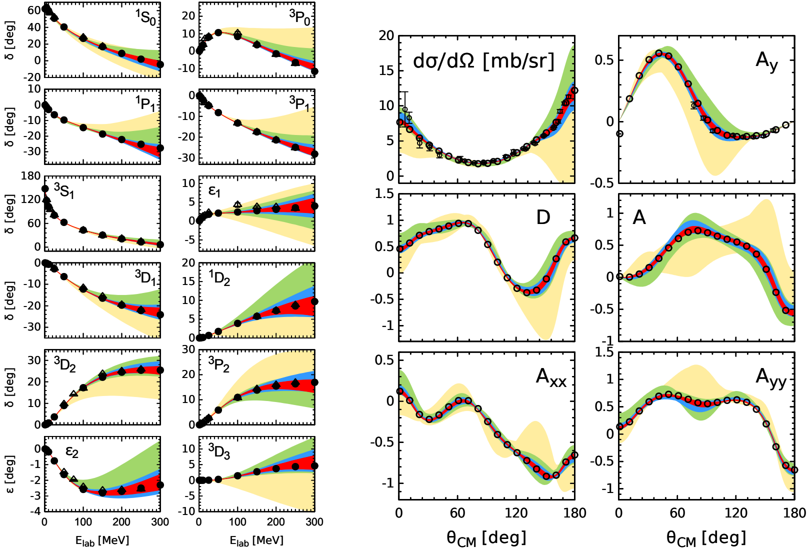
- Uncertainty for observable $X(p)$ at a given order determined from calculations at all lower orders. Example: uncertainty $\Delta X^{\mathrm{N^3LO}}(p)$ of $\mathrm{N^3LO}$ prediction $X^{\mathrm{N^3LO}}(p)$:

$$\Delta X^{\mathrm{N^3LO}}(p) = \max\Big(Q^5 \times |X^{\mathrm{LO}}(p)|,\; Q^3 \times |X^{\mathrm{LO}}(p) - X^{\mathrm{NLO}}(p)|,\; Q^2 \times |X^{\mathrm{NLO}}(p) - X^{\mathrm{N^2LO}}(p)|,\; Q \times |X^{\mathrm{N^2LO}}(p) - X^{\mathrm{N^3LO}}(p)|\Big)$$

- Figure below shows order-by-order convergence of total cross sections
- Breakdown scale when error stops improving ($R \approx 0.9\,\mathrm{fm}$)



Phase shifts and spin observables for $R = 0.9\,\mathrm{fm}$



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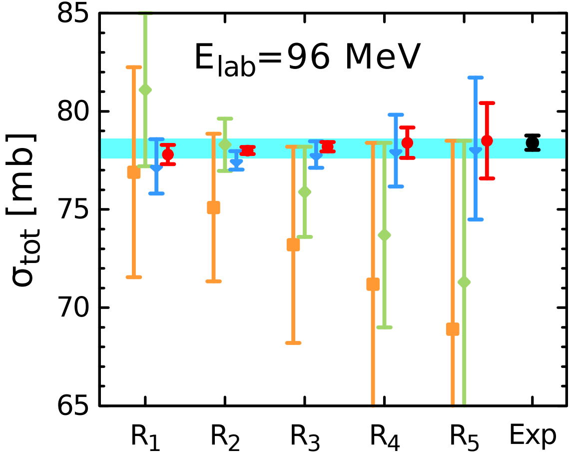

Can we justify these "error bars" in a Bayesian framework?

Estimating nuclear EFT truncation errors

- Adapt Bayesian technology used in pQCD [Cacciari and Houdeau (2011)]

up to k^{th} order: $$\sigma_{\text{QCD}} \approx \sum_{n=0}^{k} c_n \alpha_s^n \longrightarrow \sigma_{np} \approx \sigma_{\text{ref}} \sum_{n=0}^{k} c_n \left(\frac{p}{\Lambda_b}\right)^n$$

where $\Lambda_b \approx 600\,\text{MeV}$ (new: determine Λ_b self-consistently!)

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- Goal: find $\Delta_k \equiv \sum_{n=k+1}^{\infty} c_n z^n$ where $z = \alpha_s$ or p/Λ_b (or scaled)
- Underlying assumption based on naturalness: all c_n's are about the same size or have a pdf with the same upper bound, denoted $\bar{c}$.

