

Combining Physics and Bayesian Statistics to Validate Models and Infer Their Parameters

Jordan Melendez¹

Dick Furnstahl¹

Daniel Phillips²

Matt Pratola¹

Sarah Wesolowski³

August 17, 2019

¹The Ohio State University

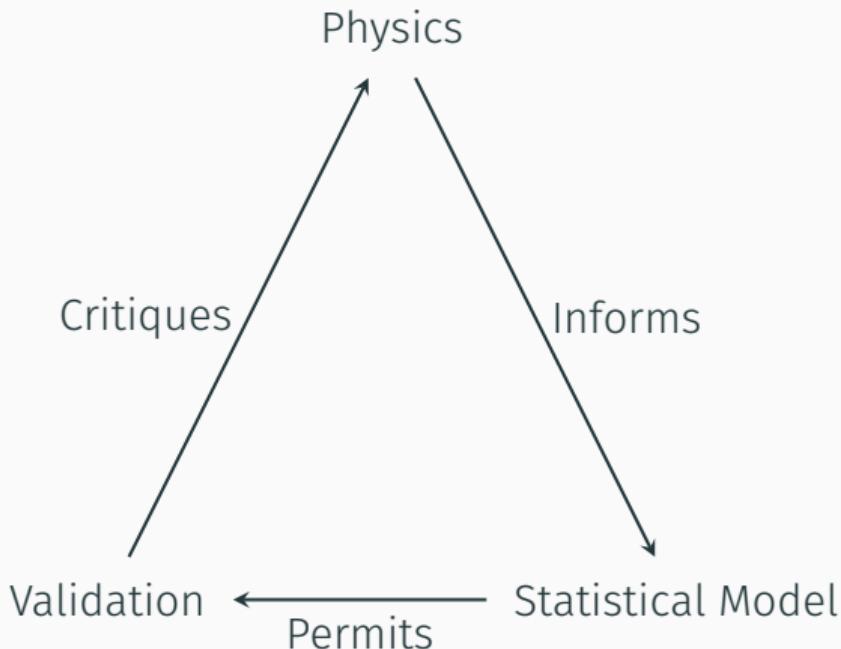
²Ohio University

³Salisbury University

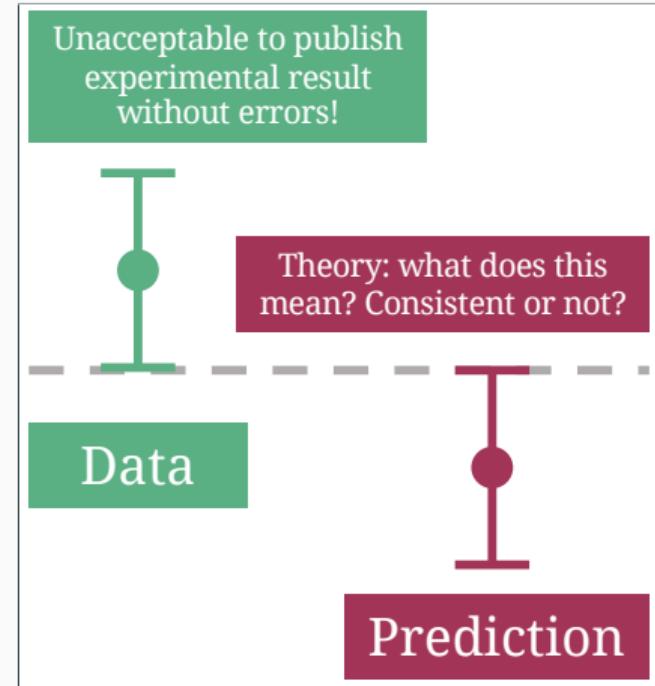
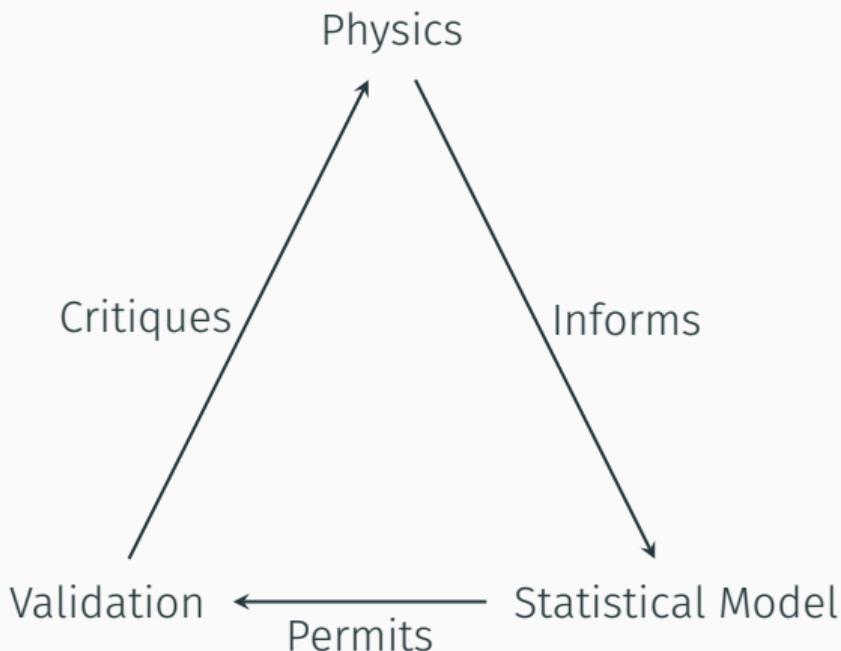


Based on: · S. Wesolowski, R. J. Furnstahl, J. A. Melendez, D. Phillips, arXiv:1808.08211; &
· J. A. Melendez, S. Wesolowski, and R. J. Furnstahl Phys. Rev. C **96**, 024003, Editors' Suggestion

Outline



Outline



Why Bayesian?



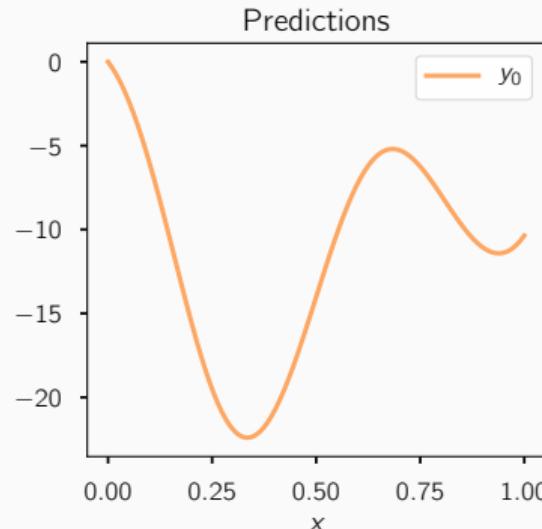
- More intuitive
 - Confidence intervals → credible intervals
 - p -values → posterior probabilities
- Conventional results often recovered as a special case
- Assumptions are made **explicit**
- Well suited for incorporating theoretical error

