Errors in Effective Field Theory and Why They Matter

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Background

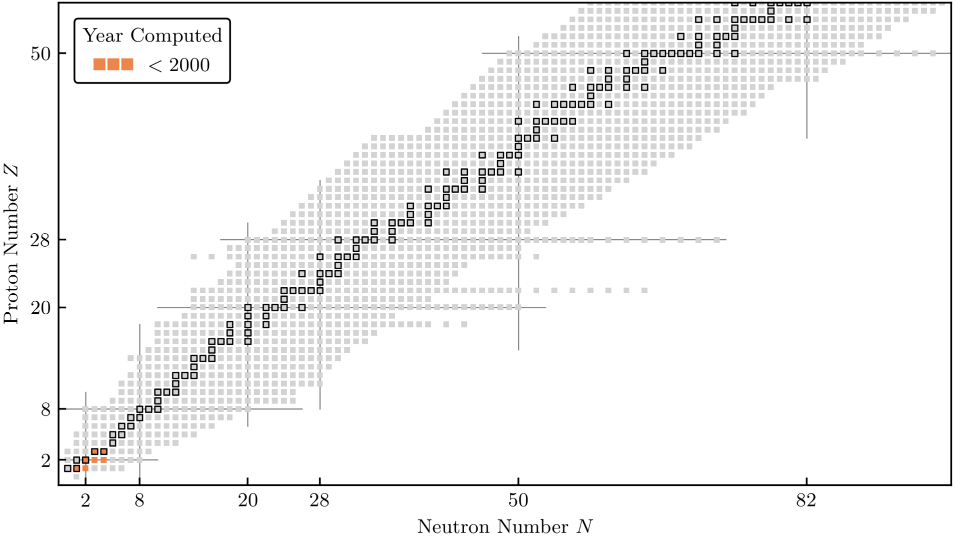
"From First Principles"

- A subset of nuclear theorists works on ab initio methods.
- Goal: predict all nuclear properties from basic assumptions

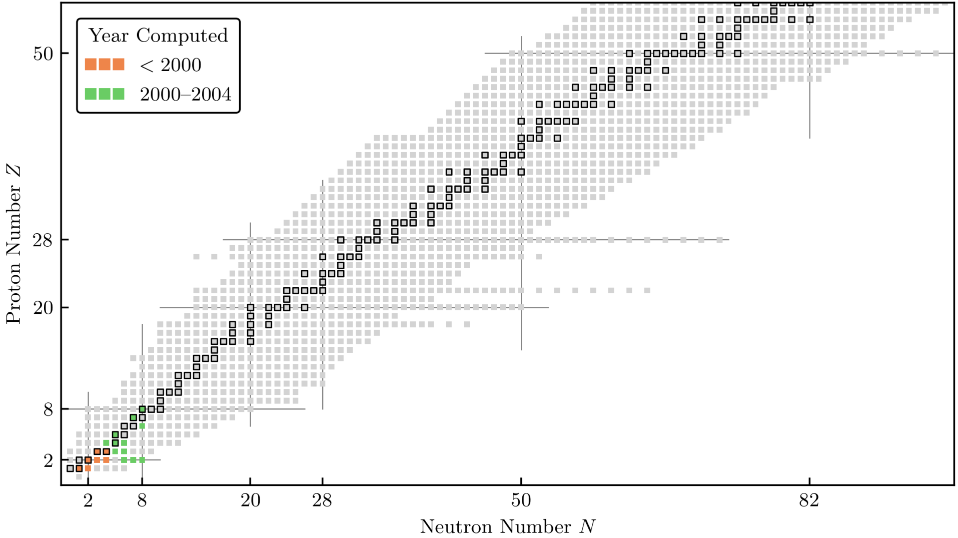
“From First Principles”

- A subset of nuclear theorists works on ab initio methods.
- Goal: predict all nuclear properties from basic assumptions
- Take protons & neutrons as given; predict everything else.
- Desire a connection to the more fundamental theory: quantum chromodynamics

The Precision Era



The Precision Era



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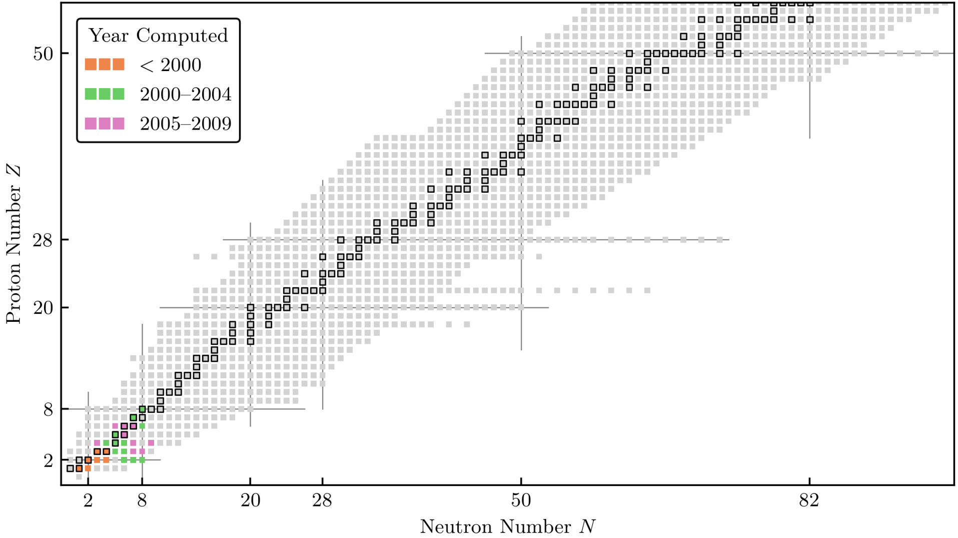

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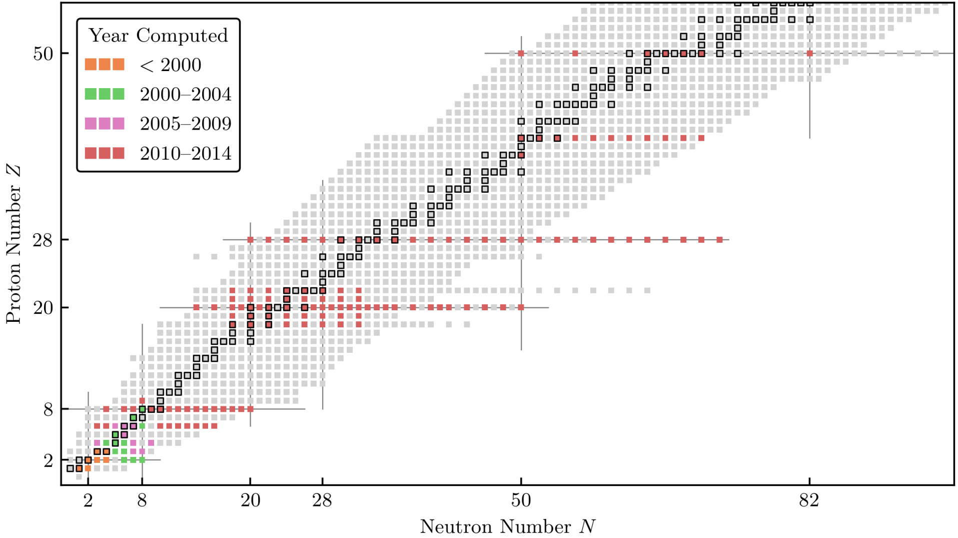

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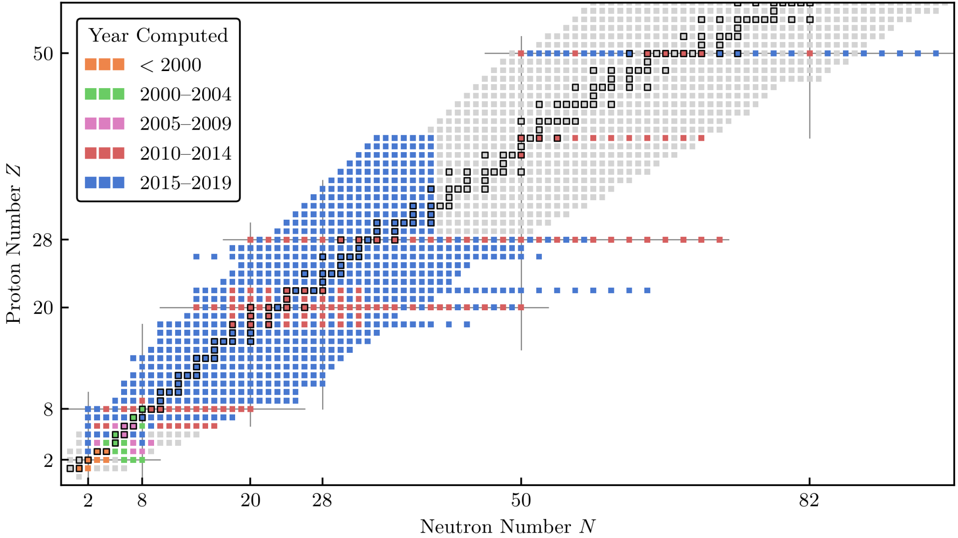

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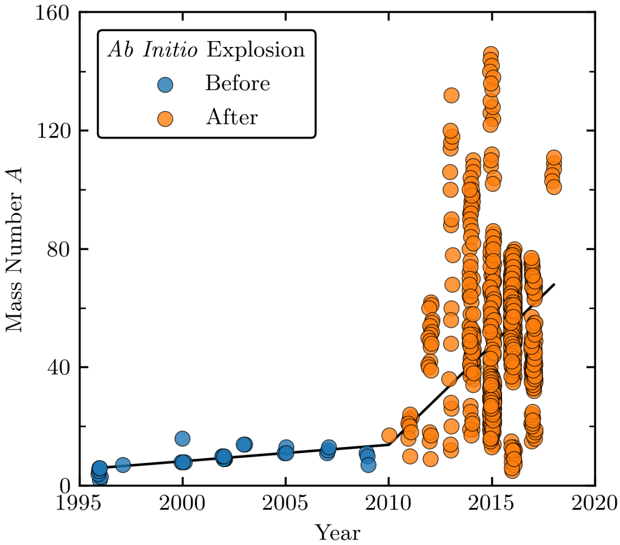

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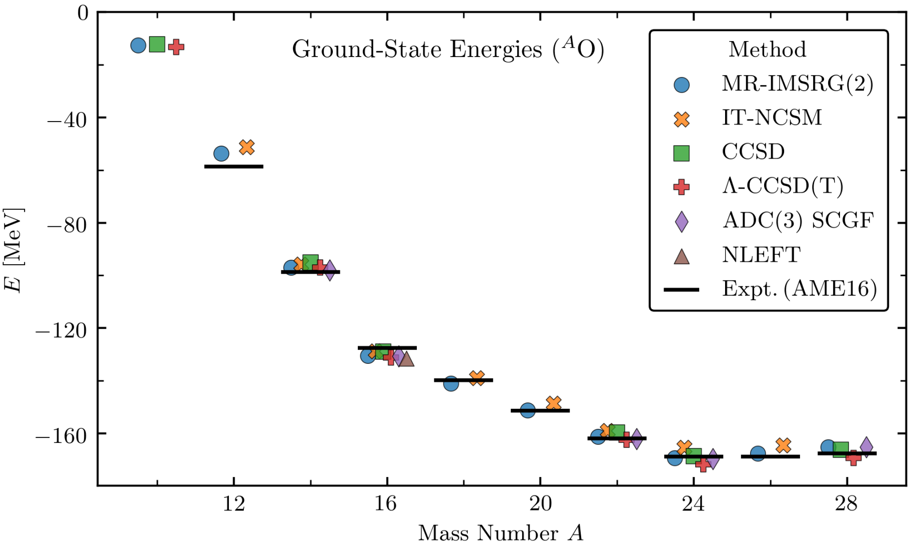

The Precision Era

- We've entered the precision era!
- $\rightarrow$ It's time to worry about the details.
- Error bars aren't just for experimentalists...

Phys. Rev. A Editorial (April 2011)

Papers presenting the results of theoretical calculations are expected to include uncertainty estimates...

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

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This work makes novel contributions to uncertainty quantification methods for nuclear predictions.