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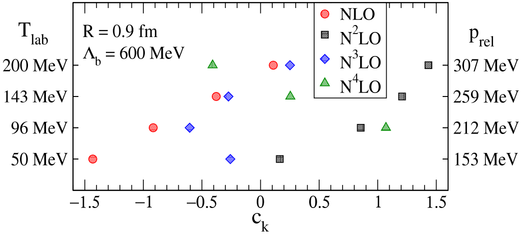
- Underlying assumption based on naturalness: all c_n's are about the same size or have a pdf with the same upper bound, denoted $\bar{c}$.
- Check whether c_n's have a bounded distribution for a chiral EFT observable: $\sigma_{np} \approx \sigma_0(1 + c_2 z^2 + c_3 z^3 + \cdots)$ with $z = p/600\,\text{MeV}$

- σ_{np} from EKM at $R = 0.9\,\text{fm}$
- Coefficients at four energies
- z from about 1/4 to 1/2
- Natural: $c_n \sim \mathcal{O}(1)$

$\Longrightarrow$ apply as Bayesian priors on c_n, $\bar{c}$



Estimating nuclear EFT truncation errors for R_2

- Determine $\mathrm{pr}(\Delta_k|c_0,\cdots,c_k)$ by Bayes' theorem and possible priors for $\bar{c}$:

set	$\mathrm{pr}(c_n\|\bar{c})$	$\mathrm{pr}(\bar{c})$
A	$\frac{1}{2\bar{c}}\,\theta(\bar{c}-\|c_n\|)$	$\frac{1}{\ln \bar{c}_>/\bar{c}_<}\,\frac{1}{\bar{c}}\theta(\bar{c}-\bar{c}_<)\theta(\bar{c}_>-\bar{c})$
B	$\frac{1}{2\bar{c}}\,\theta(\bar{c}-\|c_n\|)$	$\frac{1}{\sqrt{2\pi}\bar{c}\sigma}\,e^{-(\log\bar{c})^2/2\sigma^2}$
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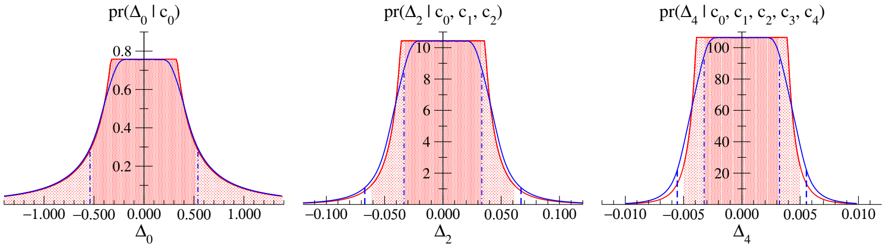
- For set A, apply Bayes' theorem and marginalization repeatedly:

$$\mathrm{pr}(\Delta_k|c_0,\ldots,c_k) \approx \left(\frac{n_c}{n_c+1}\right)\frac{1}{2z^{k+1}\bar{c}_{(k)}}\begin{cases}1 & \text{if } |\Delta_k| \le z^{k+1}\bar{c}_{(k)}\\ \left(\dfrac{z^{k+1}\bar{c}_{(k)}}{|\Delta_k|}\right)^{n_c+1} & \text{if } |\Delta_k| > z^{k+1}\bar{c}_{(k)}\end{cases}$$



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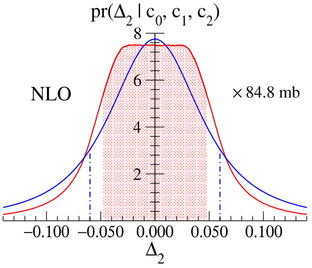

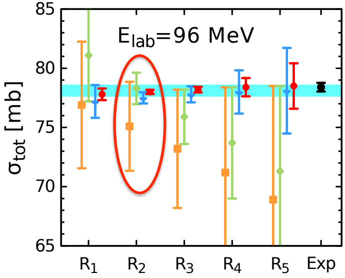

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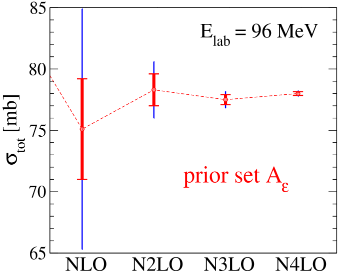