Physical Motivation

Chiral EFT in One Slide

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

$\{y_0\}$

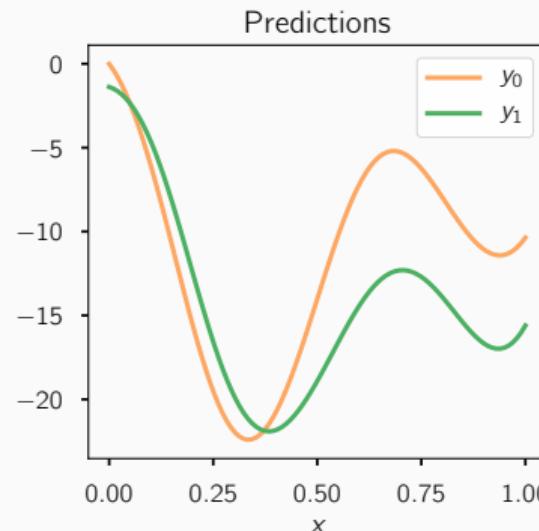


$y_0 \rightarrow \text{LO}$

Chiral EFT in One Slide

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$\{y_0, y_1\}$



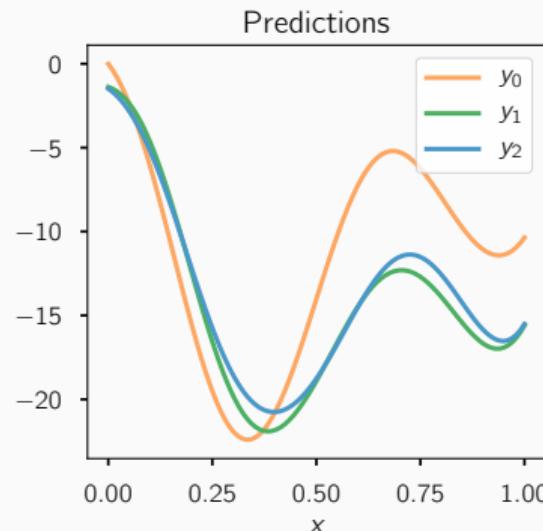
$y_0 \rightarrow \text{LO}$

$y_1 \rightarrow \text{NLO}$

Chiral EFT in One Slide

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$\{y_0, y_1, y_2\}$



$y_0 \rightarrow \text{LO}$

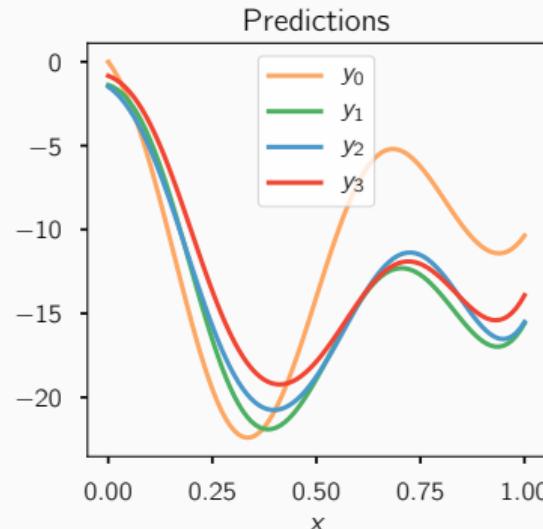
$y_1 \rightarrow \text{NLO}$

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

Chiral EFT in One Slide

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



$y_0 \rightarrow \text{LO}$

$y_1 \rightarrow \text{NLO}$

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

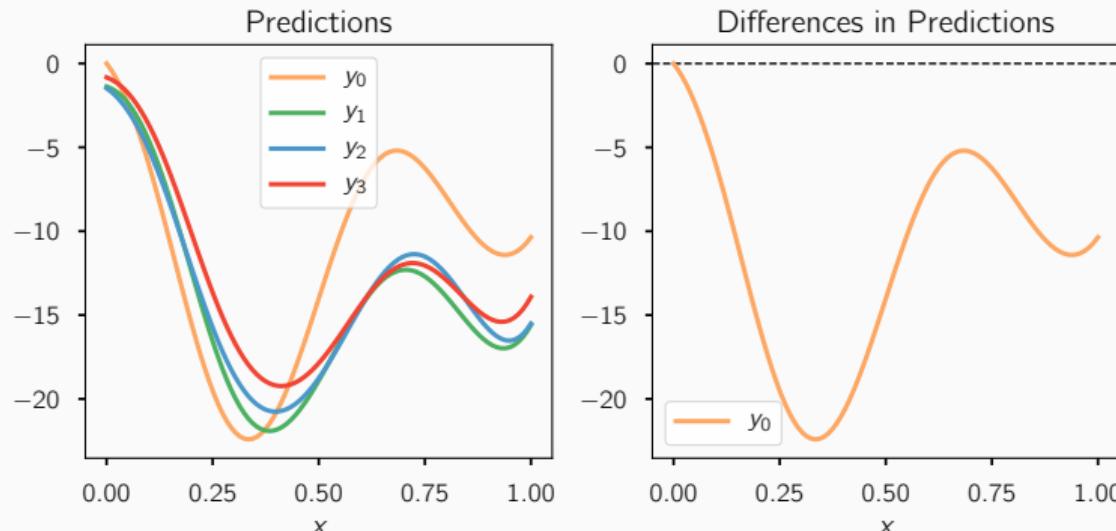
\vdots

$y_k \rightarrow \text{N}^k\text{LO}$

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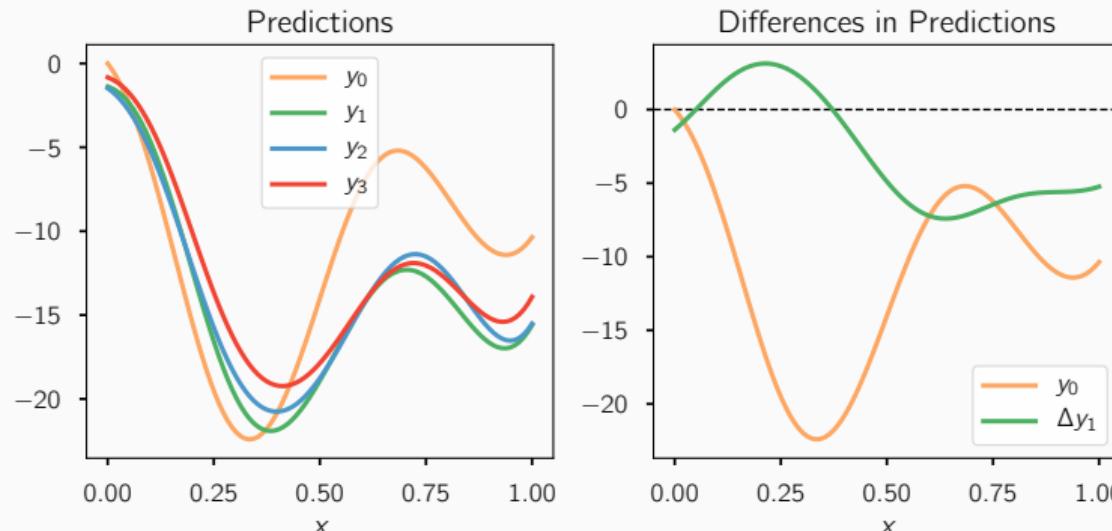
$$y_0 = \textcolor{orange}{y}_0$$



Chiral EFT in One Slide

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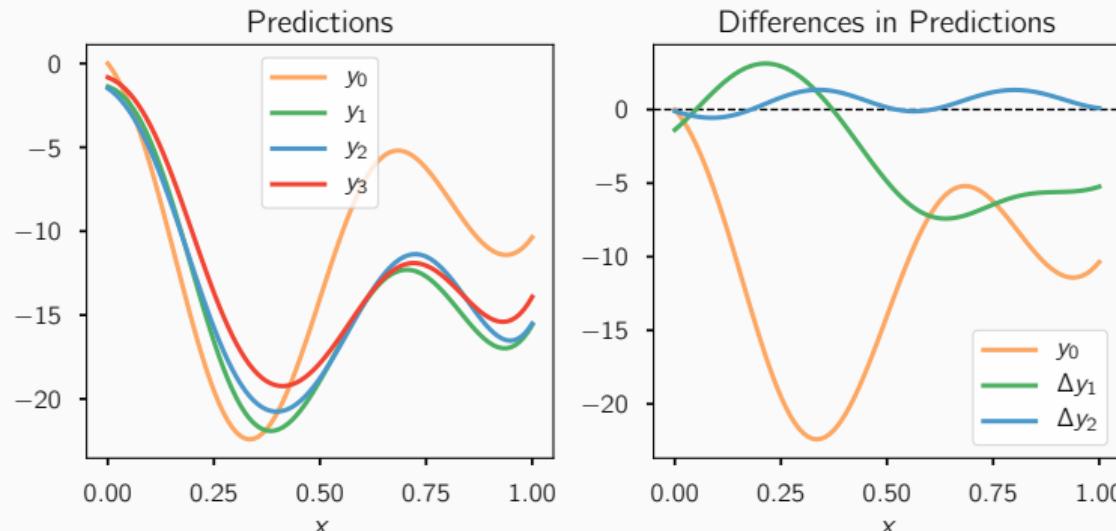
$$y_1 = y_0 + \Delta y_1$$



Chiral EFT in One Slide

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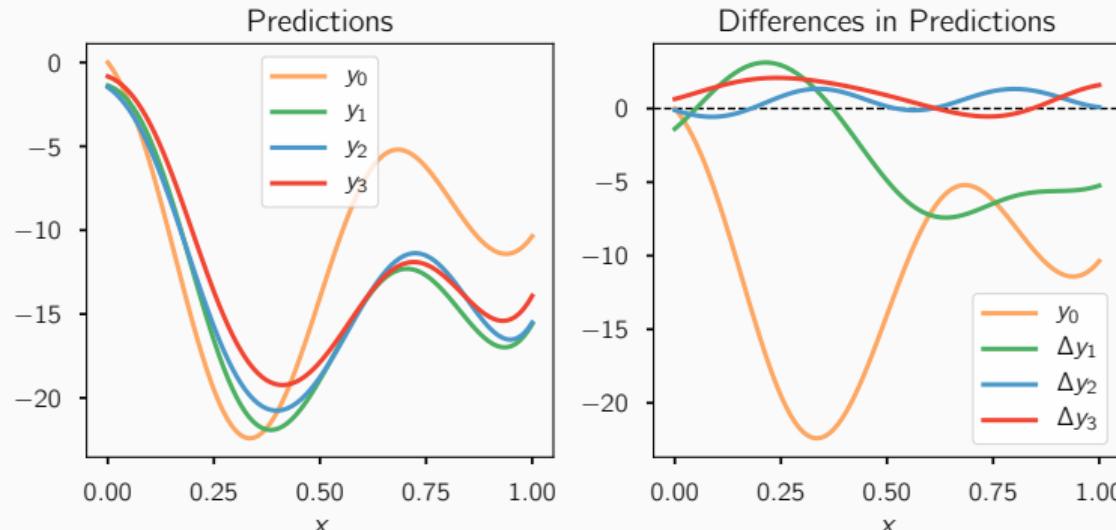
$$y_2 = y_0 + \Delta y_1 + \Delta y_2$$



Chiral EFT in One Slide

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- $\Delta y_n = y_{\text{ref}} c_n Q^n$

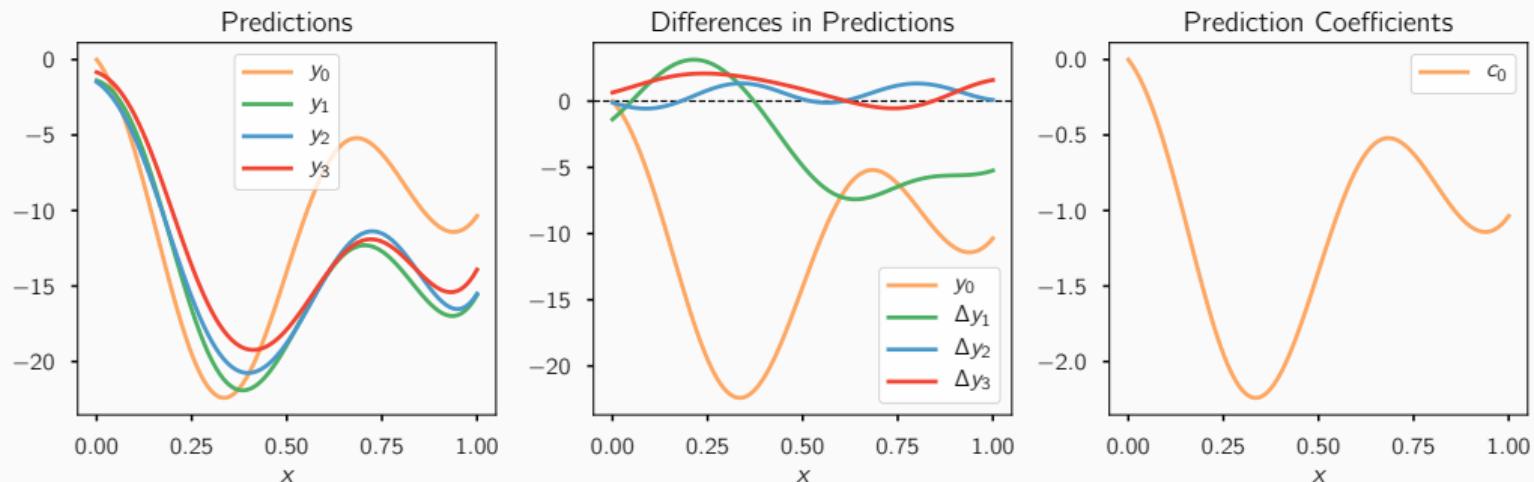
$$y_3 = y_0 + \Delta y_1 + \Delta y_2 + \Delta y_3$$



Chiral EFT in One Slide

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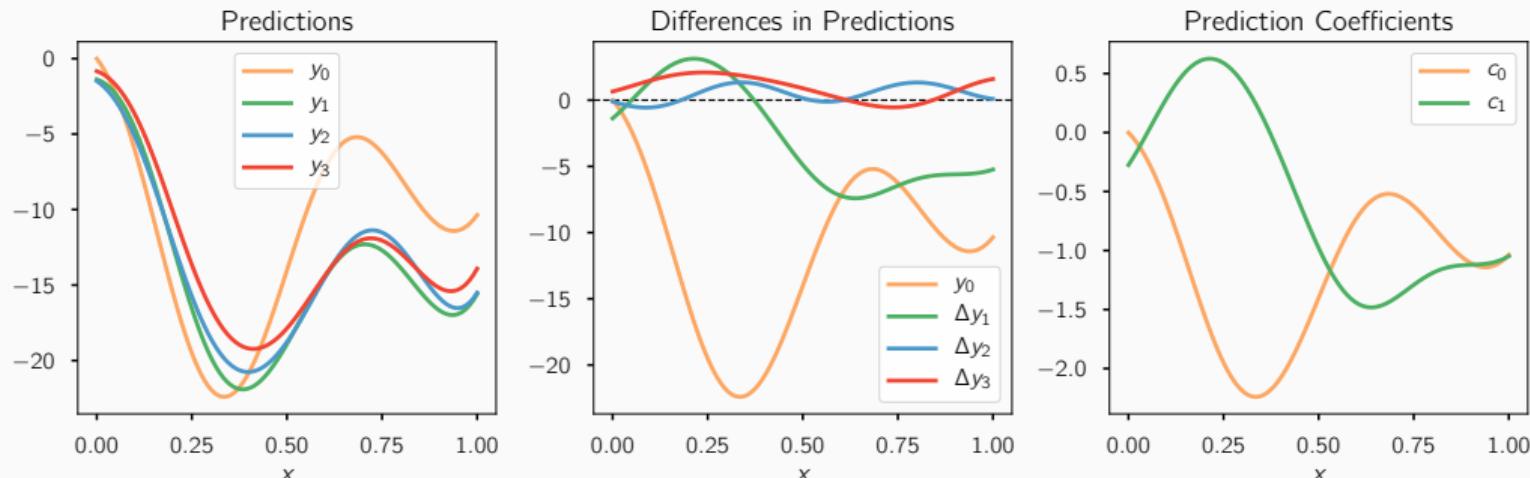
$$y_0 = y_{\text{ref}} [c_0 Q^0]$$