Figure credit: Danielle Towne

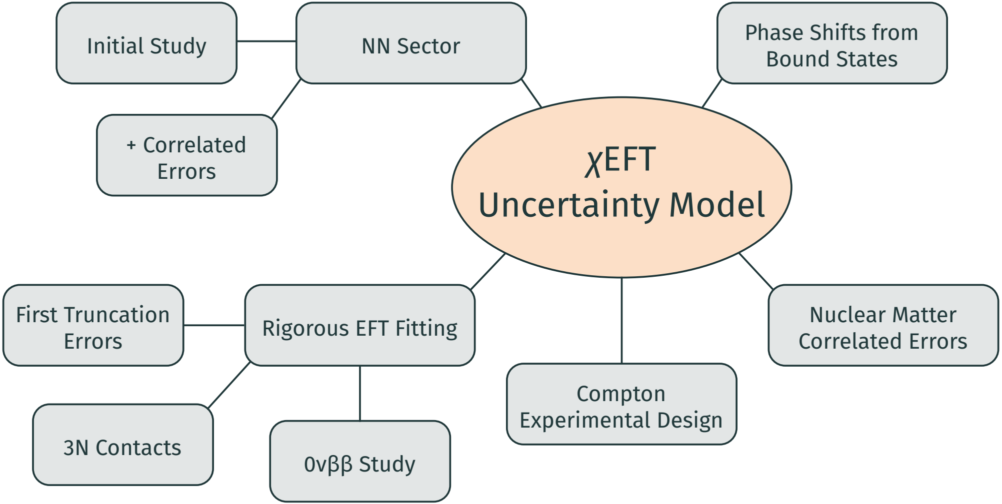
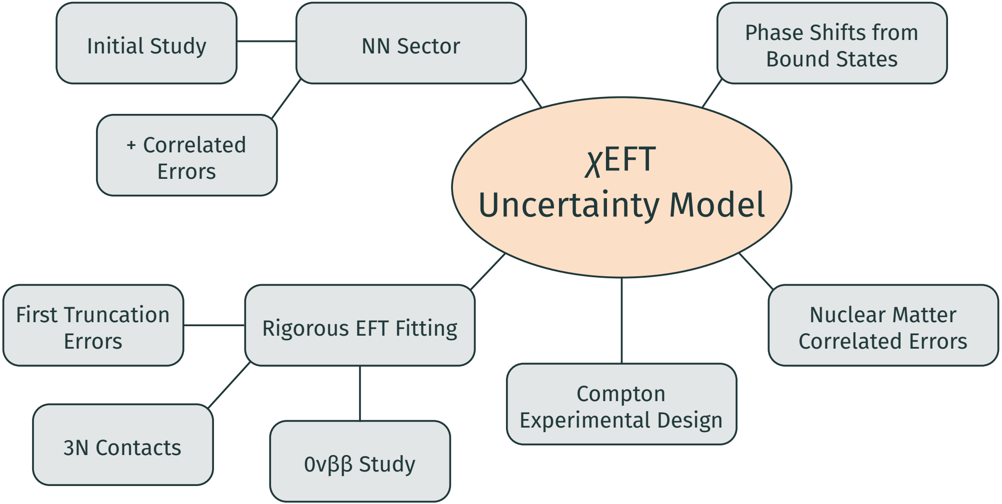


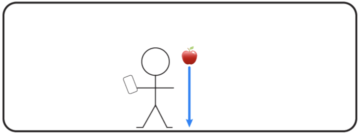
Figure credit: Danielle Towne



The codes for all published work has been made publicly available

→ reproducibility & extendability

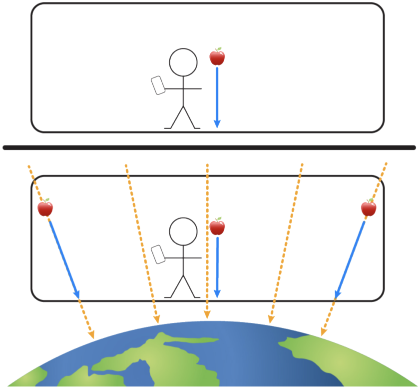
Scales in Physics



Grav. force (short distances):

$$F = -mg$$

Scales in Physics



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Grav. force (large distances):

$$F = -\frac{GMm}{r^2}$$

The laws look quite different!

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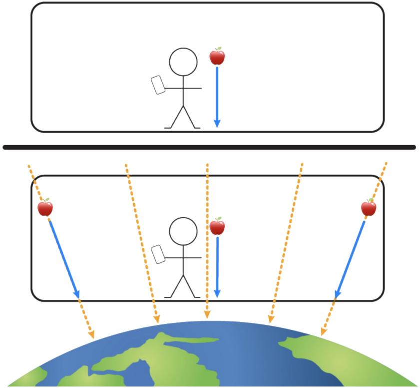

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Grav. force (large distances):

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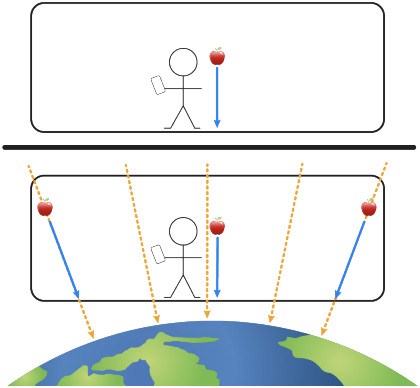
Connected via series expansion about radius of Earth R:

$$F \approx -mg + 2mg\left(\frac{r-R}{R}\right) - 3mg\left(\frac{r-R}{R}\right)^2 + \mathcal{O}\left[\left(\frac{r-R}{R}\right)^3\right]$$

Scales in Physics



Grav. force (short distances):

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Grav. force (large distances):

$$\boxed{F = -\frac{GMm}{r^2}}$$

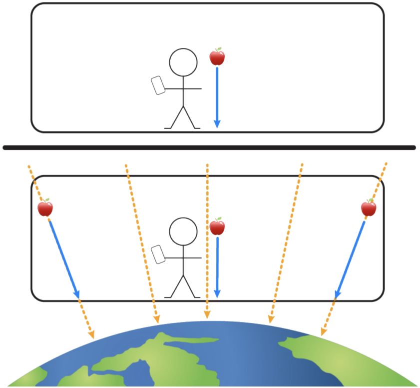
???

The laws look quite different!

Can fit unknown parameters to data $\Rightarrow$ inverse problem!

$$F \approx a_0 + a_1 \left(\frac{r-R}{R}\right) + a_2 \left(\frac{r-R}{R}\right)^2 + \mathcal{O}\left[\left(\frac{r-R}{R}\right)^3\right]$$

Scales in Physics



Grav. force (short distances):

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Grav. force (large distances):

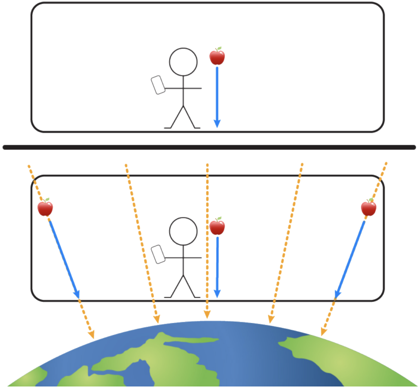
$$\boxed{F = -\frac{GMm}{r^2} \;???}$$

The laws look quite different!

Use prior info from physics:

$$F \approx mg \left\{ a_0' + a_1' \left(\frac{r-R}{R} \right) + a_2' \left(\frac{r-R}{R} \right)^2 + \mathcal{O}\left[\left(\frac{r-R}{R} \right)^3 \right] \right\}$$

Scales in Physics



Grav. force (short distances):

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$$\boxed{F = -\frac{GMm}{r^2}}$$

???

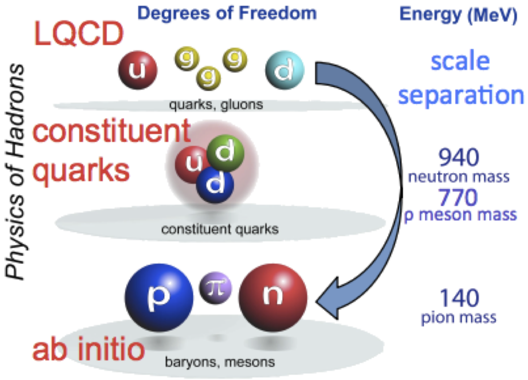
The laws look quite different!

Propagate full uncertainty

$$F \approx mg\left\{a'_0 + a'_1\left(\frac{r-R}{R}\right) + a'_2\left(\frac{r-R}{R}\right)^2 + \mathcal{O}\left[\left(\frac{r-R}{R}\right)^3\right]\right\}$$

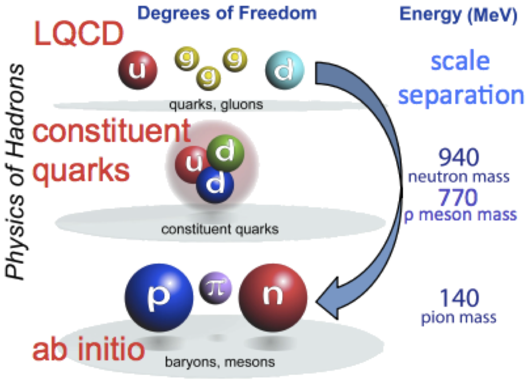
Predictions in Low-Energy Nuclear Physics

- There is interesting physics at all scales



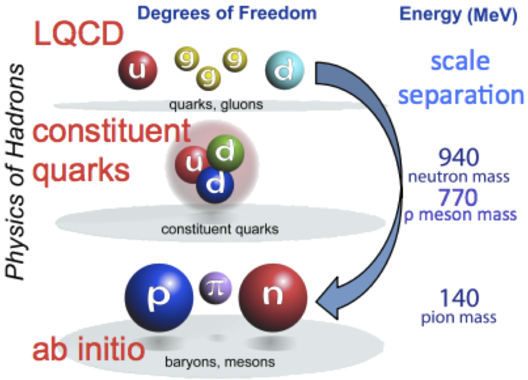
Predictions in Low-Energy Nuclear Physics

- There is interesting physics at all scales
- Fine details at one level of analysis do not affect the physics at a coarser level of analysis



Predictions in Low-Energy Nuclear Physics

- There is interesting physics at all scales
- Fine details at one level of analysis do not affect the physics at a coarser level of analysis
- Start simple $\rightarrow$ add corrections to reach desired precision.



$$y_{\mathrm{exp}}(x) = y_{\mathrm{th}}(x, \vec{a}) + \delta y_{\mathrm{th}}(x) + \delta y_{\mathrm{exp}}$$

To theorists, magic

$$y_{\text{exp}}(x) = y_{\text{th}}(x, \vec{a}) + \delta y_{\text{th}}(x) + \delta y_{\text{exp}}$$

Parameters

Discrepancy

$$\overset{\chi^2 \text{ fit}}{y_{\text{exp}}(x) = y_{\text{th}}(x, \vec{a})} \qquad\qquad + \delta y_{\text{exp}}$$

$$\overbrace{y_{\mathrm{exp}}(x) = y_{\mathrm{th}}(x, \vec{a}}^{\text{rigorous fit}}) + \delta y_{\mathrm{th}}(x) + \delta y_{\mathrm{exp}}$$

$$y_{\mathrm{exp}}(x) = \overbrace{y_{\mathrm{th}}(x, \vec{a}) + \delta y_{\mathrm{th}}(x)}^{\text{Full Prediction}} + \delta y_{\mathrm{exp}}$$

$$y_{\mathrm{exp}}(x) = y_{\mathrm{th}}(x, \vec{a}) + \underbrace{\delta y_{\mathrm{th}}(x)}_{\substack{\text{Can we build this?} \\ \text{Can we use it?}}} + \delta y_{\mathrm{exp}}$$

$$y_{\text{exp}}(x) = y_{\text{th}}(x, \vec{a}) + \underbrace{\delta y_{\text{th}}(x)} + \delta y_{\text{exp}}$$

Can we build this?

Can we use it?

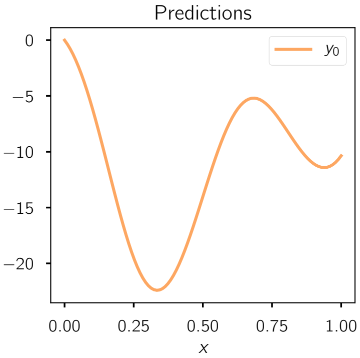
Takeaway info about our δy_{th} model:

Built in		Results in
Physics-based	$\longleftrightarrow$	Discovery
Energy degradation	$\longleftrightarrow$	E_{max} insensitivity
Correlations	$\longleftrightarrow$	Derivatives (& More!)
Smart priors	$\longleftrightarrow$	Easy & analytic!