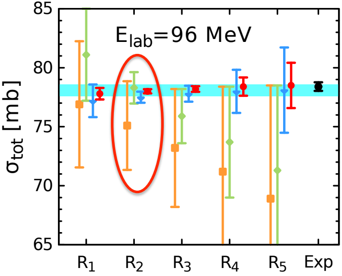

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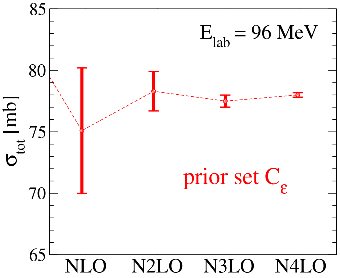

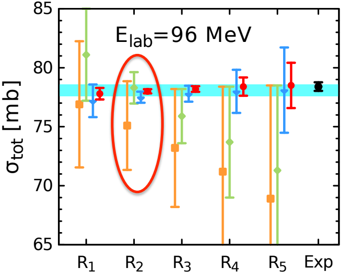

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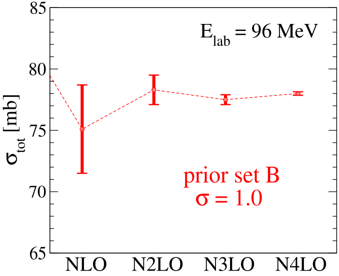

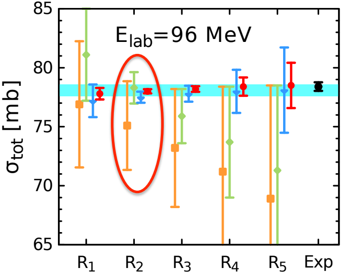

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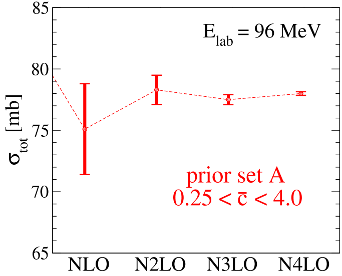

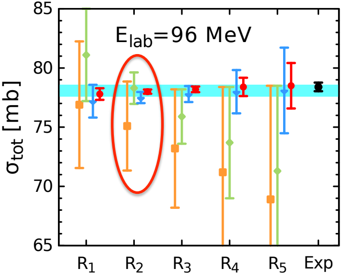

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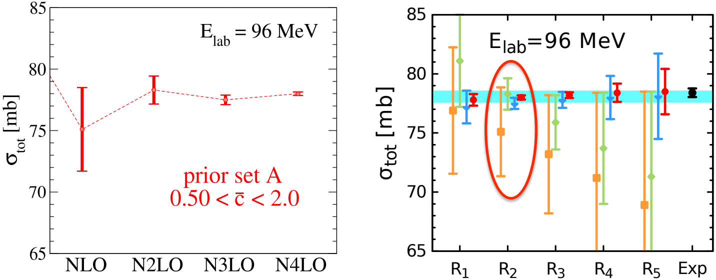

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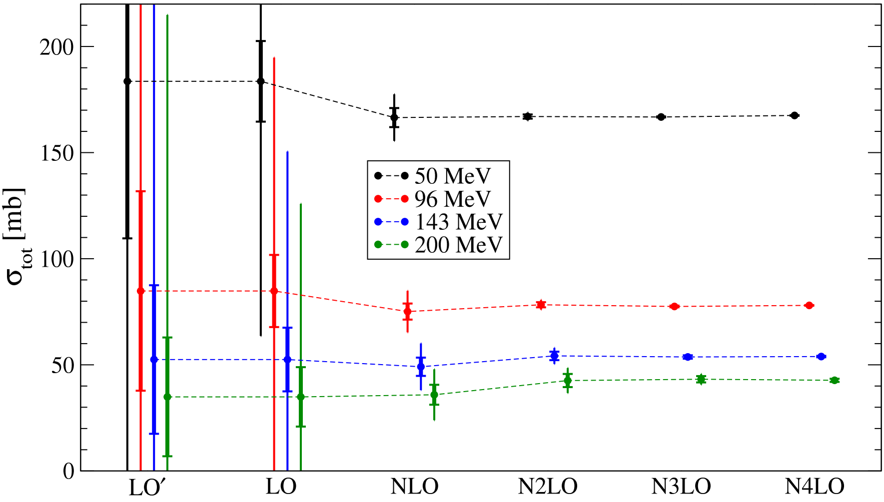
Full results from analytic prior (set A_ϵ)