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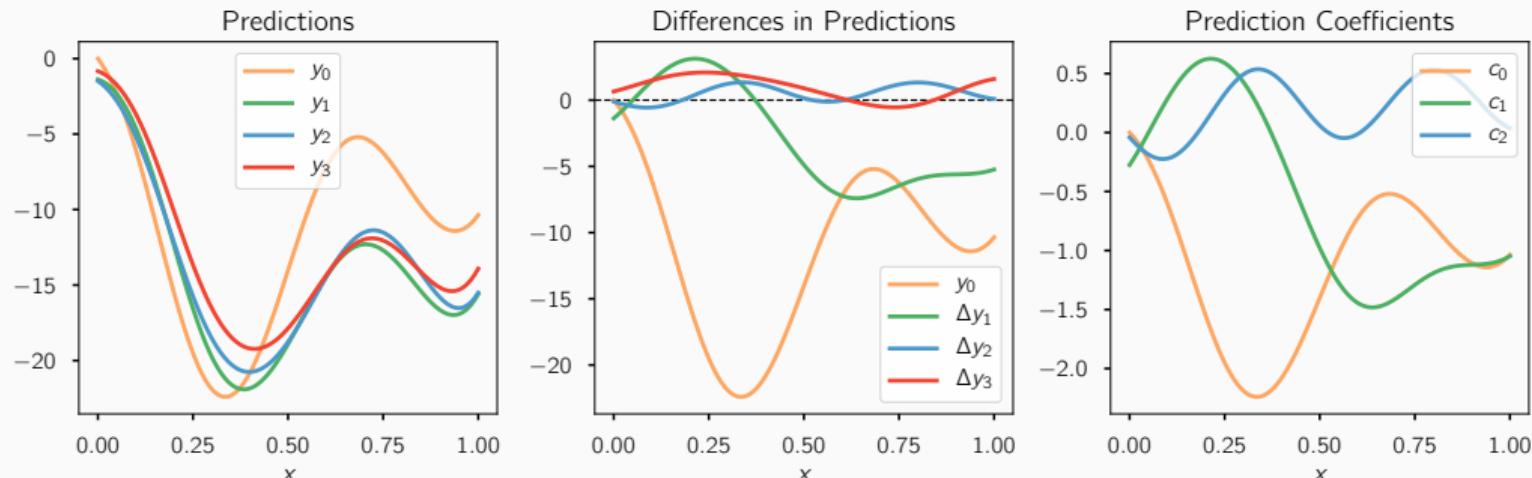
$$y_1 = y_{\text{ref}} [c_0 Q^0 + c_1 Q^1]$$



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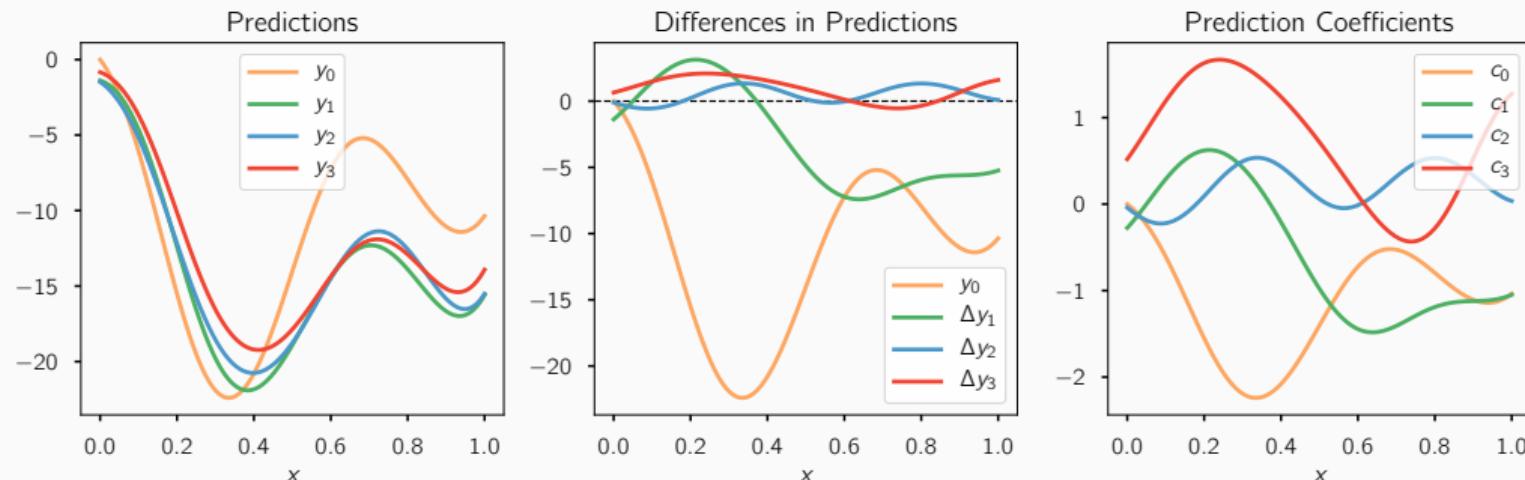
$$y_2 = y_{\text{ref}} [c_0 Q^0 + c_1 Q^1 + c_2 Q^2]$$



Chiral EFT in One Slide

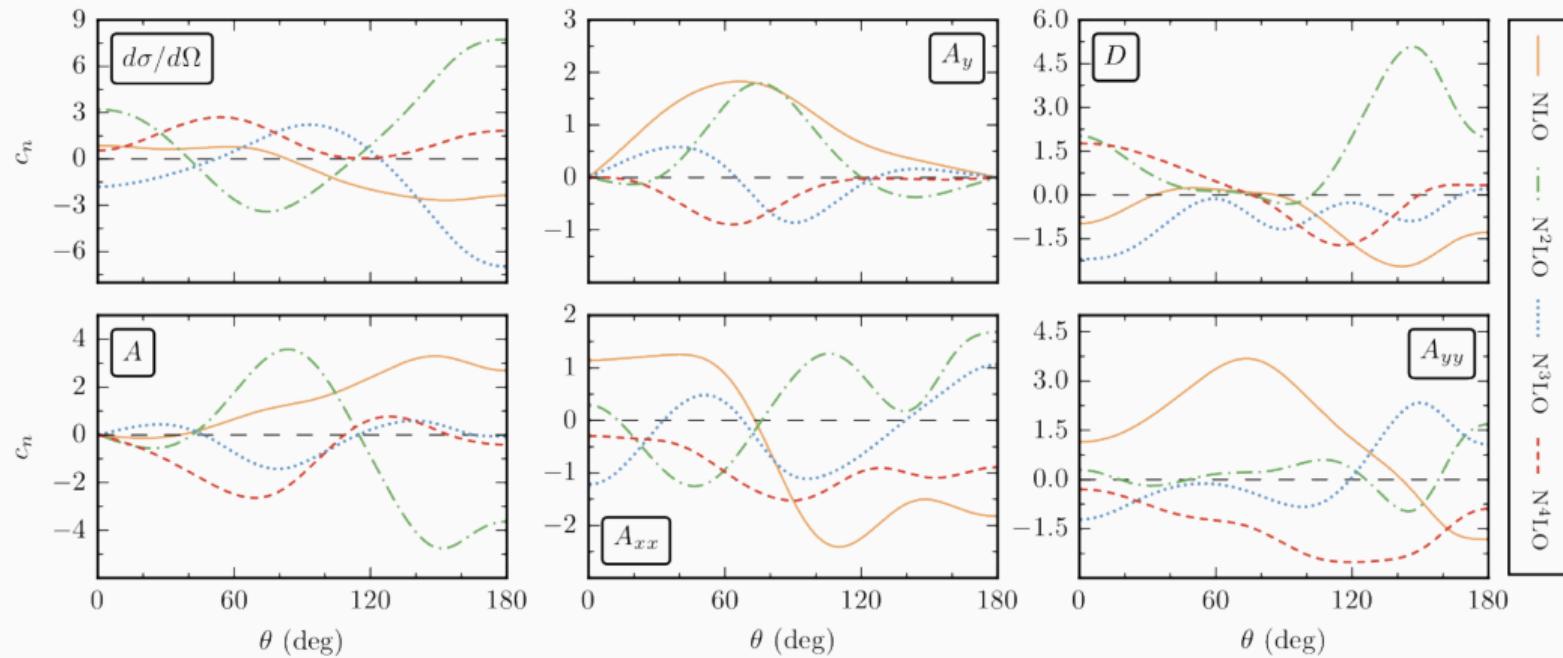
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$$y_3 = y_{\text{ref}} [c_0 Q^0 + c_1 Q^1 + c_2 Q^2 + c_3 Q^3]$$



Real Life (Neutron-Proton Scattering)

Coefficients from NN scattering look like the example on the previous slide!



Statistical Model

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

To theorists, magic

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

Parameters

Discrepancy

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

$\chi^2 \text{ fit}$



rigorous fit


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

Full Prediction

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

$$y_{\text{exp}}(x) = y_{\text{th}}(x, \vec{a}) + \underbrace{\delta y_{\text{th}}(x)}_{\text{How do we design this?}} + \delta y_{\text{exp}}$$

How does it affect fitting \vec{a} ?