Chiral EFT in One Slide

- $V_{NN}(\vec{a}) = V_{LO} + V_{NLO} + \cdots + V_{N^kLO} \Longrightarrow \boxed{\text{Schrödinger Eq.}} \Longrightarrow y_k(x; \vec{a})$

$$\{y_0\}$$



$y_0 \to \text{LO}$

Chiral EFT in One Slide

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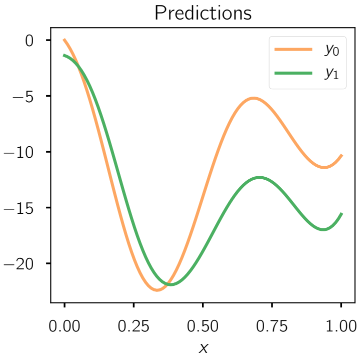
$$\{y_0, y_1\}$$



$y_0 \to \text{LO}$

$y_1 \to \text{NLO}$

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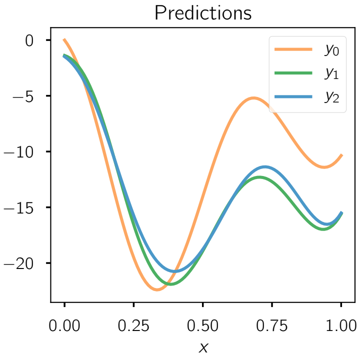
- $V_{NN}(\vec{a}) = V_{LO} + V_{NLO} + \cdots + V_{N^kLO} \Longrightarrow \boxed{\text{Schrödinger Eq.}} \Longrightarrow y_k(x; \vec{a})$

$$\{y_0, y_1, y_2\}$$



$y_0 \rightarrow \text{LO}$

$y_1 \rightarrow \text{NLO}$

$y_2 \rightarrow \text{N}^2\text{LO}$

Chiral EFT in One Slide

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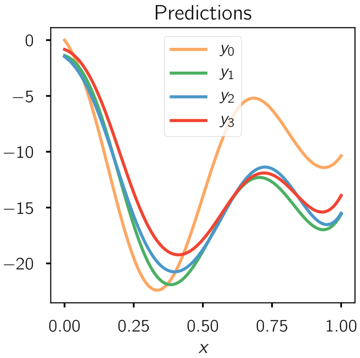
$$\{y_0, y_1, y_2, y_3\}$$



$y_0 \to$ LO

$y_1 \to$ NLO

$y_2 \to$ N^{2}LO

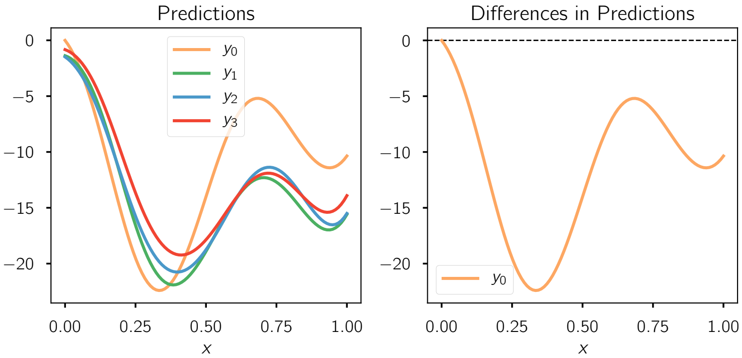
$\vdots$

$y_k \to$ N^{k}LO

Chiral EFT in One Slide

- $V_{NN}(\vec{a}) = V_{LO} + V_{NLO} + \cdots + V_{N^kLO} \Longrightarrow \boxed{\text{Schrödinger Eq.}} \Longrightarrow y_k(x; \vec{a})$
- One can change variables for convenience/insight.

$$y_0 = y_0$$



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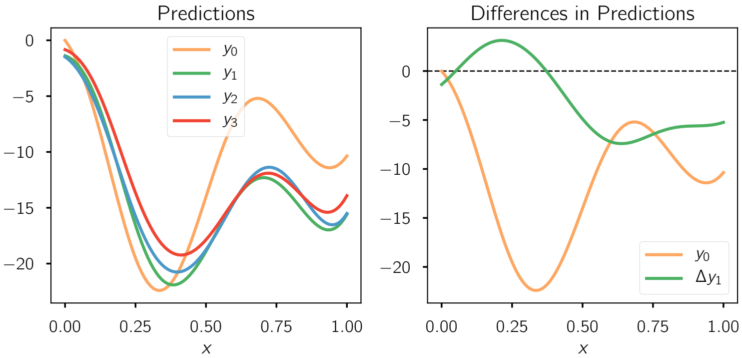
$$y_1 = y_0 + \Delta y_1$$



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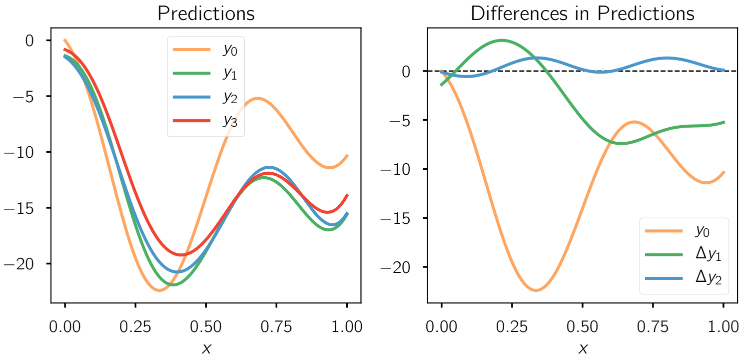
- One can change variables for convenience/insight.

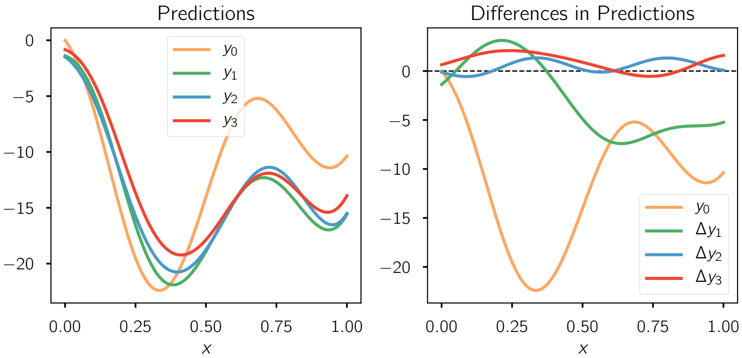
$$y_2 = y_0 + \Delta y_1 + \Delta y_2$$



Chiral EFT in One Slide

- $V_{NN}(\vec{a}) = V_{LO} + V_{NLO} + \cdots + V_{N^kLO} \implies \boxed{\text{Schrödinger Eq.}} \implies y_k(x; \vec{a})$
- One can change variables for convenience/insight.
- $\Delta y_n = y_{\text{ref}} c_n Q^n$

$$y_3 = y_0 + \Delta y_1 + \Delta y_2 + \Delta y_3$$



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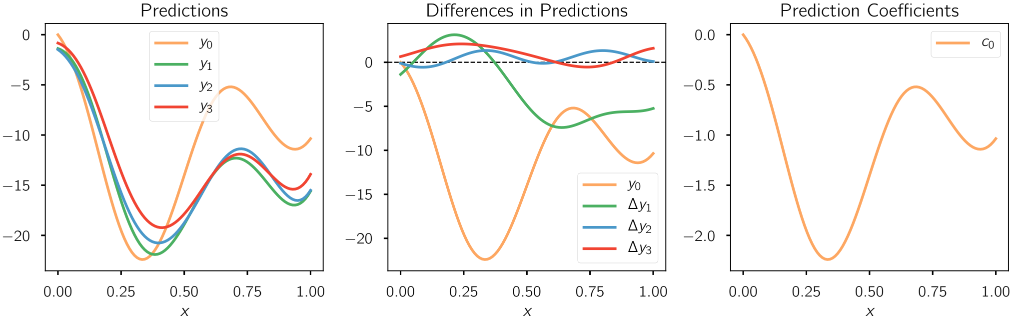
$$y_0 = y_{\text{ref}} \left[c_0 Q^0\right]$$



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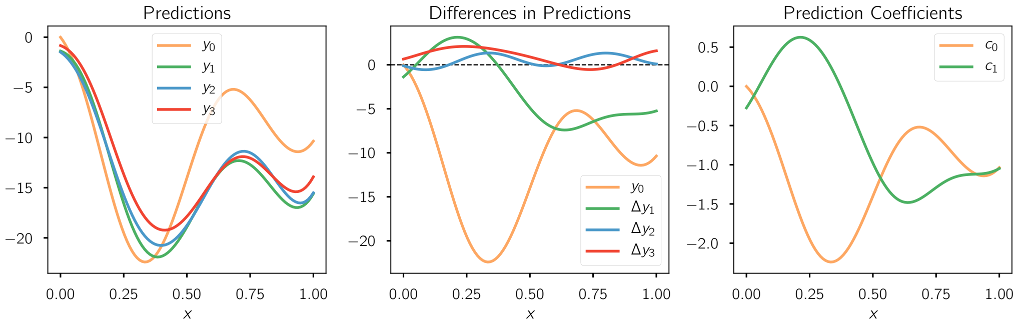
$$y_1 = y_{\text{ref}} \left[c_0 Q^0 + c_1 Q^1 \right]$$



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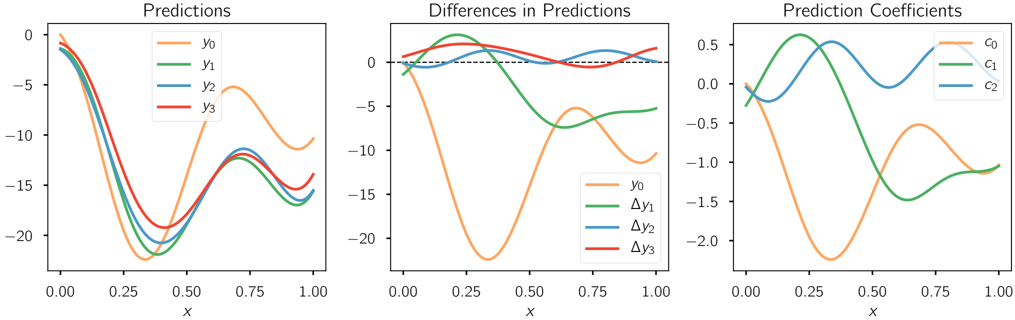
$$y_2 = y_{\mathrm{ref}}\left[c_0 Q^0 + c_1 Q^1 + c_2 Q^2\right]$$



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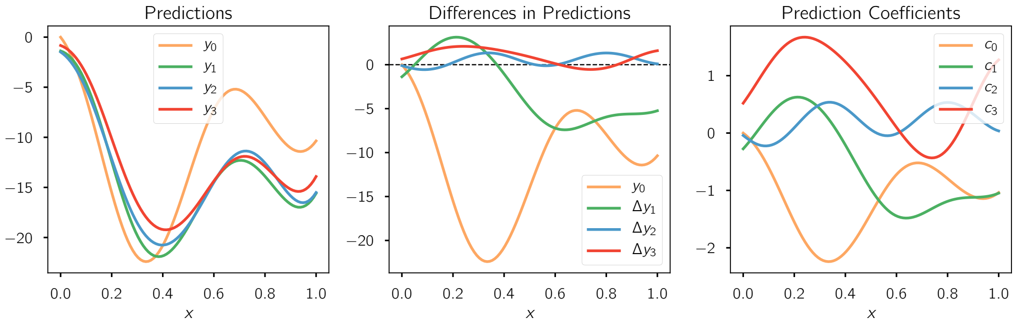
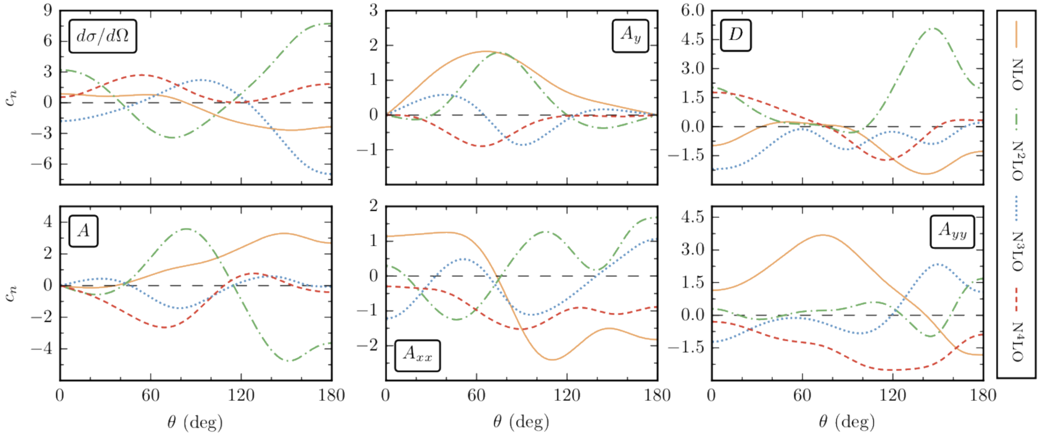
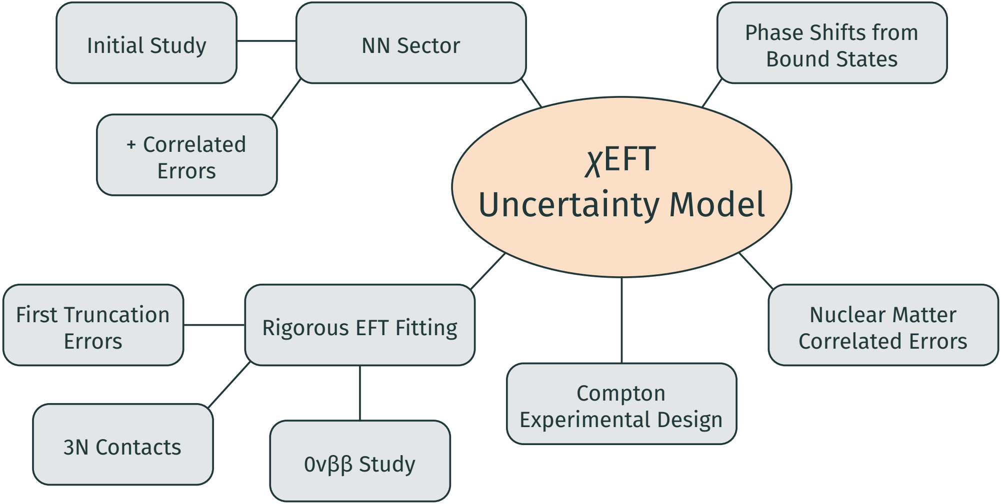
$$y_3 = y_{\mathrm{ref}}\left[c_0 Q^0 + c_1 Q^1 + c_2 Q^2 + c_3 Q^3\right]$$



Real Life

Coefficients from NN scattering look like our toy model!