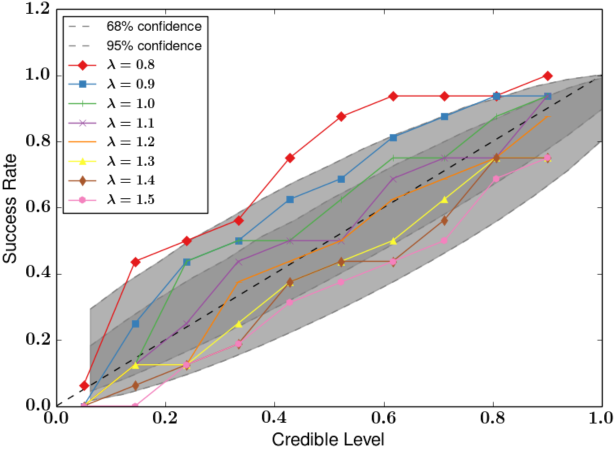


- Bold error bars are 68% credibility intervals
- Thin error bars are 95% credibility intervals

Can we find Λ_b from order-by-order observables?

- Consistency method as part of $\overline{\text{CH}}$ protocol
- Compare "success rate" of next order prediction against expectation from credibility interval as a function of scaling parameter λ:

$$\sigma_{np} \approx \sigma_{\text{ref}} \sum_{n=0}^{k} c_n \left(\frac{p}{\lambda\Lambda_b}\right)^n$$

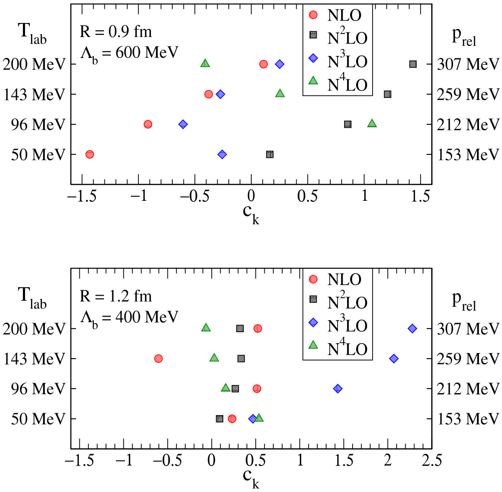


What about other R values?

- Recall the expansion of σ_{np} (for $p > m_\pi$):

$$\sigma_{np} \approx \sigma_{\rm ref} \sum_{n=0}^{k} c_n \left(\frac{p}{\Lambda_b}\right)^n$$

- Compare c_n's for $R = 0.9$ fm and $R = 1.2$ fm (note Λ_b's)
- Can also use alternative $\sigma_{\rm ref}$
- How do we assess the distribution for $R = 1.2$ fm, which has regulator artifacts?
- Need more data!



Derivation of analytic posterior for Δ_k

1. Marginalize over the coefficients for omitted terms (cf. insert complete states)

$$\mathrm{pr}(\Delta_k|c_0,\ldots,c_k) = \int \mathrm{pr}(\Delta_k|c_{k+1},c_{k+2},\ldots)\,\mathrm{pr}(c_{k+1},c_{k+2},\ldots|c_0,\ldots,c_k)\,dc_{k+1}\,dc_{k+2}\cdots$$

$$= \int \Big[\delta(\Delta_k - \sum_{n=k+1}^{\infty} c_n z^n)\Big]\,\mathrm{pr}(c_{k+1},c_{k+2},\ldots|c_0,\ldots,c_k)\,dc_{k+1}\,dc_{k+2}\cdots$$