The Hierarchical Model

- Decompose prediction

$$y_k = y_0 + \sum_{n=1}^k \Delta y_n \quad \left. \right\}$$



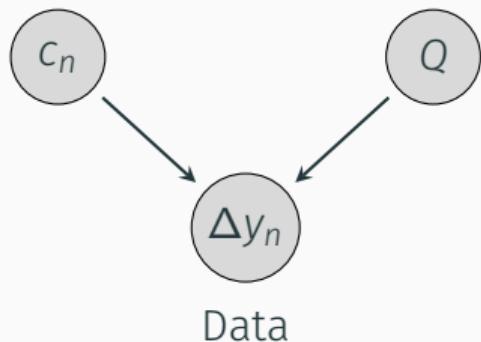
Data

The Hierarchical Model

- Decompose prediction

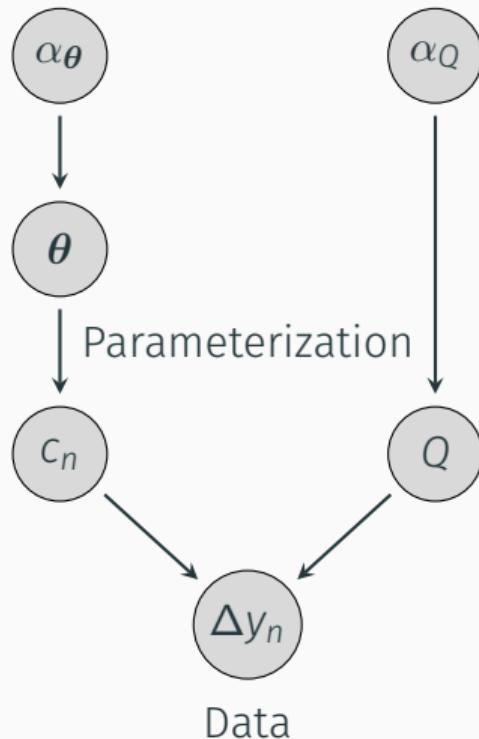
$$\left. \begin{aligned} y_k &= y_0 + \sum_{n=1}^k \Delta y_n \\ &= y_{\text{ref}} \sum_{n=0}^k c_n Q^n \end{aligned} \right\}$$

Parameterization



The Hierarchical Model

Hyperparameters



- Decompose prediction

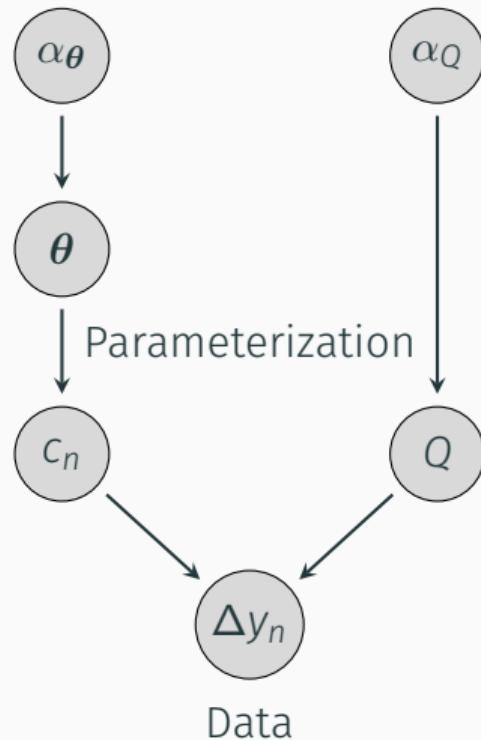
$$\left. \begin{aligned} y_k &= y_0 + \sum_{n=1}^k \Delta y_n \\ &= y_{\text{ref}} \sum_{n=0}^k c_n Q^n \end{aligned} \right\} \implies \delta y_k = y_{\text{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$$

- Promote c_n (and Q) to random variables

$$\text{pr}(c_n | \theta) \stackrel{\text{iid}}{\sim} \mathcal{GP}(\mu, \sigma^2 R_\ell)$$

The Hierarchical Model

Hyperparameters



- Decompose prediction

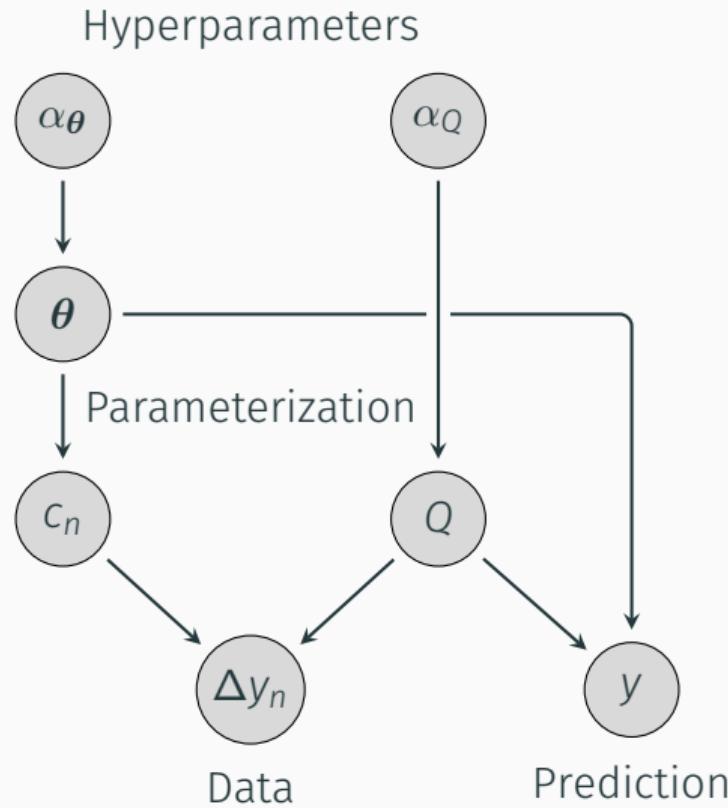
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- Train statistical parameters (θ and Q) and LECs \vec{a} on data

The Hierarchical Model



- Decompose prediction

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- Train statistical parameters (θ and Q) and LECs \vec{a} on data
- Compare $y_k + \delta y_k$ to experiment y_{exp}

```

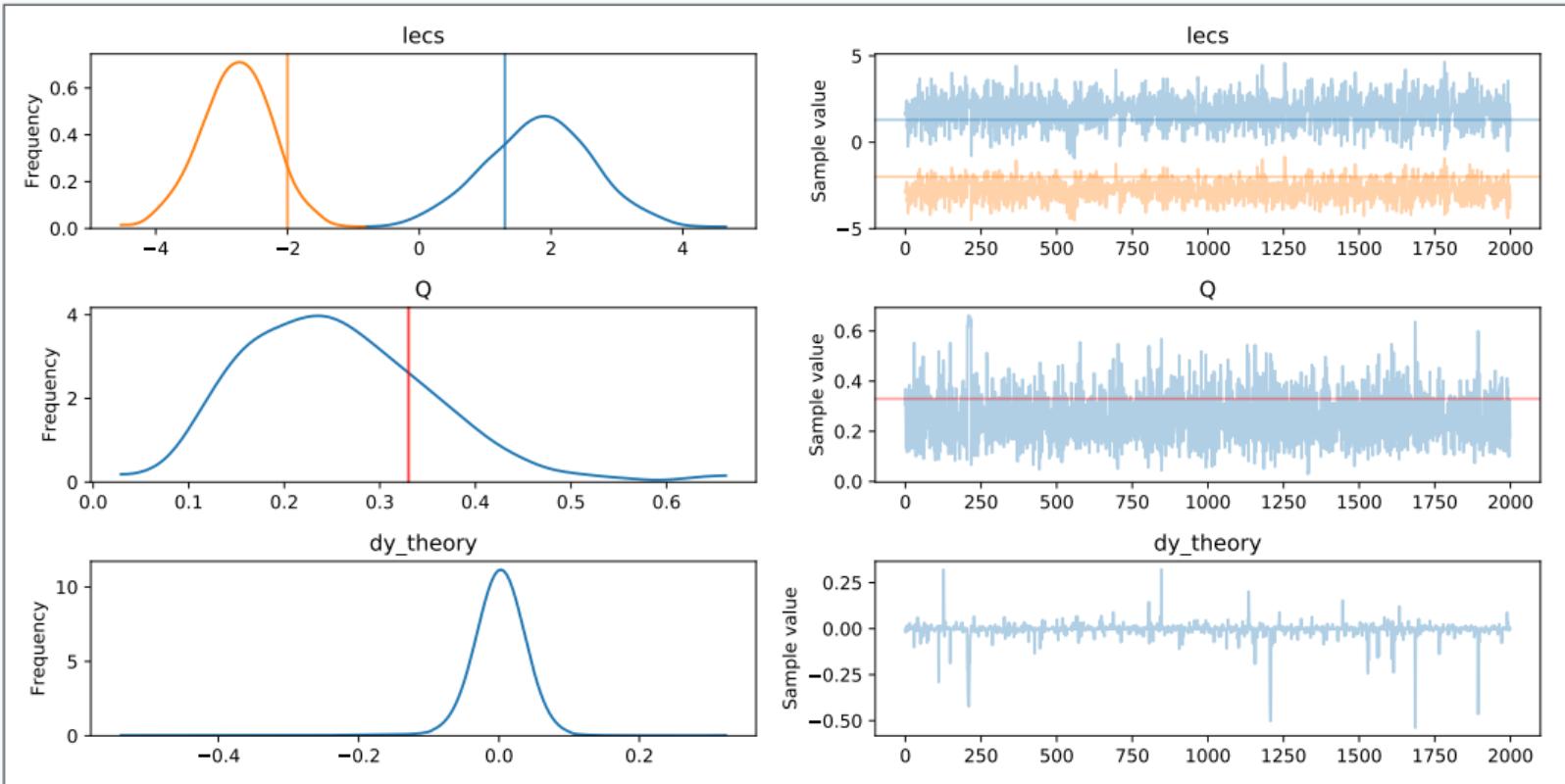
# Setup code goes up here ...
with Model() as model: # Build statistical model with PyMC3
    Q = Beta('Q', alpha=5, beta=15) # Priors
    sigma = Lognormal('sigma', mu=0, sd=1)
    c_n = Normal('c_n', mu=0, sd=sigma, shape=(n_high_ords, 1))
    dy_theory = Deterministic('dy_theory',
        tt.sum(c_n * Q**higher_orders, axis=0)) #  $\sum c_n Q^n$ 

    # Setup chiral EFT variables:  $y_k(x; \vec{a}) + \delta y_k(x)$  and prior  $pr(\vec{a})$ .
    lecs = MvNormal('lecs', mu=0, cov=np.identity(2), shape=2)
    y_theory = compute_observable(X, lecs) + dy_theory

    # Fit chiEFT parameters and statistical parameters
    MvNormal('y_exp', mu=y_theory, cov=exp_cov, observed=exp_data)
    MvNormal('c_n_obs', mu=0, cov=sigma**2 * R, observed=coeffs)
    trace = sample(draws=500)

```

Toy Results



Physics Results

So far we've

- added a model discrepancy term δy_{th}
- adopted a Bayesian approach

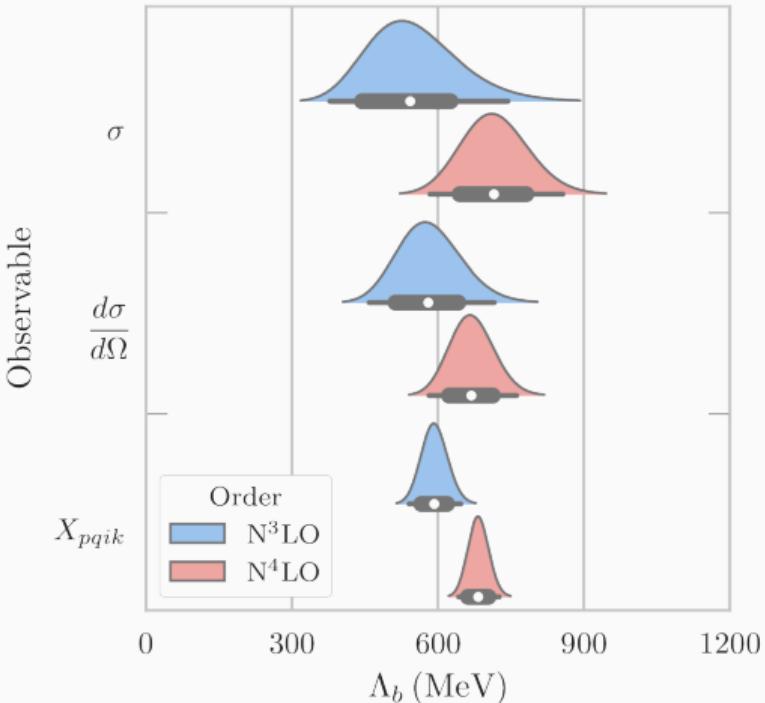
So what?