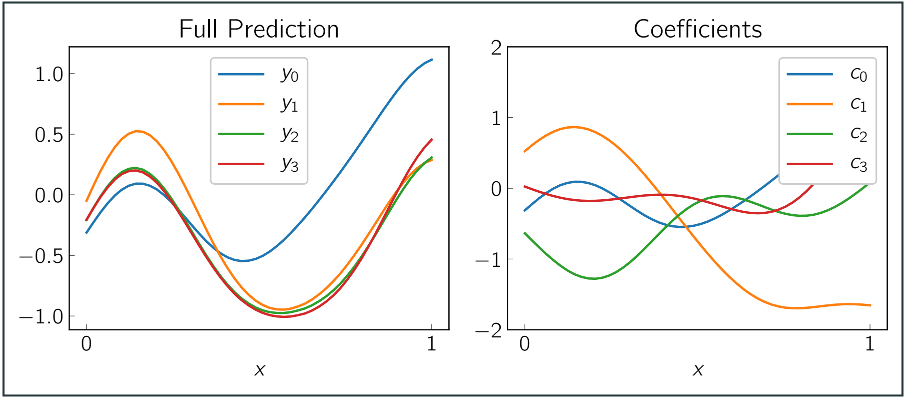

χEFT Uncertainty Model
NN Sector
Initial Study
+ Correlated Errors
Phase Shifts from Bound States
Rigorous EFT Fitting
First Truncation Errors
3N Contacts
0νββ Study
Compton Experimental Design
Nuclear Matter Correlated Errors

Model Building

Main equation

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

$$c_n \equiv \frac{y_n - y_{n-1}}{y_{\text{ref}} Q^n}$$



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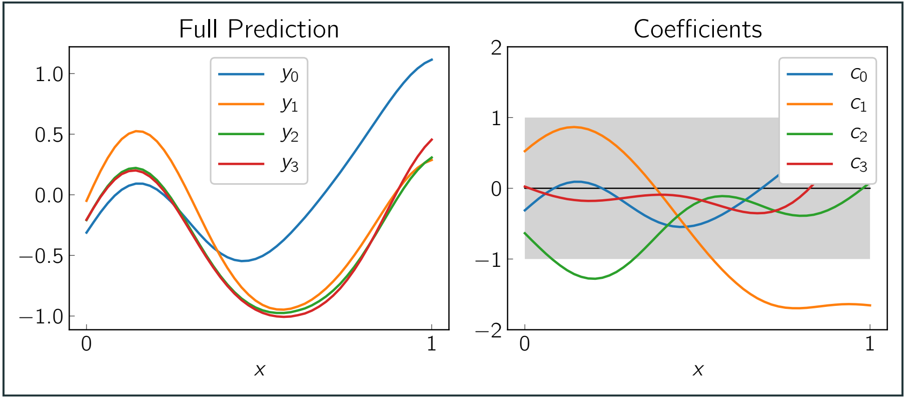
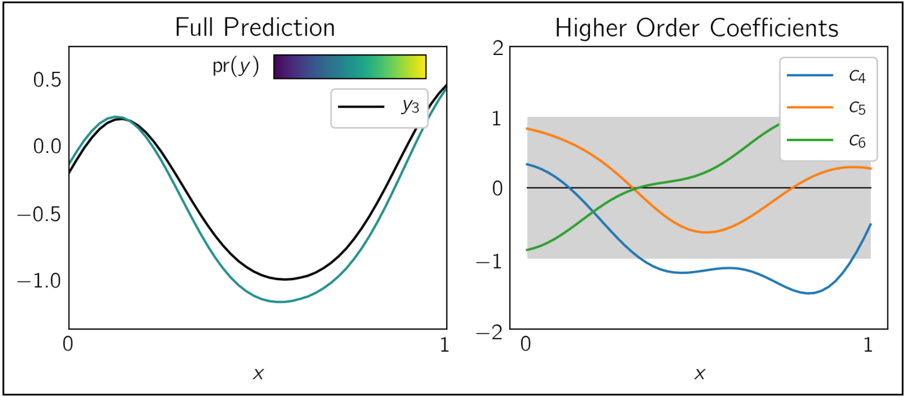


Model Building

Main equation

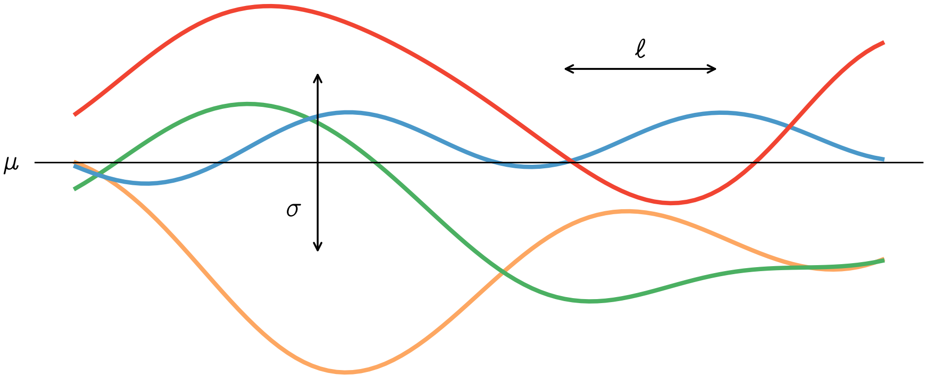
$$y = y_{\text{ref}} \sum_{n=0}^{\infty} c_n Q^n$$

$$c_n \equiv \frac{y_n - y_{n-1}}{y_{\text{ref}} Q^n}$$



Gaussian Processes: How We Induct on the c_n

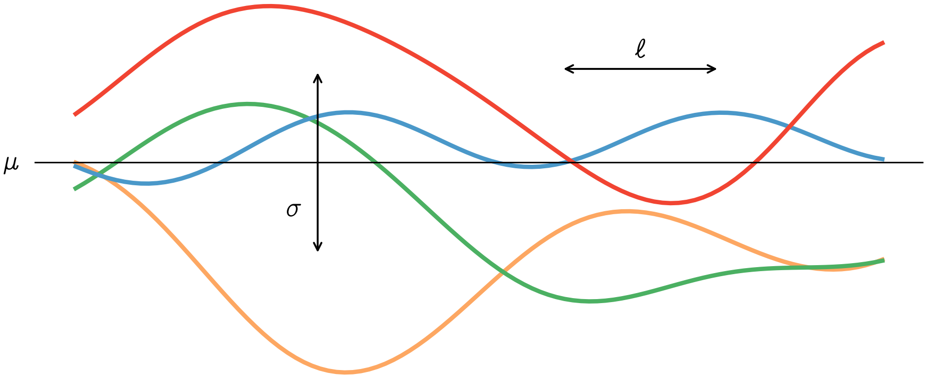
What are Gaussian processes?



Gaussian Processes: How We Induct on the c_n

What are Gaussian processes?

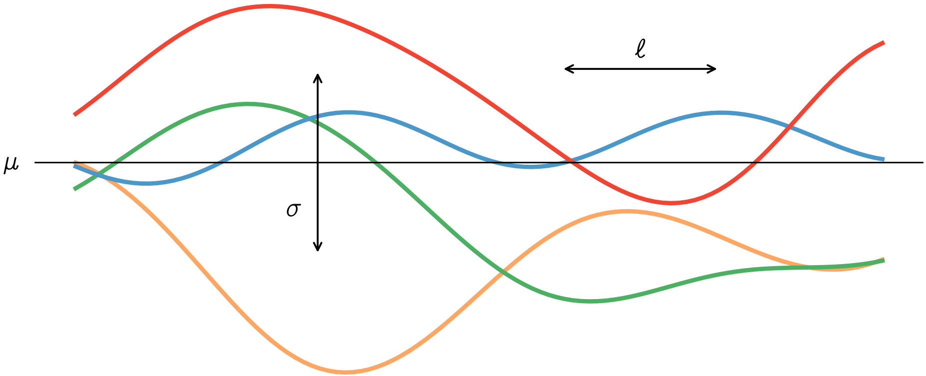
- An infinite dimensional generalization of the Gaussian distribution (??)



Gaussian Processes: How We Induct on the c_n

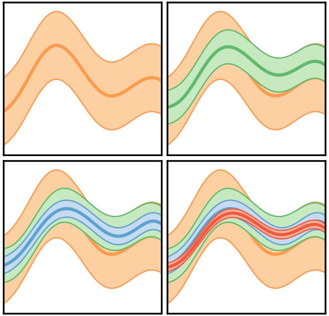
What are Gaussian processes?

- An infinite dimensional generalization of the Gaussian distribution (??)
- A popular machine learning tool for non-parametric regression



Quantifying Truncation Uncertainty

Inexpensive Prediction



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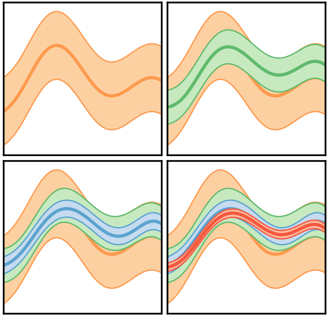
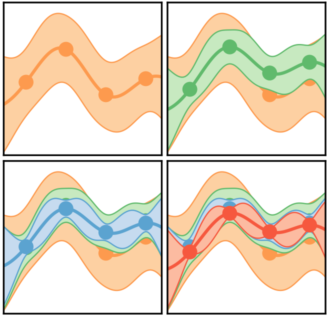