2. Insert $\bar{c}$ (marginalize) and apply independence assumption

$$\mathrm{pr}(c_{k+1},c_{k+2},\ldots|c_0,\ldots,c_k) = \int \mathrm{pr}(c_{k+1},c_{k+2},\ldots|\bar{c})\,\mathrm{pr}(\bar{c}|c_0,\ldots,c_k)\,d\bar{c}$$

$$= \int \Big[\prod_{n=k+1}^{\infty} \mathrm{pr}(c_n|\bar{c})\Big]\mathrm{pr}(\bar{c}|c_0,\ldots,c_k)\,d\bar{c}$$

3. Assume (for now) the error is dominated by the first omitted term

$$\mathrm{pr}(\Delta_k|c_0,\ldots,c_k) = \int \big[\delta(\Delta_k - c_{k+1}z^{k+1})\big]\mathrm{pr}(c_{k+1}|\bar{c})\,\mathrm{pr}(\bar{c}|c_0,\ldots,c_k)\,d\bar{c}\,dc_{k+1}$$

$$= \frac{1}{z^{k+1}} \int \mathrm{pr}(c_{k+1} = \Delta_k/z^{k+1}|\bar{c})\,\mathrm{pr}(\bar{c}|c_0,\ldots,c_k)\,d\bar{c}$$

Derivation of analytic posterior for Δ_k (cont.)

4. Apply Bayes' theorem and the independence assumptions

$$
\begin{aligned}
\mathrm{pr}(\bar{c}|c_0,\ldots,c_k) &= \frac{\mathrm{pr}(c_0,\ldots,c_k|\bar{c})\,\mathrm{pr}(\bar{c})}{\int \mathrm{pr}(c_0,\ldots,c_k|\bar{c}')\,\mathrm{pr}(\bar{c}')\,d\bar{c}'} \\
&= \frac{\left[\prod_{n=0}^{k} \mathrm{pr}(c_n|\bar{c})\right]\mathrm{pr}(\bar{c})}{\int \left[\prod_{n=0}^{k} \mathrm{pr}(c_n|\bar{c}')\right]\mathrm{pr}(\bar{c}')\,d\bar{c}'}
\end{aligned}
$$

5. Put it all together:

$$
\mathrm{pr}(\Delta_k|c_0,\ldots,c_k) = \frac{\int \mathrm{pr}(c_{k+1} = \Delta_k/z^{k+1}|\bar{c})\left[\prod_{n=0}^{k} \mathrm{pr}(c_n|\bar{c})\right]\mathrm{pr}(\bar{c})\,d\bar{c}}{z^{k+1}\int \left[\prod_{n=0}^{k} \mathrm{pr}(c_n|\bar{c}')\right]\mathrm{pr}(\bar{c}')\,d\bar{c}'}
$$

6. Substitute your choice of priors and integrate (analytic for set A_ϵ). Relaxing the assumption of first-omitted-term dominance is straightforward.

Outline

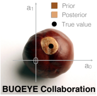
Theory errors and nuclear EFT

Bayesian methods applied to a model problem

Application to chiral EFT $\Longrightarrow$ building on EKM

Going forward . . .

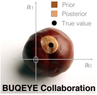
Goals of UQ for EFT calculations



- Reflect *all* sources of uncertainty in an EFT prediction
- Compare theory predictions and experimental results statistically
- Distinguish uncertainties from IR (long-range) vs. UV (short-range) physics
- Guidance on how to extract EFT parameters (LECs)
- Test whether EFT is working as advertised— do our predictions exhibit the anticipated systematic improvement?

Goals of UQ for EFT calculations

BUQEYE ("Bayesian Uncertainty Quantification: Errors in Your EFT")



"A recipe for EFT uncertainty quantification in nuclear physics," J. Phys. G

- Reflect *all* sources of uncertainty in an EFT prediction
  $\Longrightarrow$ likelihood or prior for each
- Compare theory predictions and experimental results statistically
  $\Longrightarrow$ error bands as Bayesian credibility intervals
- Distinguish uncertainties from IR (long-range) vs. UV (short-range) physics
  $\Longrightarrow$ separate priors (?); avoid overfitting
- Guidance on how to extract EFT parameters (LECs)
  $\Longrightarrow$ Bayes propagates new info (e.g., will an additional or better measurement or lattice calculation help and by how much?)
- Test whether EFT is working as advertised— do our predictions exhibit the anticipated systematic improvement?
  $\Longrightarrow$ Trends of credibility interval; model selection

The Bayesian framework lets us consistently achieve our UQ goals!