Rigorous Estimation of Unknown Quantities

- The breakdown scale of the EFT Λ_b :

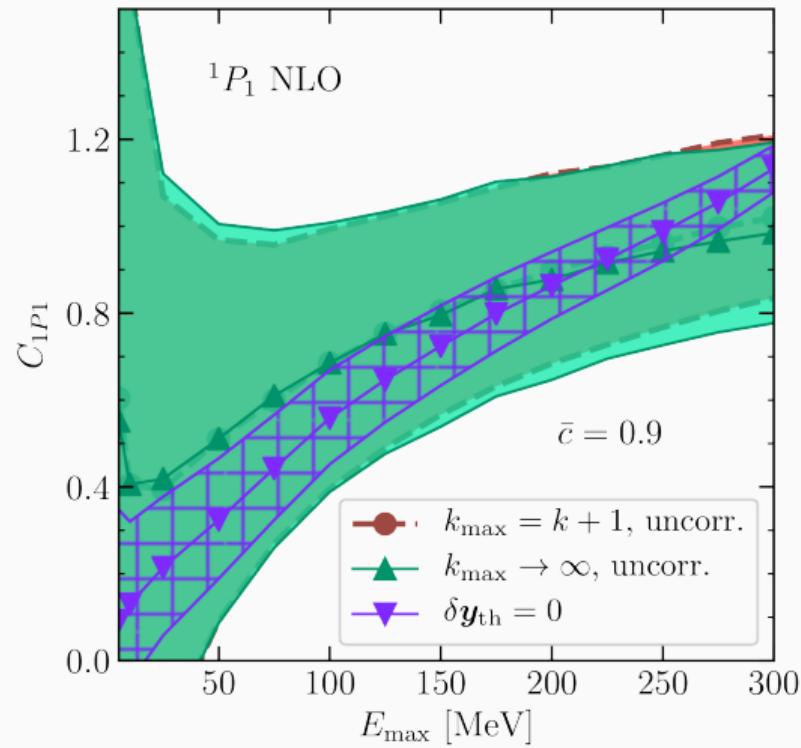
$$Q \approx \frac{f(p, m_\pi)}{\Lambda_b}$$

- Once energies approach Λ_b , the EFT no longer works.
- By promoting Λ_b to a random variable, its posterior can be produced as a byproduct of δy_{th} estimation.



Adding Theory Error Reduces Bias

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

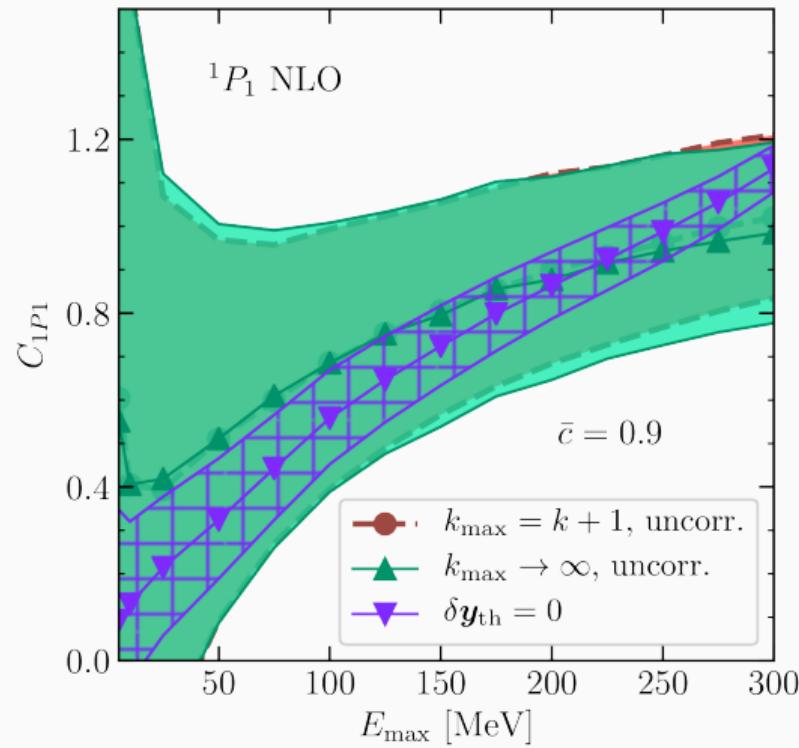


Adding Theory Error Reduces Bias

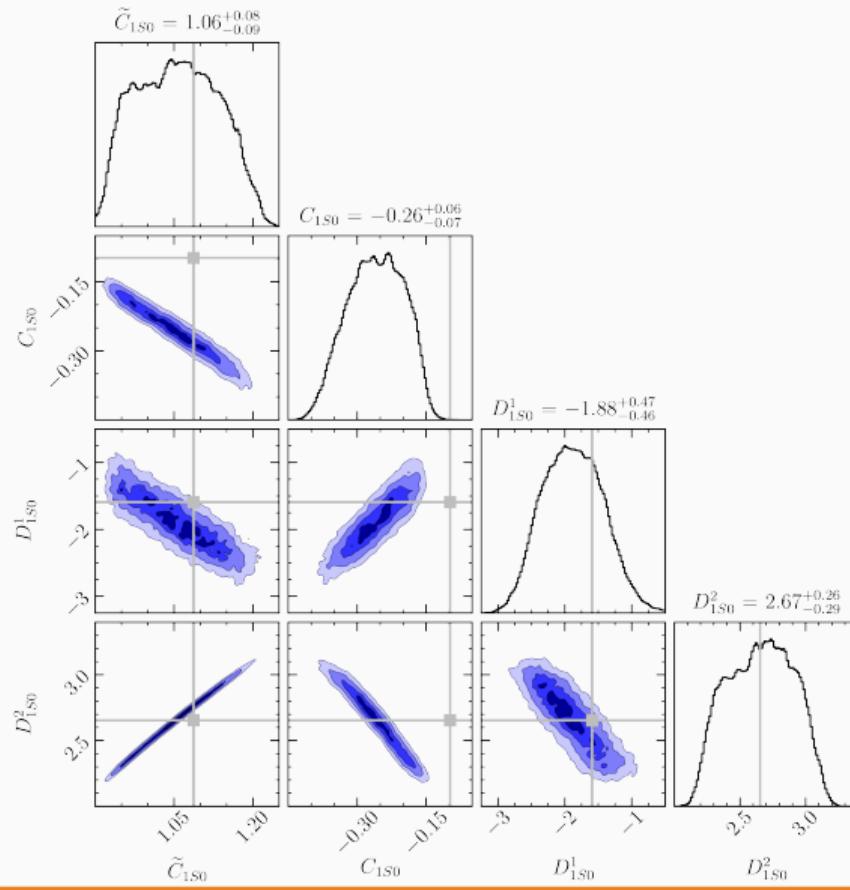
- y axis: posterior median $\pm 1\sigma$
- x axis: max energy of data in fit
- Q , and hence δy_{th} , grows with energy

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

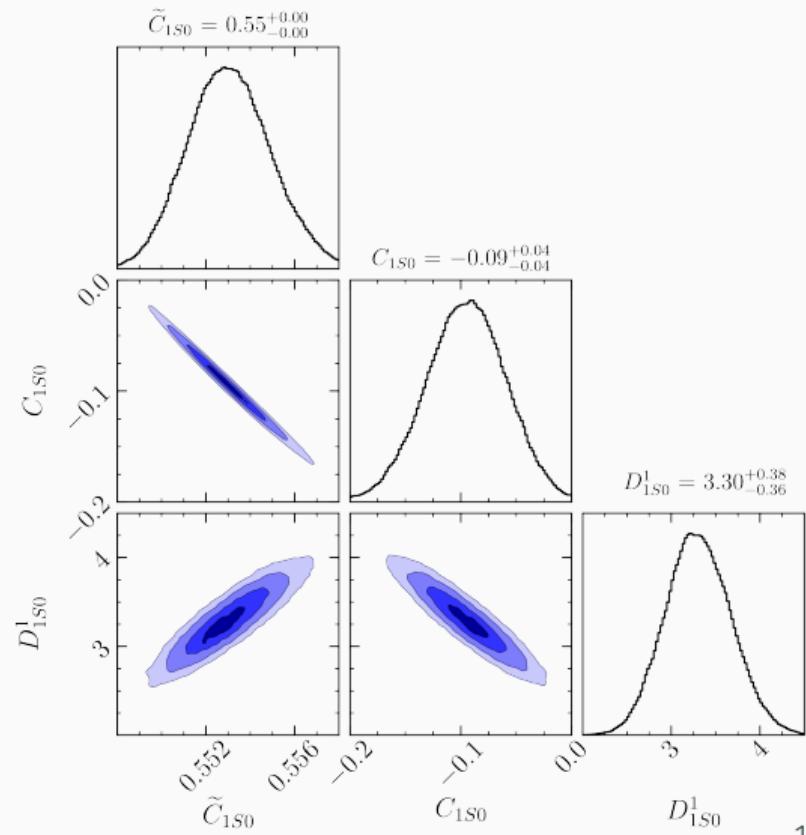
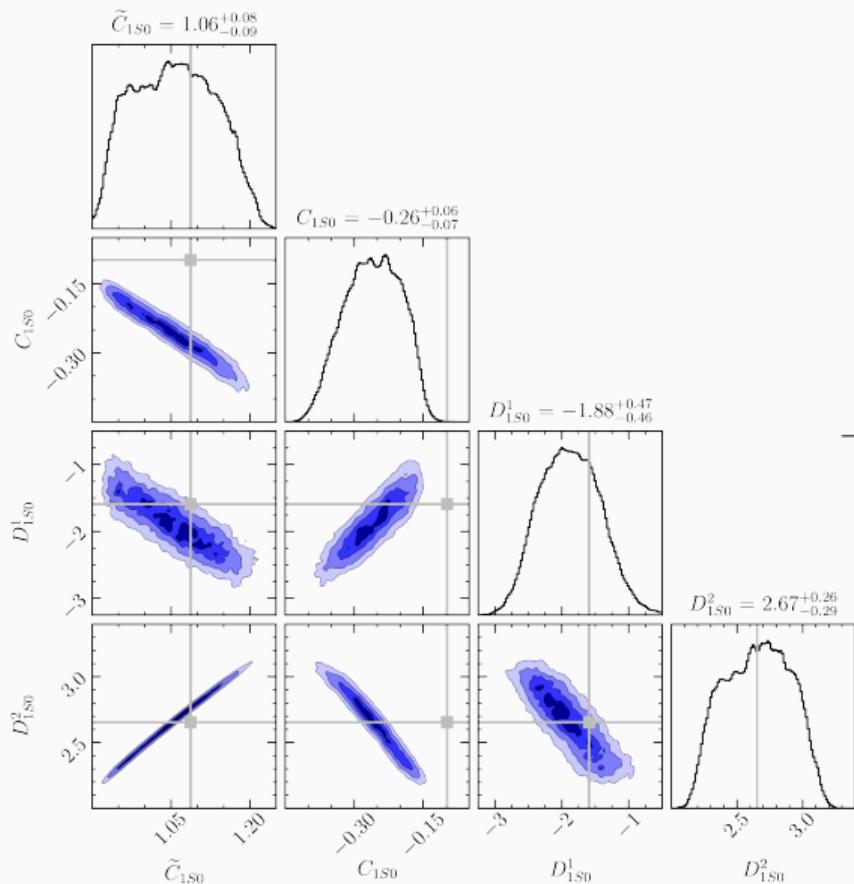
- This weights high energy data less!
- Stabilizes LEC fit as a function of E
- LEC uncertainty is more realistic



Discovering Physics (Redundant LECs)



Discovering Physics (Redundant LECs)



(Also: 2018 Reinert, P. and Krebs, H. and Epelbaum, E.)