Expensive Prediction

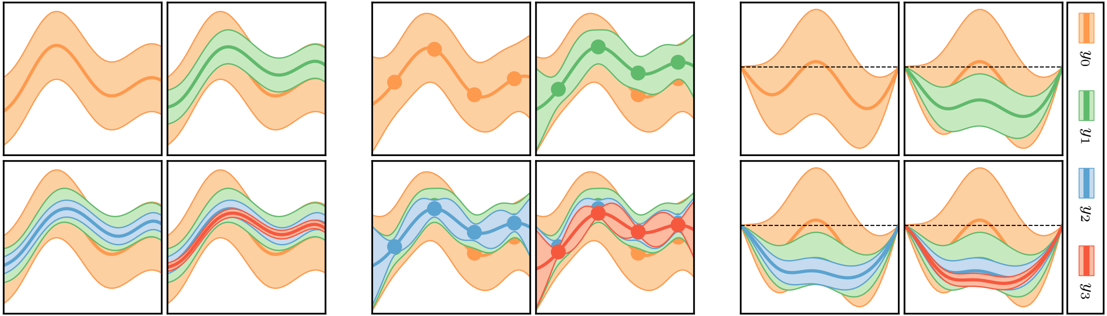


Quantifying Truncation Uncertainty

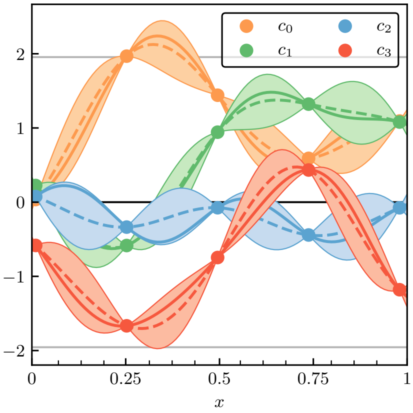
Inexpensive Prediction

Expensive Prediction

Symmetry Constraints

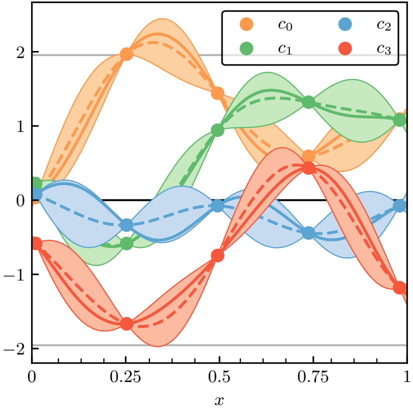


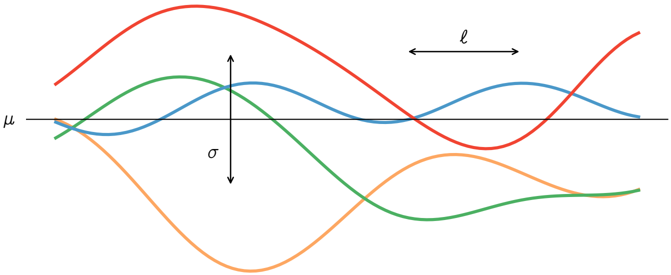
Beyond Truncation Errors



Beyond Truncation Errors

$$y_3 = y_{\mathrm{ref}}\left[c_0 Q^0 + c_1 Q^1 + c_2 Q^2 + c_3 Q^3\right]$$





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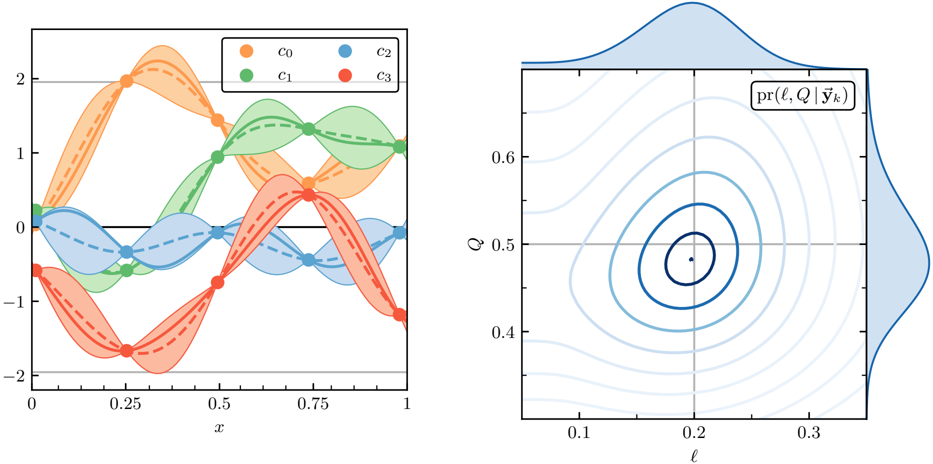

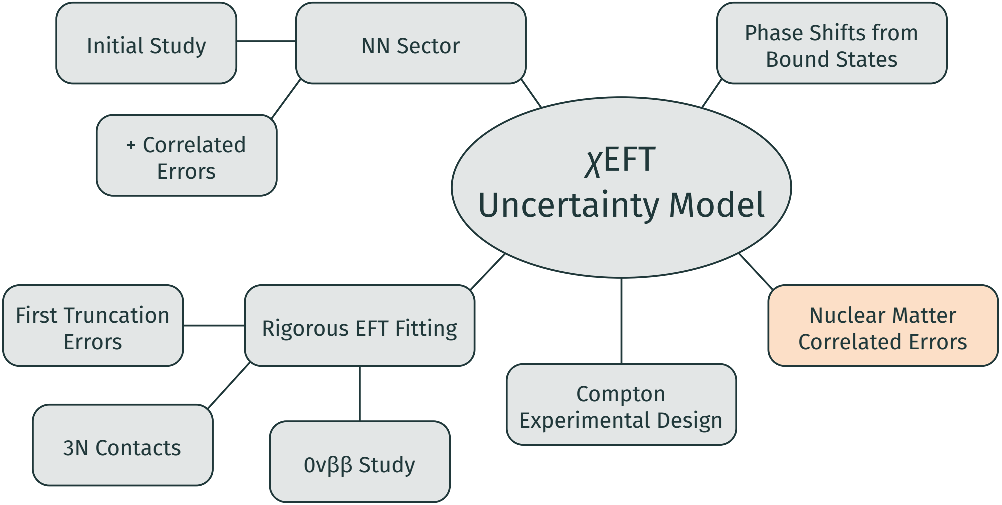

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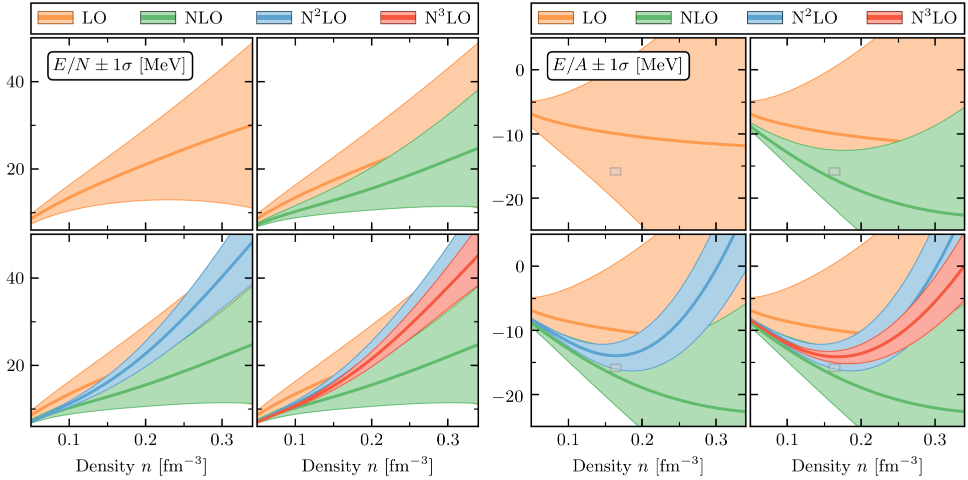
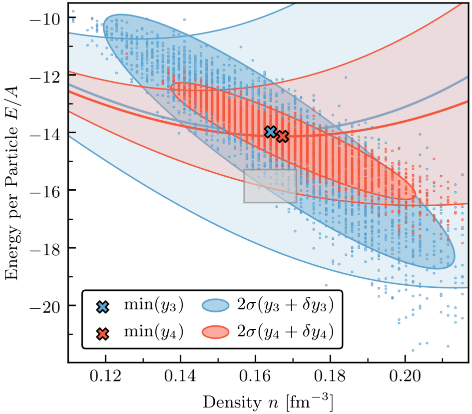
An important bridge from the nucleon-nucleon interaction to neutron-rich matter



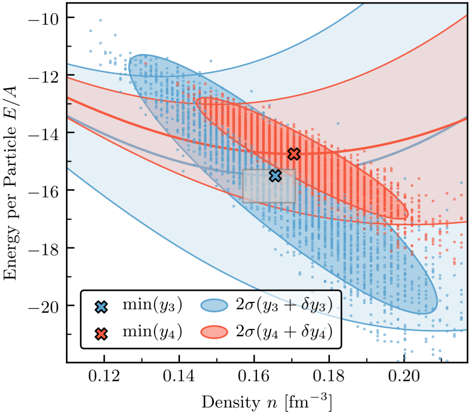
Saturation Properties

Using the Entem, Machleidt, and Nosyk potential with two momentum cutoffs:

$\Lambda = 500\,\text{MeV}$

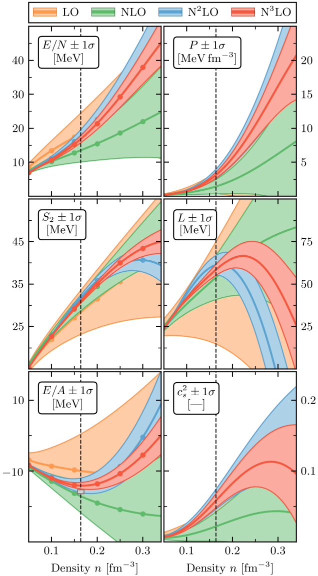


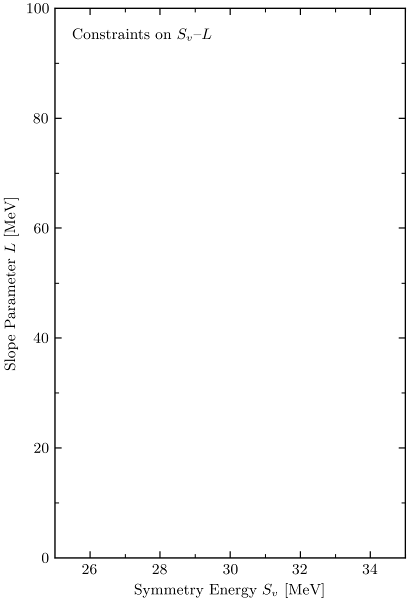
$\Lambda = 450\,\text{MeV}$



Obtaining Derivatives

- Correlated errors permit derivatives
- The first rigorous uncertainty propagation
- Furthermore, the convergence pattern of E/N is correlated with that of E/A.
- So the uncertainty in $S_2 = E/N - E/A$ is smaller than naively expected




Constraints on S_v–L
Slope Parameter L [MeV]
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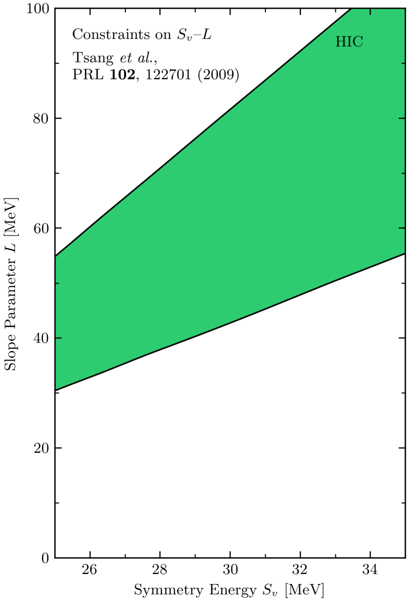
Symmetry Energy S_v [MeV]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Tsang *et al.*,
PRL **102**, 122701 (2009)
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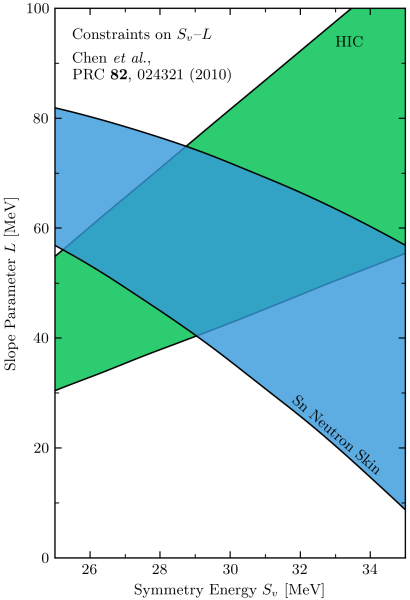
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Chen *et al.*,
PRC **82**, 024321 (2010)
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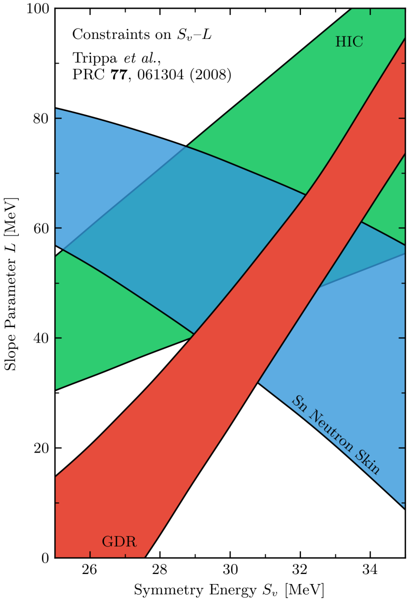
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PRC **77**, 061304 (2008)
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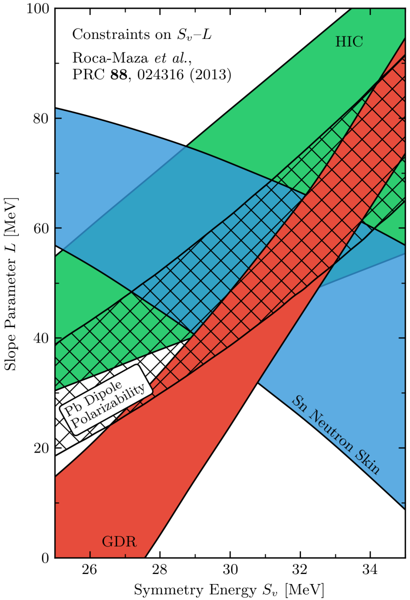
Constraints on S_v–L
Roca-Maza *et al.*,
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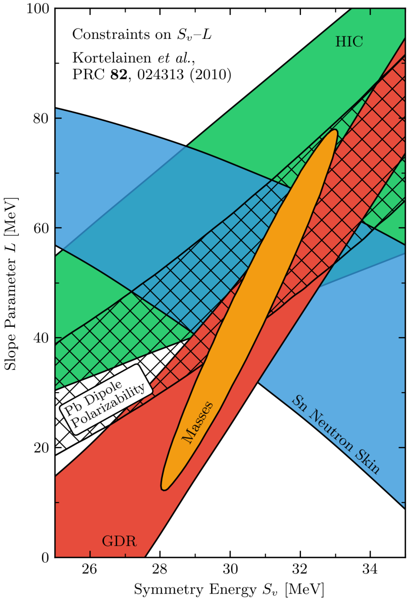
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Kortelainen *et al.*,
PRC **82**, 024313 (2010)
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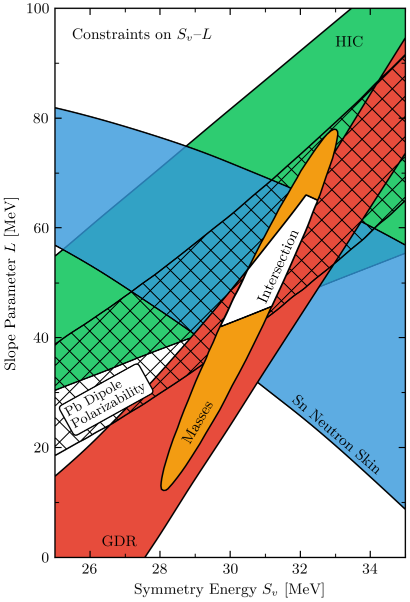
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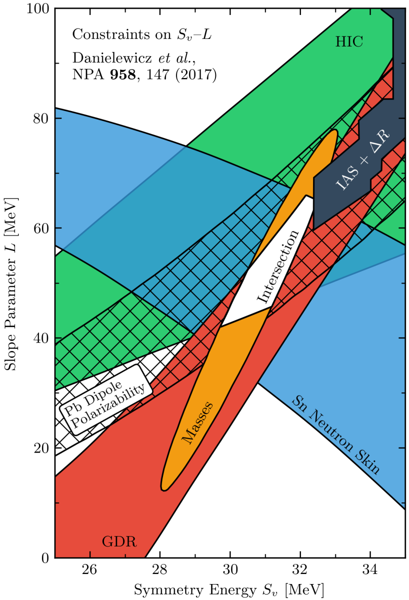