Next steps and open questions

- Apply full Bayesian framework to EFT fitting
  - First NN, then NNN
  - Computationally feasible?
- Test full propagation of EFT errors order-by-order
- Try applying Bayesian model selection (what's that?)
- (Some) future questions to address:
  - When are standard alternatives (theory penalties) ok?
  - What are the best measurements to better constrain LECs?
  - Is it ever ok to fine-tune an observable?
  - Is the EFT working as advertised?
  - Can nuclei resolve pions?
  - How well can lattice calculations constrain LECs?

Bayesian model selection

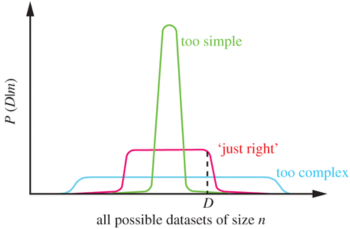
Determine the evidence for different models M_1 and M_2 via marginalization by integrating over possible sets of parameters **a** in different models, same D and information I.

The evidence ratio for two different model:

$$\frac{\mathrm{pr}(M_1|D,I)}{\mathrm{pr}(M_2|D,I)} = \frac{\mathrm{pr}(D|M_1,I)\,\mathrm{pr}(M_1|I)}{\mathrm{pr}(D|M_2,I)\,\mathrm{pr}(M_2|I)}$$

The Bayes Ratio (implements Occam's Razor):

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



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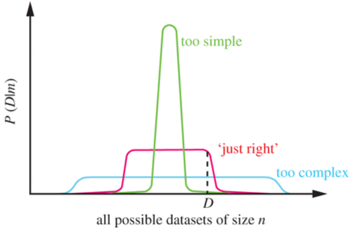
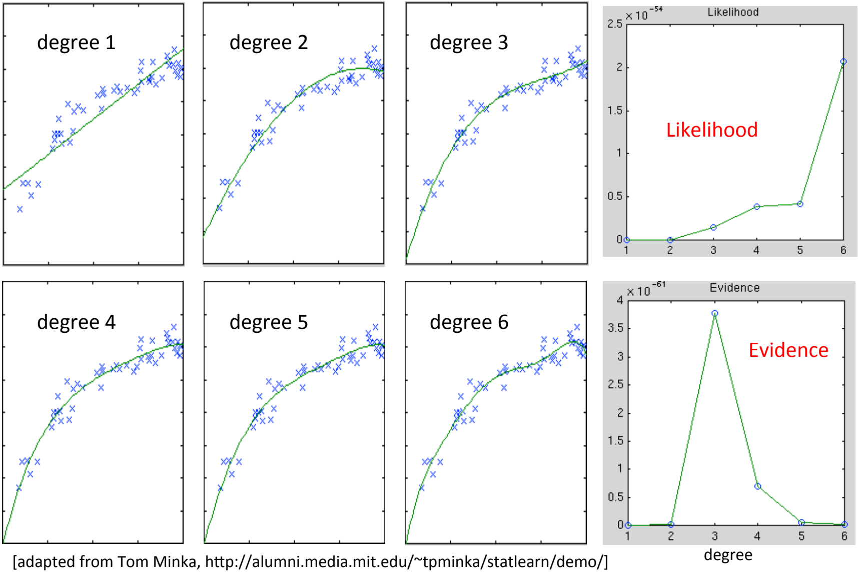


Examples of how we could use this in EFT context:

- Which EFT parameters $\Longrightarrow$ improve the fit to data?
- Which EFT power counting is more effective? (cf. more parameters)
- Pionless vs. chiral EFT?

Bayesian model selection: polynomial fitting



[adapted from Tom Minka, http://alumni.media.mit.edu/~tpminka/statlearn/demo/]

The likelihood considers the single most probable curve, and always increases with increasing degree. The evidence is a maximum at 3, the true degree!