Model Validation

Model Validation

*As far as the laws of mathematics refer to reality, they are not certain,
and as far as they are certain, they do not refer to reality.*

— Albert Einstein

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

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Custom Tests

1. Are the theory error bands actually working?

Bayesian Solution

1. Use the posterior predictive $\text{pr}(y | M)$ to generate fake data

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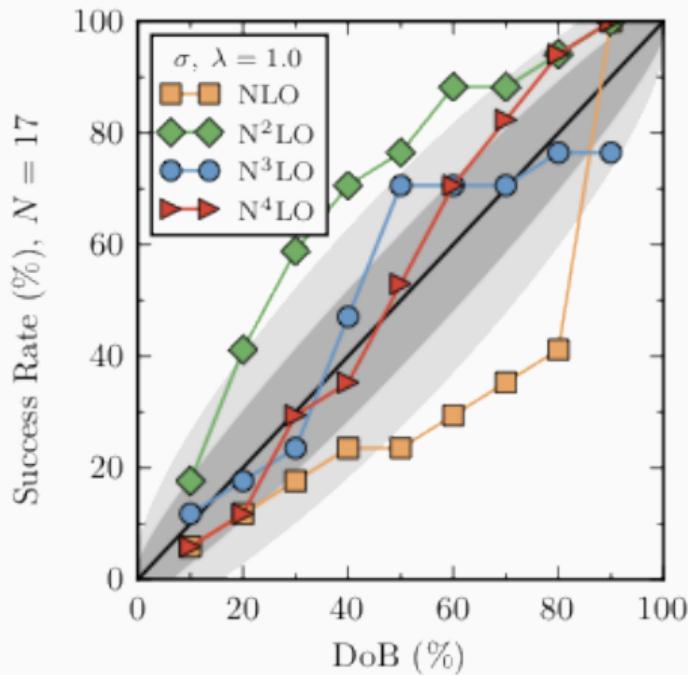
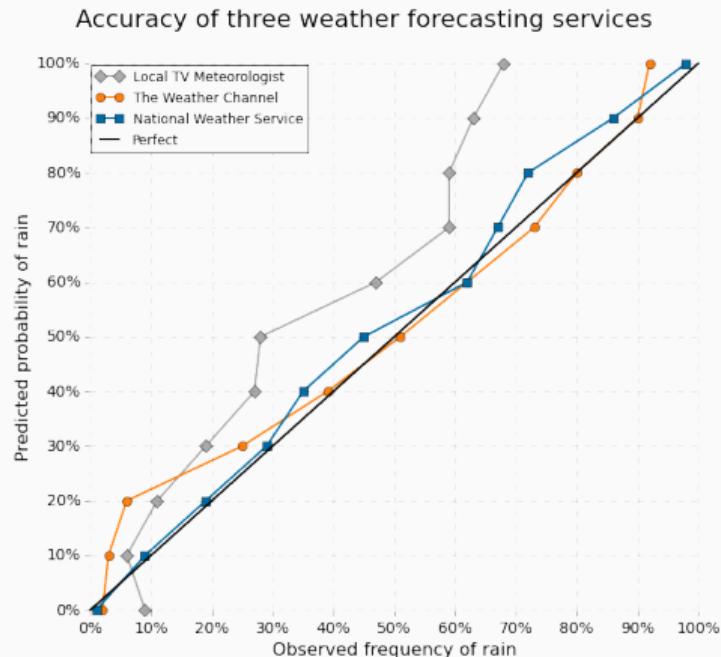
1. Are the theory error bands actually working?
2. Are the EFT parameters sufficient? Are they overfitting?

Bayesian Solution

1. Use the posterior predictive $\text{pr}(y | M)$ to generate fake data
2. Can assign probabilities to **models**

Credible Interval Diagnostics

Are our error bands working as advertised? Requires a **reference** distribution.

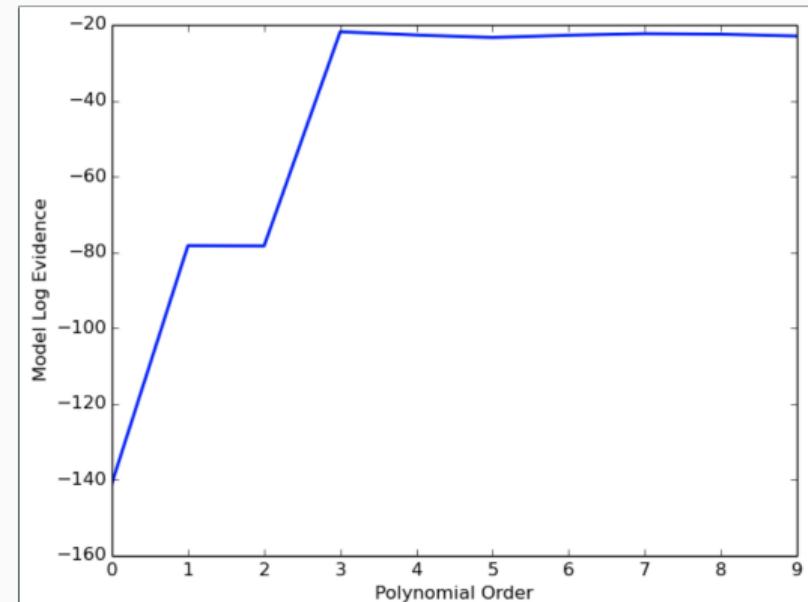


Source: "The Signal and the Noise" by Nate Silver | Author: Randy Olson (randalolson.com / @randal_olson)

Model Selection: Bayes Factors

- Which model is better supported by the data, M_0 or M_1 ?

$$\frac{\text{pr}(M_1 | \mathcal{D})}{\text{pr}(M_0 | \mathcal{D})} = \frac{\text{pr}(\mathcal{D} | M_1)}{\text{pr}(\mathcal{D} | M_0)} \frac{\text{pr}(M_1)}{\text{pr}(M_0)}$$

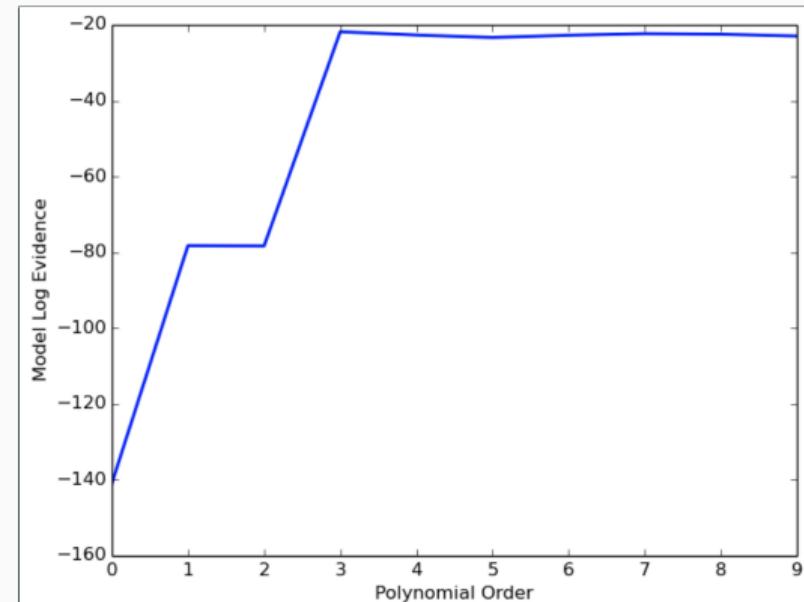


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- Requires computation of evidence $\text{pr}(\mathcal{D} | M)$ which can be tricky
- But can be used to prevent overfitting, and to choose between competing models!



Takeaway Points

Building Statistical Models

Building Statistical Models

- List what you know and what you don't

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

Building Statistical Models

- List what you know and what you don't
- Build it in the language of random variables

$$\text{pr}(c_n | \boldsymbol{\theta}) \stackrel{\text{iid}}{\sim} \mathcal{GP}(\mu, \sigma^2 R_\ell)$$

Takeaway Points

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What is Gained

- Full accounting of uncertainty (keeps experimentalists happy)

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- Can uncover physics and falsify models

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Building Statistical Models

- List what you know and what you don't
- Build it in the language of random variables
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What is Gained

- Full accounting of uncertainty (keeps experimentalists happy)
- Can uncover physics and falsify models
- Is easy due to new computational tools, like PyMC3

Thank you!