Constraints on S_v–L
Danielewicz *et al.*,
NPA **958**, 147 (2017)
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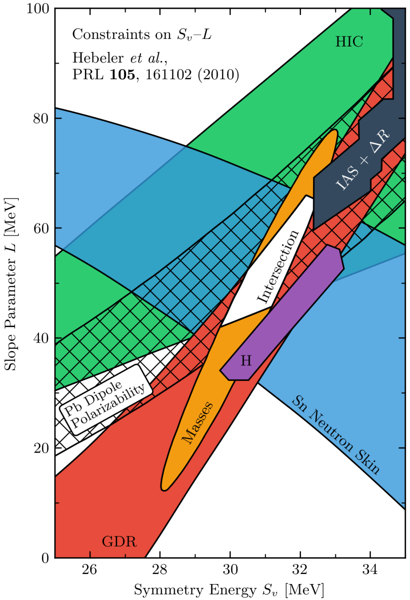

Constraints on S_v–L
Hebeler *et al.*,
PRL **105**, 161102 (2010)
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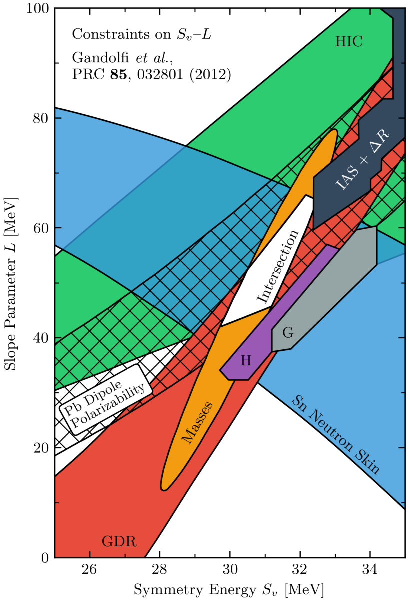

Constraints on S_v–L
Gandolfi *et al.*,
PRC **85**, 032801 (2012)
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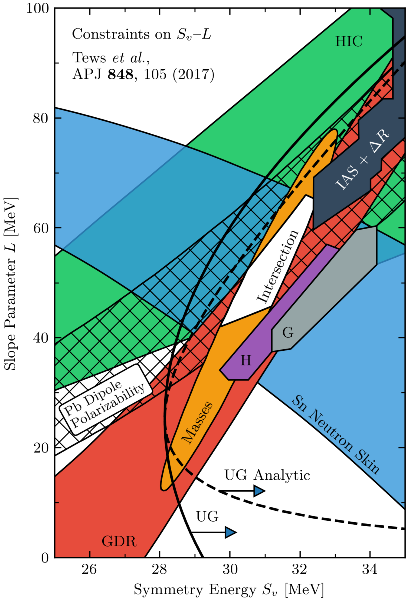

Constraints on S_v–L
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APJ **848**, 105 (2017)
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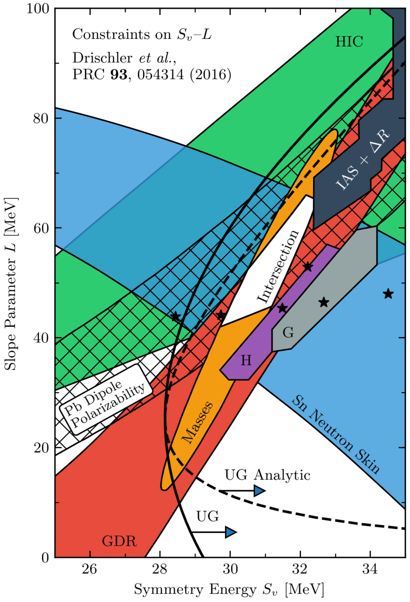

Constraints on S_v–L
Drischler *et al.*,
PRC **93**, 054314 (2016)
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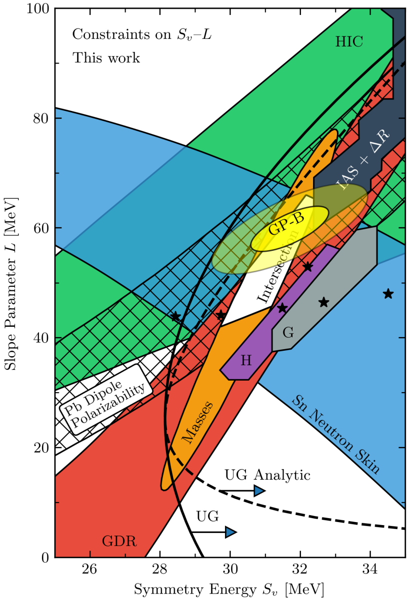
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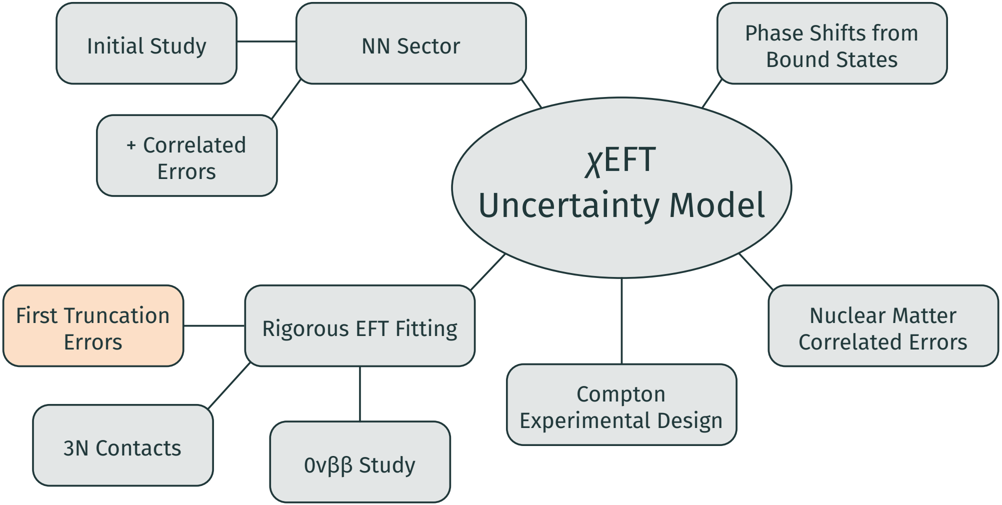

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Posterior for Low-Energy Constants

The truncation error model:

$$y_{\mathrm{exp}}(x) = y_{\mathrm{th}}(x, \vec{a}) + \delta y_{\mathrm{th}}(x) + \delta y_{\mathrm{exp}}$$

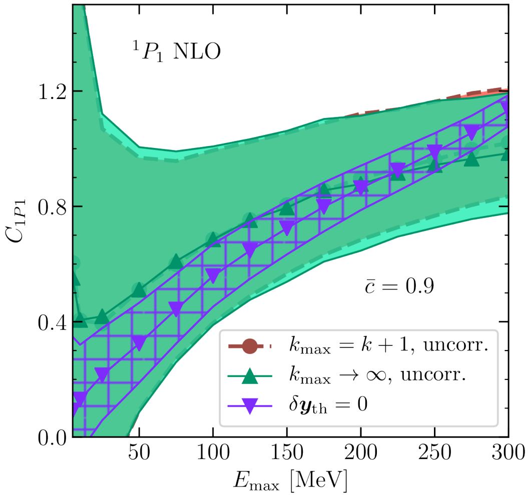
With Bayes' theorem, leads to

$$\mathrm{pr}(\vec{a} \,|\, y_{\mathrm{exp}}) \propto \mathrm{pr}(y_{\mathrm{exp}} \,|\, \vec{a}) \times \mathrm{pr}(\vec{a})$$
$$\mathrm{pr}(y_{\mathrm{exp}} \,|\, \vec{a}) = \mathcal{N}[y_k(\vec{a}), \Sigma_{\mathrm{exp}} + \Sigma_{\mathrm{th}}]$$

This can be sampled using MCMC for full uncertainty propagation

What You Get for Free: Max Energy Insensitivity

- y axis: posterior median $\pm 1\sigma$
- x axis: max energy of data in fit



What You Get for Free: Max Energy Insensitivity

- y axis: posterior median $\pm 1\sigma$
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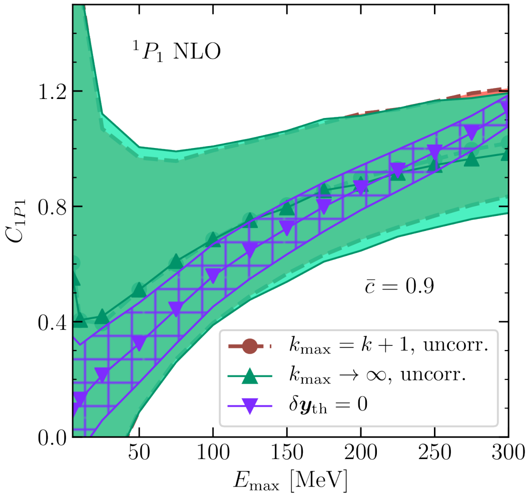
- Q, and hence δy_{th}, grows with energy

$$\delta y_{\mathrm{th}} = y_{\mathrm{ref}} \sum_{n=k+1}^{k_{\max}} c_n Q^n$$

- This weights high energy data less!
- Stabilizes LEC fit as a function of E



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- This weights high energy data less!
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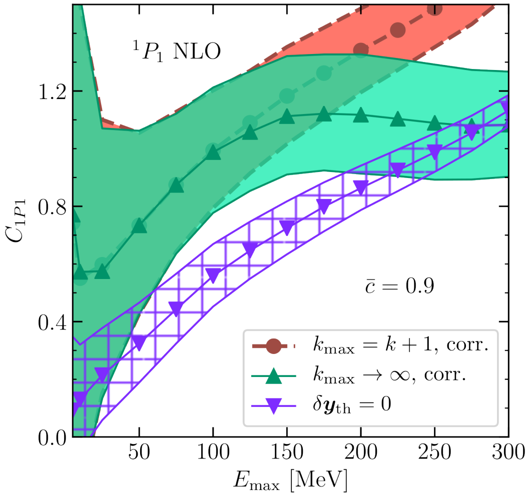
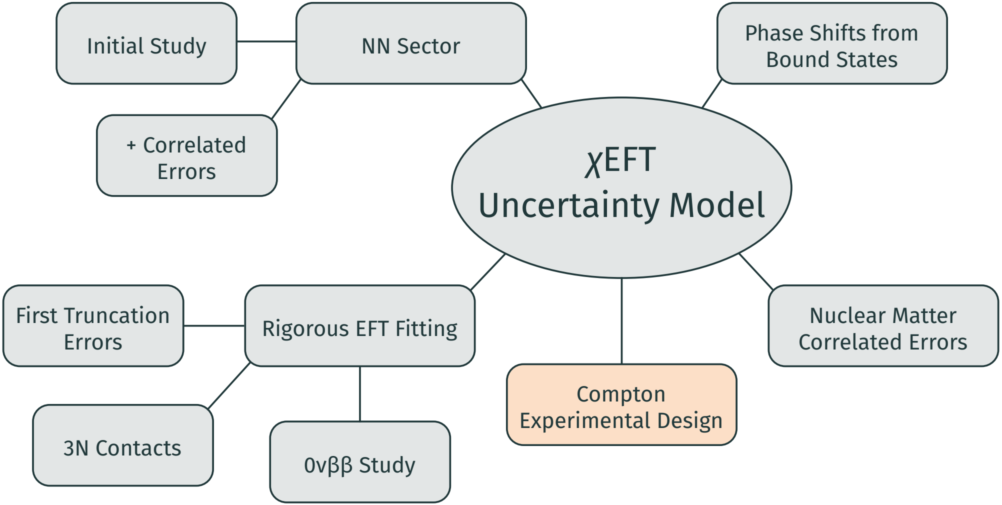
- Correlation assumptions can lead to different results

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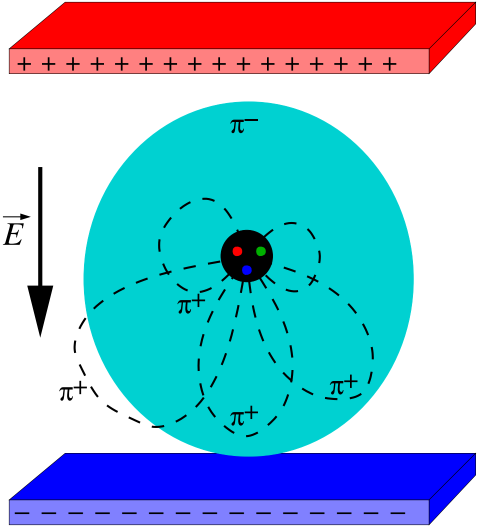
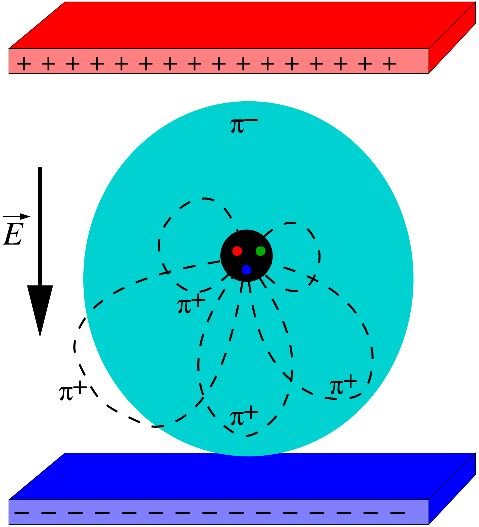
Compton Background

- Nuclear polarizabilities: a fundamental property
- Can be probed by Compton scattering: light off nucleon



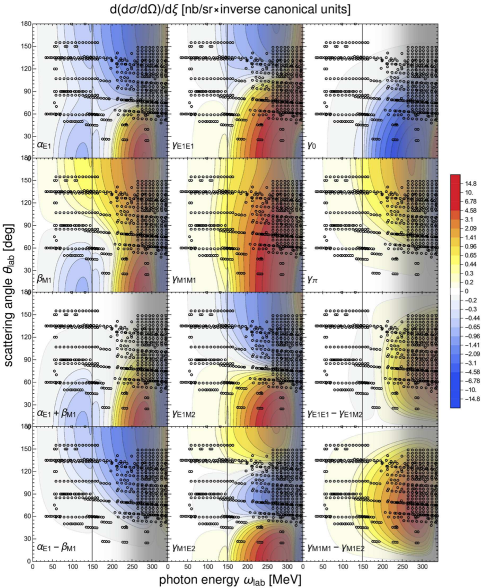
But Where to Measure?

- Beam time is not cheap...
- Experimental difficulties vary
- Theoretical difficulties vary
- How do we balance these constraints?
  - Plan effective experiments
  - Test theory



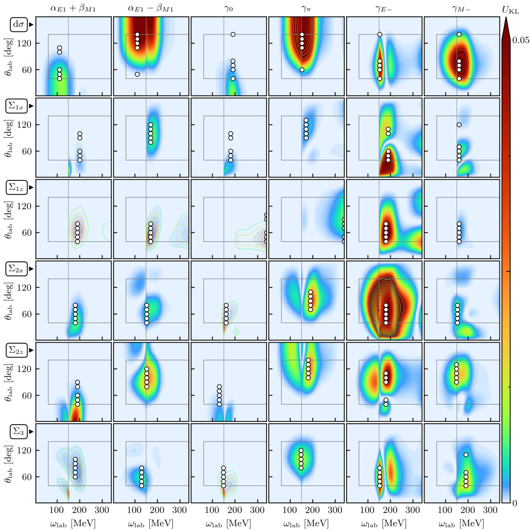
Prior Work

- Grießhammer *et al.* (2018) EPJA
- Chart shows sensitivity of χEFT diff. cross section at a range of energies and angles.
- Looked at sensitivities of theory to polarizabilities (think derivatives)
- Does not account for experimental hardships or theory uncertainty
- Cannot estimate the utility of any given experiment

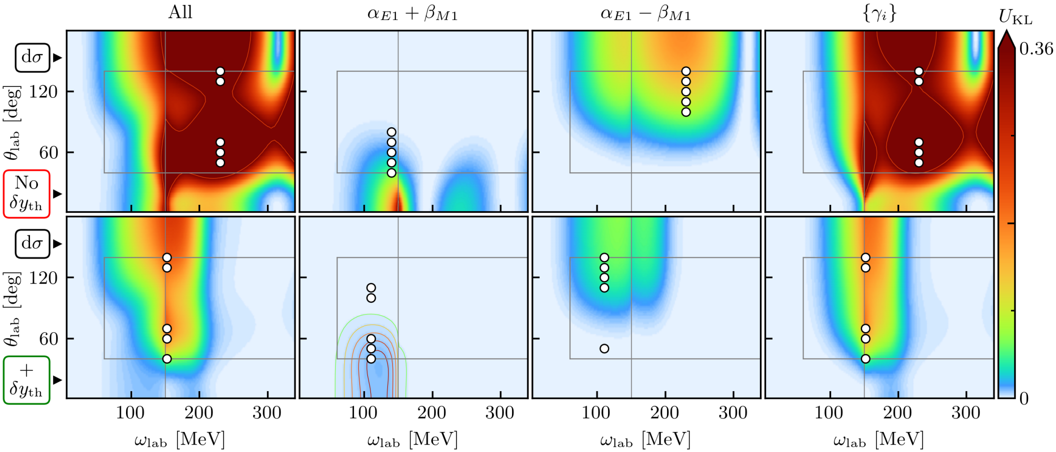


Bayesian Experimental Design

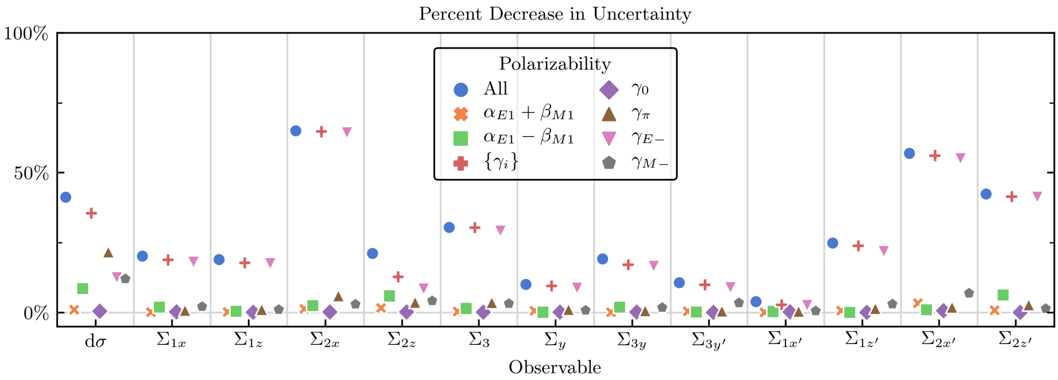
- Includes experimental and correlated theory errors
- Includes symmetry constraints on the truncation error (0th, 1st, *and* 2nd derivatives)
- Can answer questions like:
  - Is extra precision worth the cost?
  - Measure one point well or multiple points less well?
  - What is the benefit of jointly constraining polarizabilities?
  - . . .



The Effect of EFT Errors



Is an Experiment Worth It?



Takeaway Points

Truncation Model

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- Truncation and interpolation error informed by convergence pattern

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Implications

- To progress, science must reason under uncertainty

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- This work is important step for such reasoning in EFTs

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- All code is publicly available

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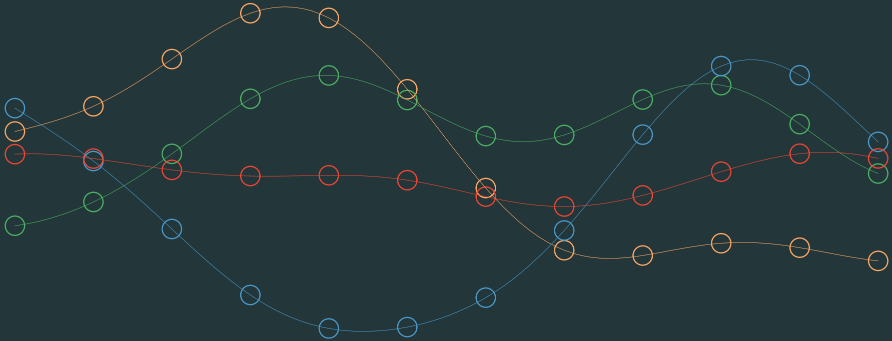
- To progress, science must reason under uncertainty
- This work is important step for such reasoning in EFTs
- All code is publicly available
- This promotes reproducibility and extendability

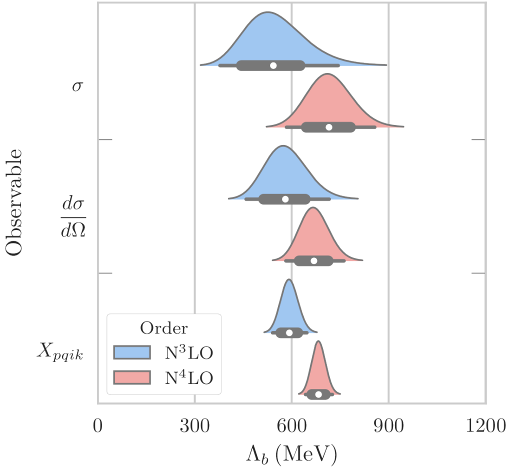
Thank you!