arxiv:1904.10581

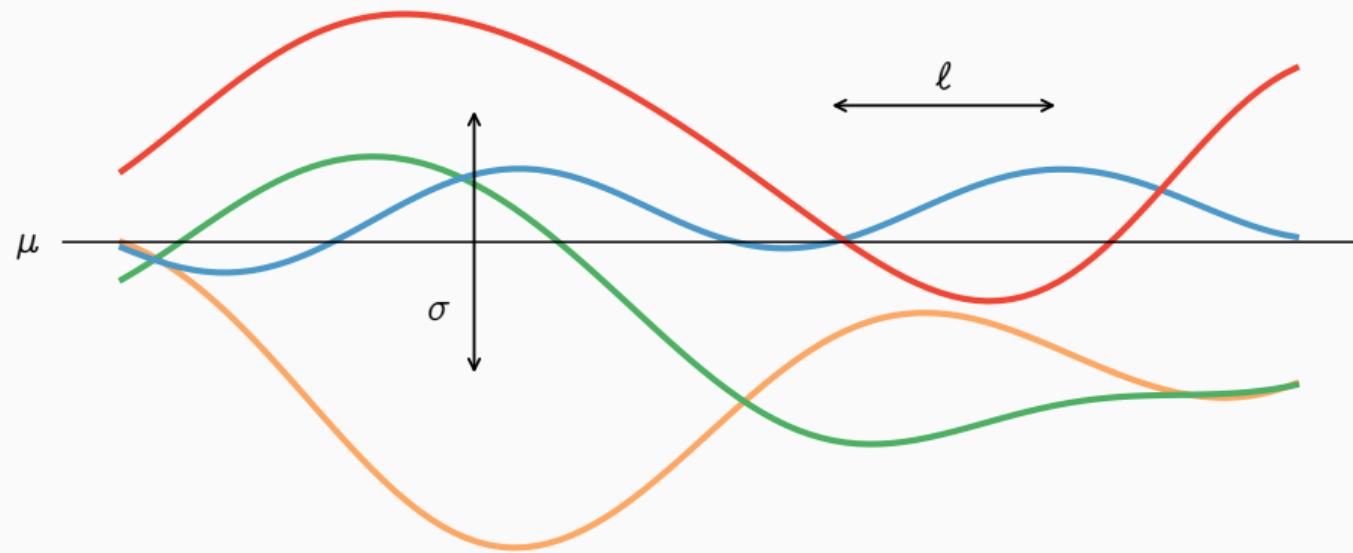
arXiv:1808.08211

arXiv:1704.03308



Gaussian Process Priors on Observable Coefficients

$$c_n | \theta \stackrel{\text{iid}}{\sim} \mathcal{GP}(\mu, \sigma^2 R_\ell)$$

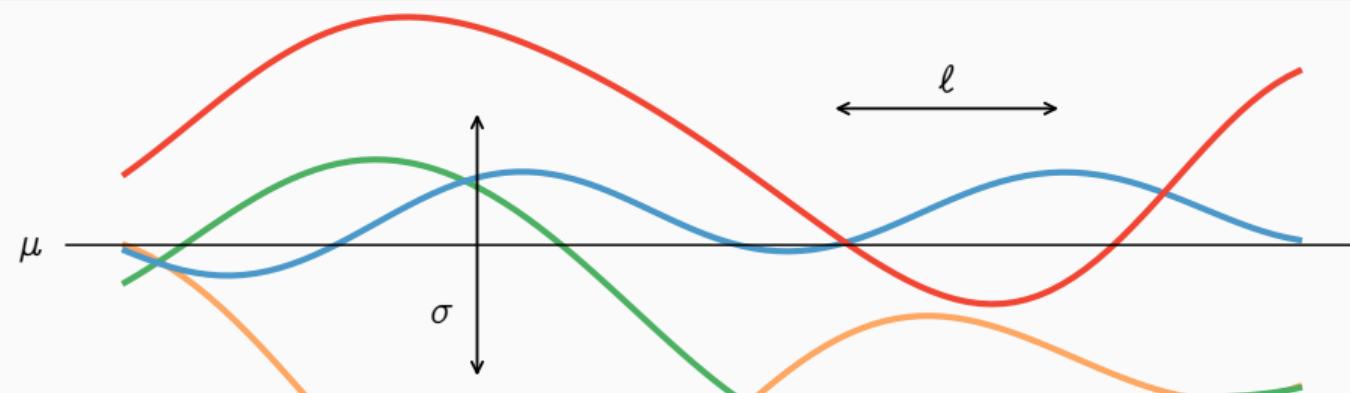


Gaussian Process Priors on Observable Coefficients

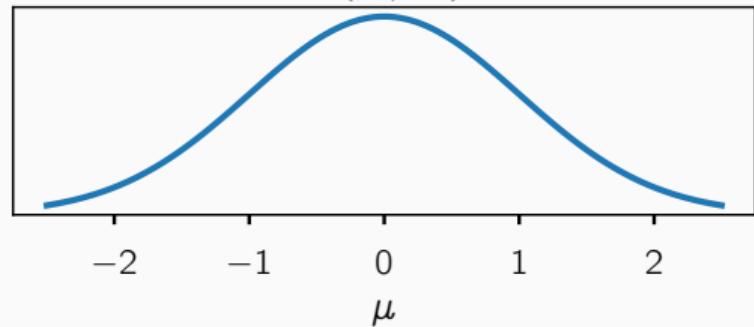
$$c_n | \theta \stackrel{\text{iid}}{\sim} \mathcal{GP}(\mu, \sigma^2 R_\ell)$$

Conjugate priors:

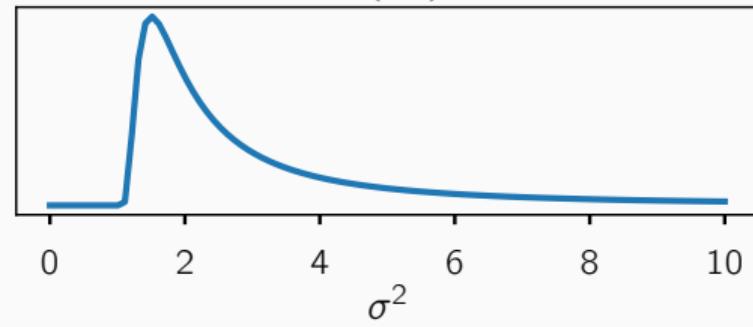
$$\begin{aligned}\mu | \sigma^2 &\sim \mathcal{N}(m, \sigma^2 V) \\ \sigma^2 &\sim \text{IG}(a, b)\end{aligned}$$



$$\text{pr}(\mu | \sigma^2)$$



$$\text{pr}(\sigma^2)$$



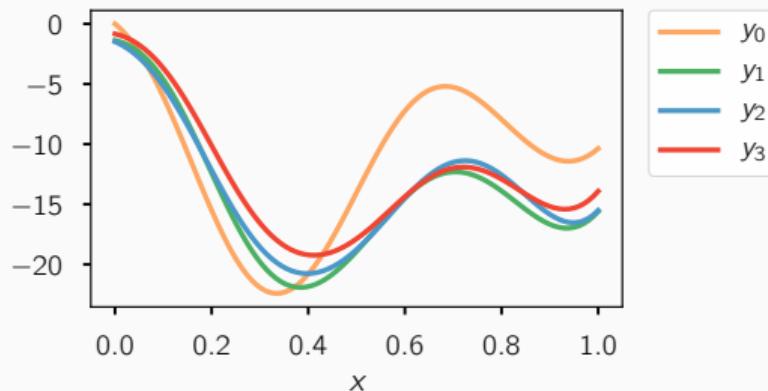
Model Building

Main equation

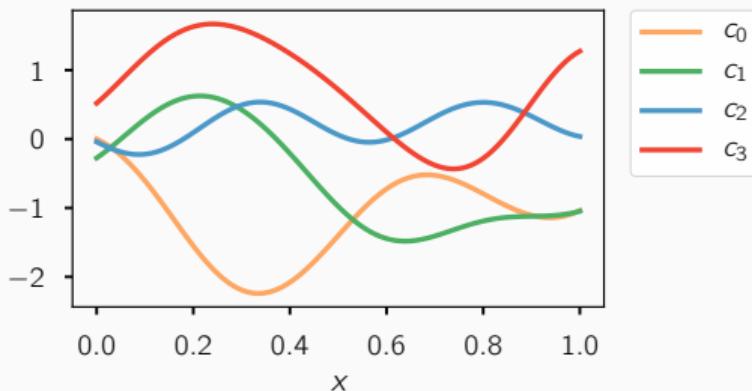
$$y_k = y_{\text{ref}} \sum_{n=0}^k c_n Q^n$$

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

Predictions



Prediction Coefficients

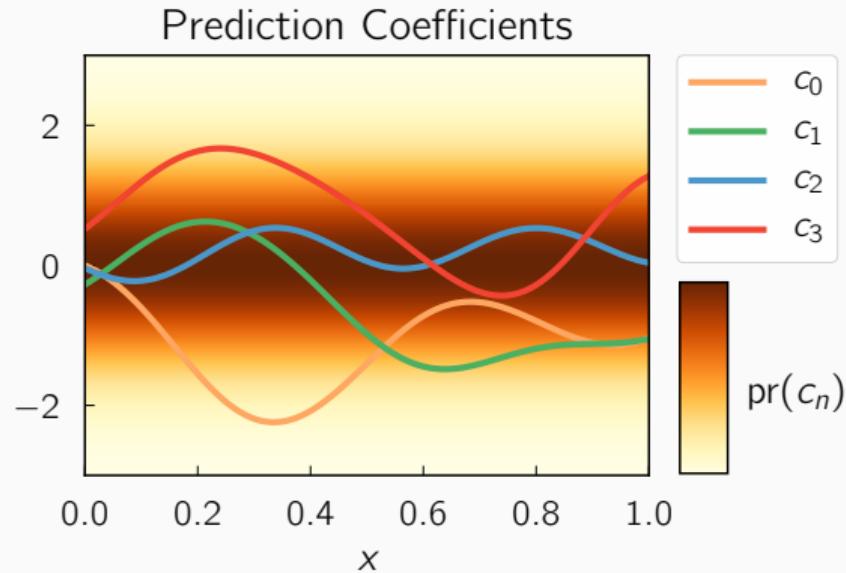
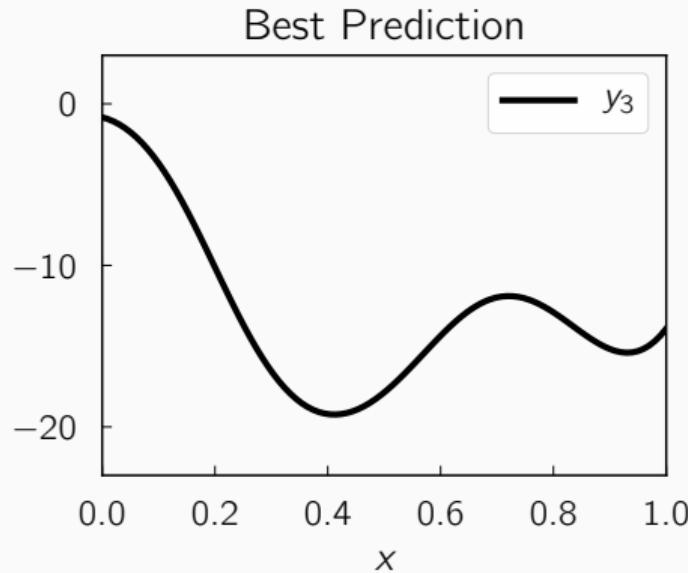


Model Building

Main equation

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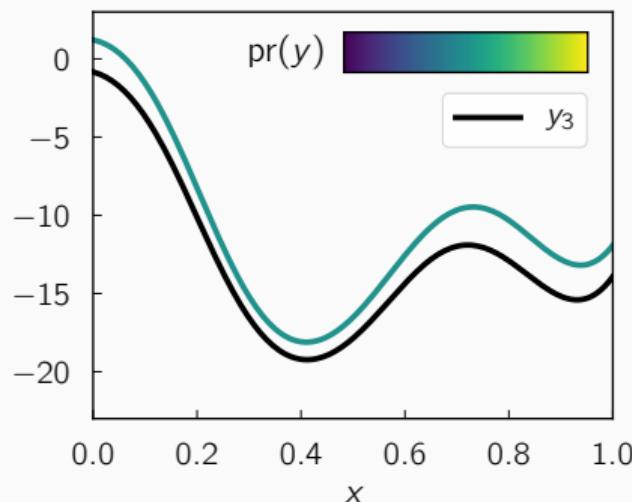
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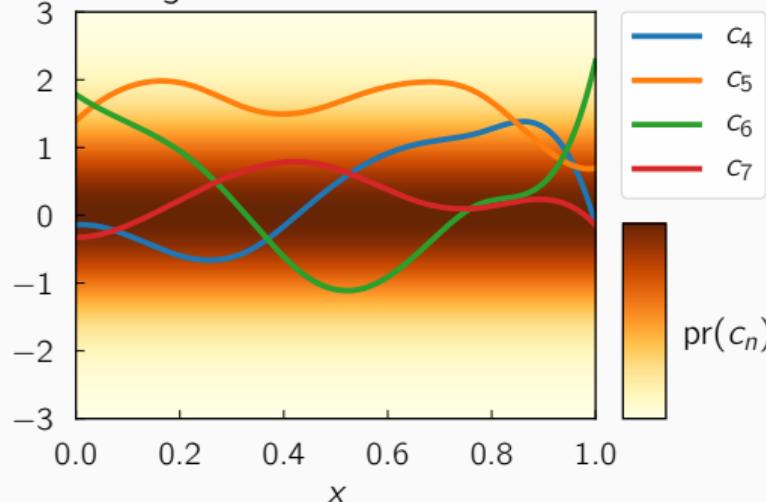
$$y = y_{\text{ref}} \sum_{n=0}^{\infty} c_n Q^n$$