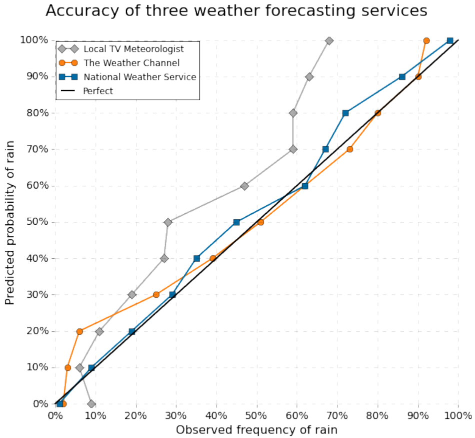
buqeye.github.io



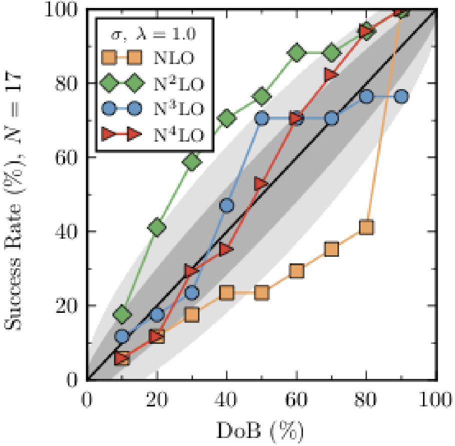
Uncorrelated Posteriors

Assumes that the variance of the c_n is independent at each point





Source: "The Signal and the Noise" by Nate Silver | Author: Randy Olson (randalolson.com / @randal_olson)



Implications for EFT Fitters

Standard χ^2

$$\sum_i \frac{[y_{\text{exp},i} - y_{\text{th},i}(\vec{a})]^2}{\sigma^2_{\text{exp}}} = \sum_i \frac{r(x_i, \vec{a})^2}{\sigma^2_{\text{exp}}}$$

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χ^2 + Theory Error

$$\chi^2_{\mathrm{mod}}(\vec{a}) = \vec{r}^{\,\mathsf{T}}(\vec{a})(\Sigma_{\mathrm{th}} + \Sigma_{\mathrm{exp}})^{-1}\vec{r}(\vec{a})$$

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$$y_{\text{exp}}(x) \overset{?}{\approx} y_{\text{th}}(x, \vec{a})$$

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Prediction + Theory Error

$$\mathrm{pr}(y_{\mathrm{exp}}) = \mathcal{N}[y_{\mathrm{th}}(x, \vec{a}) + \mu_{\mathrm{th}}, \Sigma_{\mathrm{th}}]$$

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Prediction + Theory Error

$$\text{pr}(y_{\text{exp}}) = \mathcal{N}[y_{\text{th}}(x, \vec{a}) + \mu_{\text{th}}, \Sigma_{\text{th}}]$$

- Gaussian process correlations propagate via Σ_{th} matrix (computed once!)

Implications for EFT Fitters

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$$\cancel{\sum_i \frac{[y_{\mathrm{exp},i} - y_{\mathrm{th},i}(\vec{a})]^2}{\sigma^2_{\mathrm{exp}}} = \sum_i \frac{r(x_i, \vec{a})^2}{\sigma^2_{\mathrm{exp}}}}$$

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$$\cancel{y_{\mathrm{exp}}(x) \overset{?}{\approx} y_{\mathrm{th}}(x, \vec{a})}$$

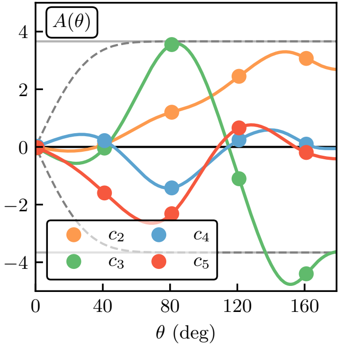
Prediction + Theory Error

$$\mathrm{pr}(y_{\mathrm{exp}}) = \mathcal{N}[y_{\mathrm{th}}(x, \vec{a}) + \mu_{\mathrm{th}}, \Sigma_{\mathrm{th}}]$$

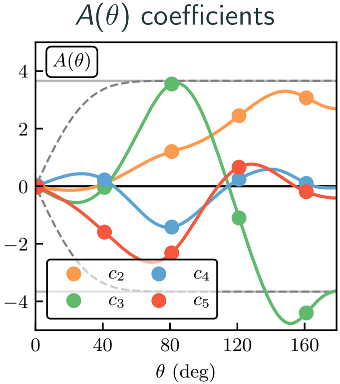
- Gaussian process correlations propagate via Σ_{th} matrix (computed once!)
- Different correlation assumptions $\rightarrow$ different results!

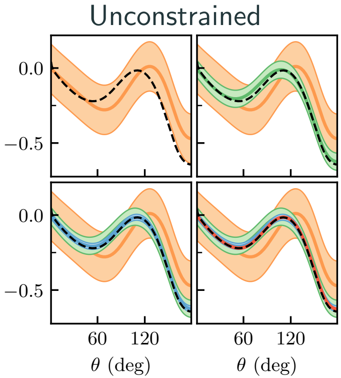
NN Scattering Errors (with Constraint)

$A(\theta)$ coefficients

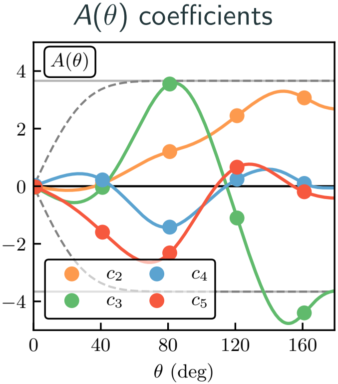


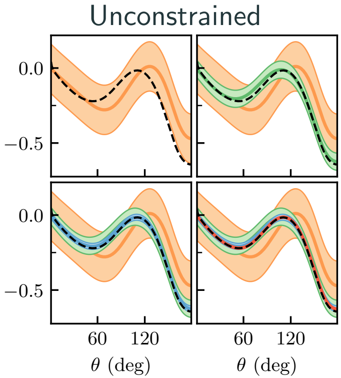
NN Scattering Errors (with Constraint)

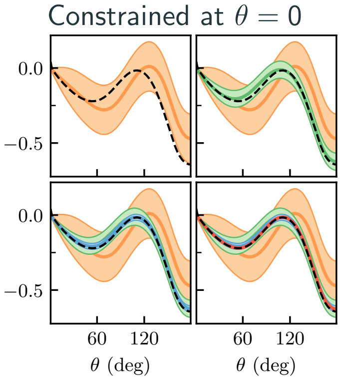




NN Scattering Errors (with Constraint)







Model Checking Diagnostics

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Does our model refer to reality? How can we check?

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Assumptions

1. c_n are iid stationary GPs

Tests

1. Define a metric to measure GP-ness

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Tests

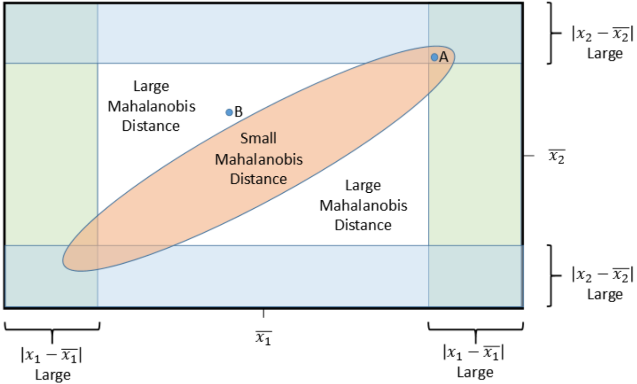
1. Define a metric to measure GP-ness
2. Credible interval diagnostic

- See Bastos & O'Hagan (2009) "Diagnostics for Gaussian Process Emulators"
- But we have multiple curves on which to test

Mahalanobis Distance

- Measures distance from mean, taking into account covariance structure

$$D_{MD}^2 = (y - m)^T \Sigma^{-1} (y - m)$$



https://blogs.sas.com/content/iml/2019/03/25/geomet
multivariate-univariate-outliers.html

Mahalanobis Distance

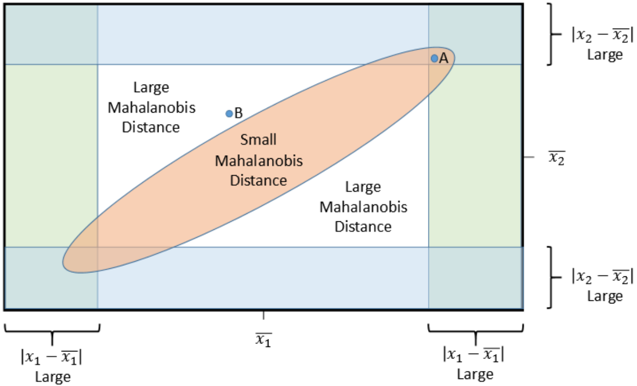
- Measures distance from mean, taking into account covariance structure

$$D_{MD}^2 = (y - m)^T \Sigma^{-1} (y - m)$$

- Can decompose scalar D_{MD}^2 into a vector D_G using $\Sigma = GG^T$

$$D_G = G^{-1}(y - m)$$

D_G can illuminate why some curves fail



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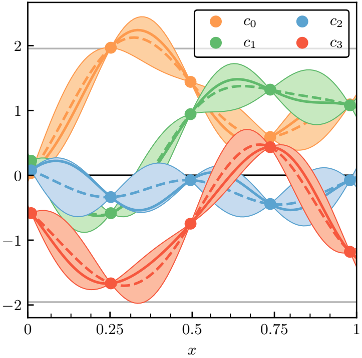
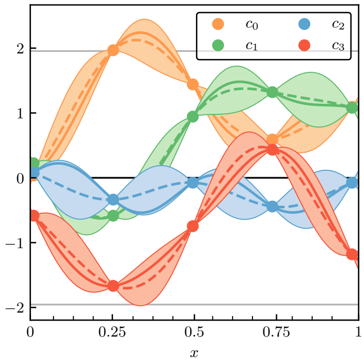
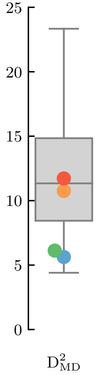
Mahalanobis Distance Toy Example



Mahalanobis Distance Toy Example





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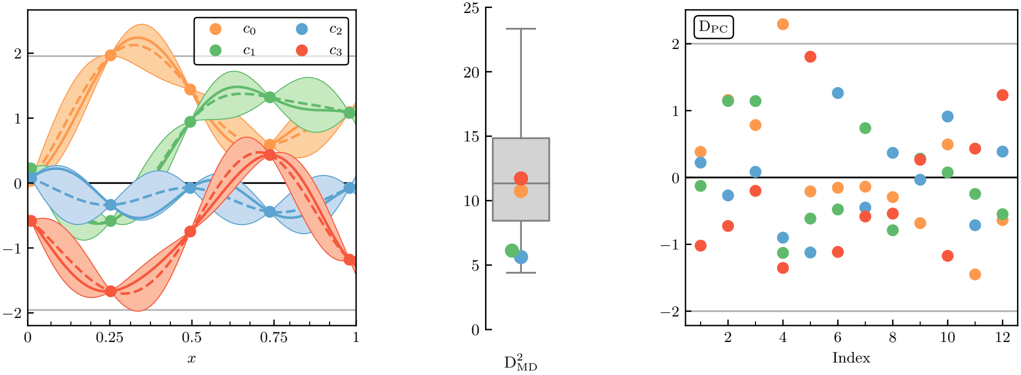
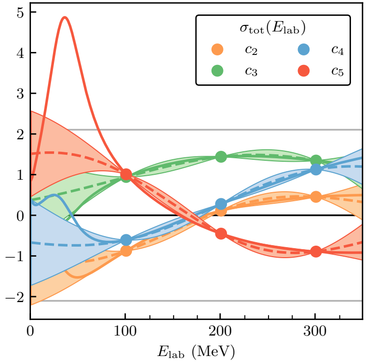


Mahalanobis Distance Real Example

EKM Semilocal ($R = 0.9\,\text{fm}$). Total cross section



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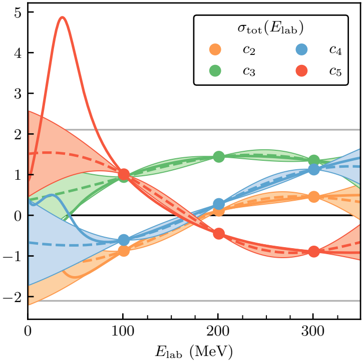

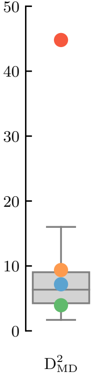

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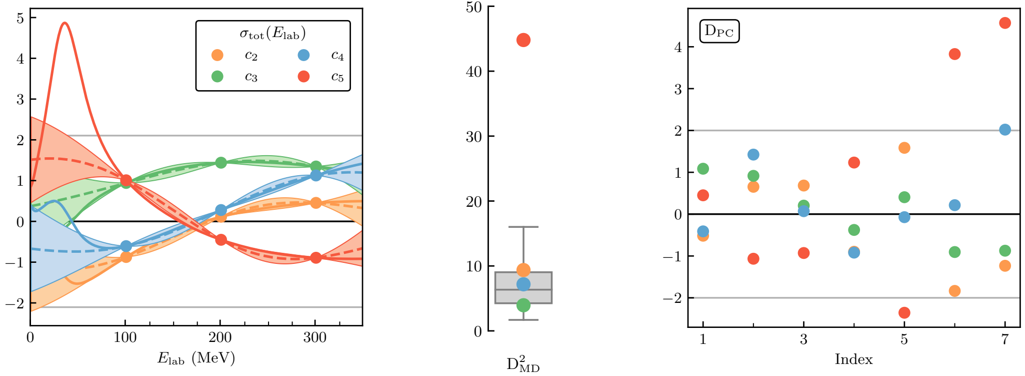

Credible Interval Diagnostics