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Full Prediction



Higher Order Coefficients



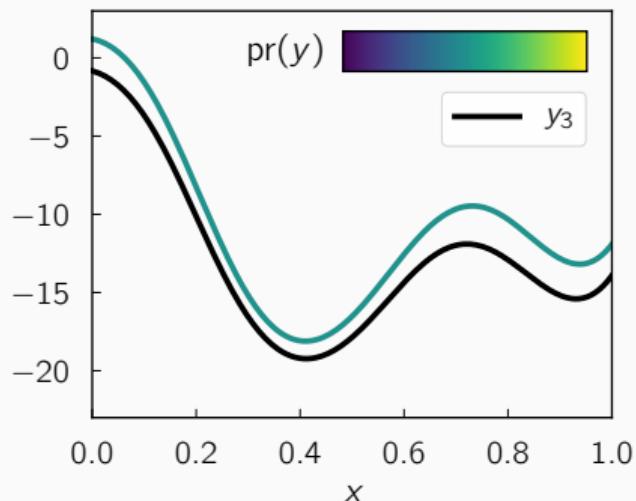
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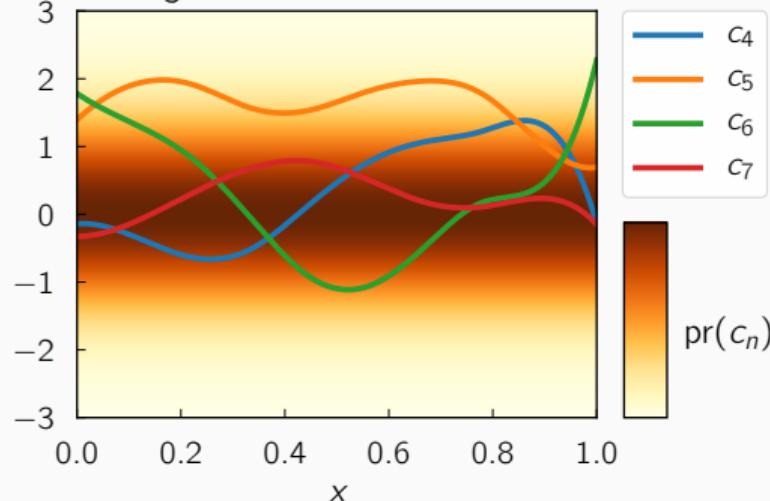
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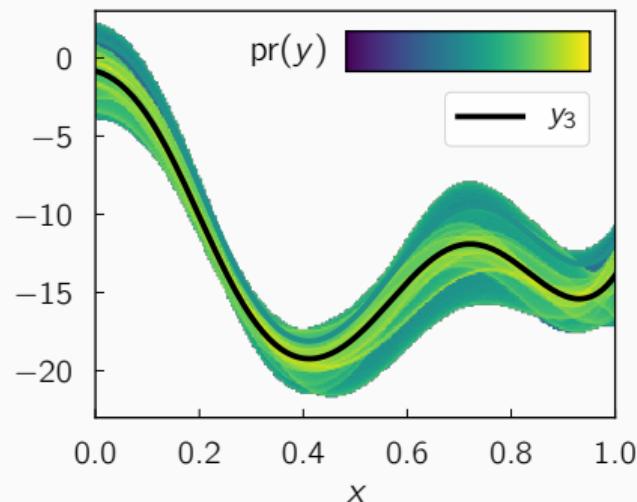
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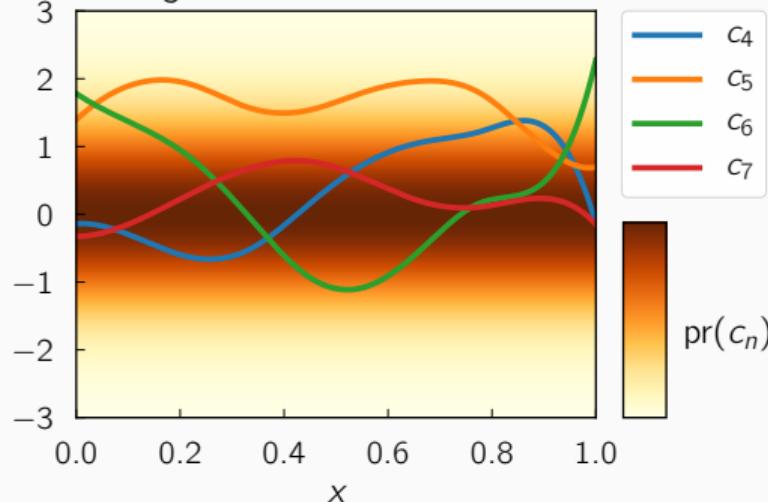
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Remember the goal:

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

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Implications for EFT Fitters

Standard χ^2

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

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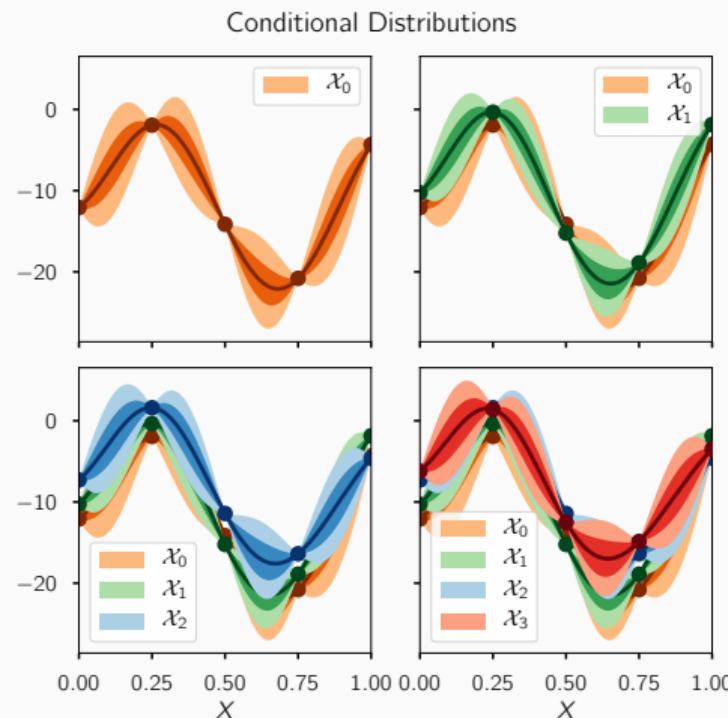
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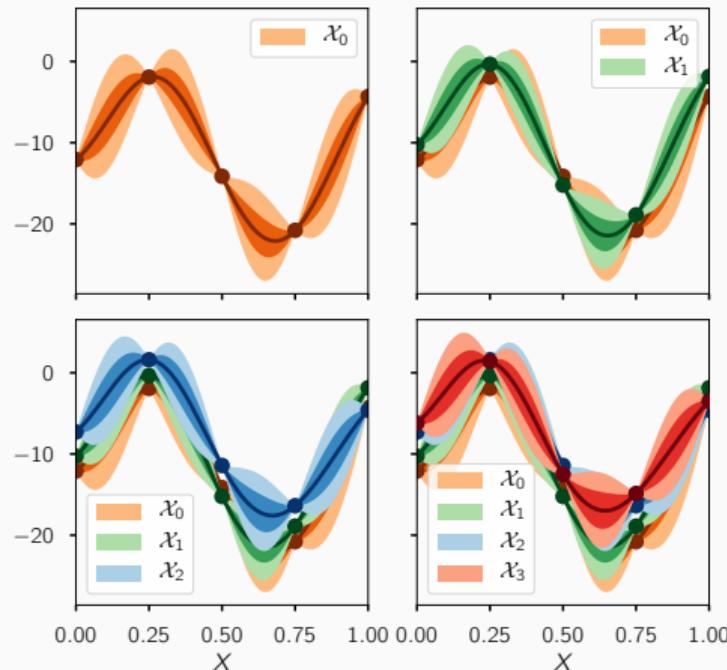
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- Different correlation assumptions \rightarrow different results!

Quantifying Truncation Uncertainty

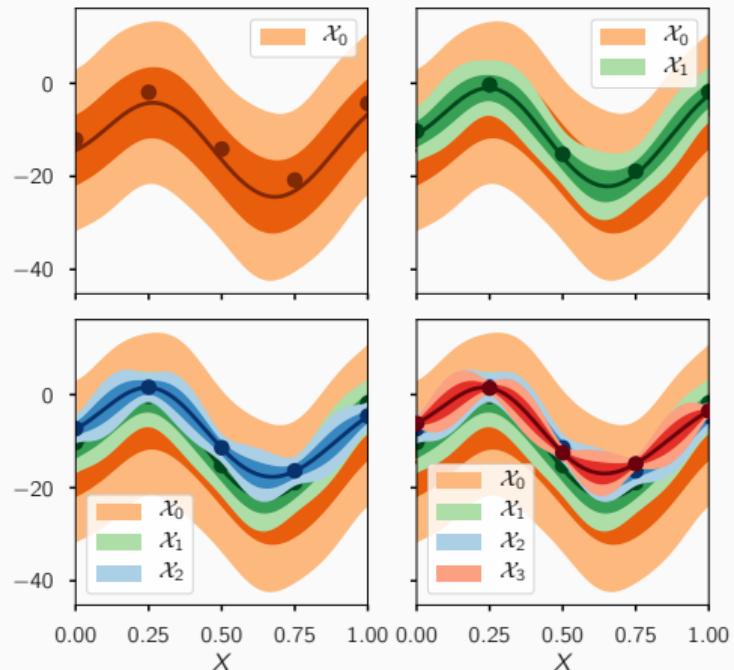


Quantifying Truncation Uncertainty

Conditional Distributions



Conditional + Error



What You Get for (Almost) Free: Evidence, Length Scale, & Breakdown Scale

This model permits mostly analytic calculation of evidence

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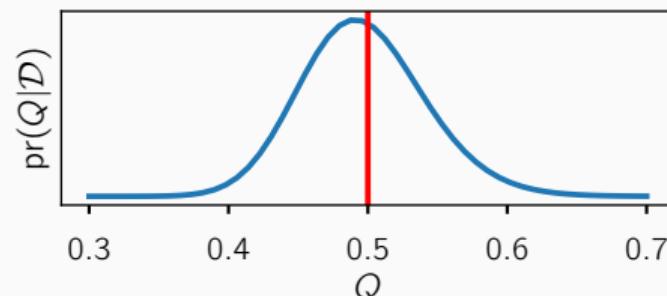
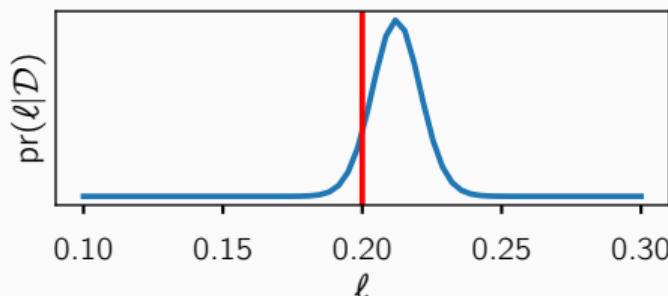
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Here, $Q \propto \frac{1}{\Lambda_b}$

