

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

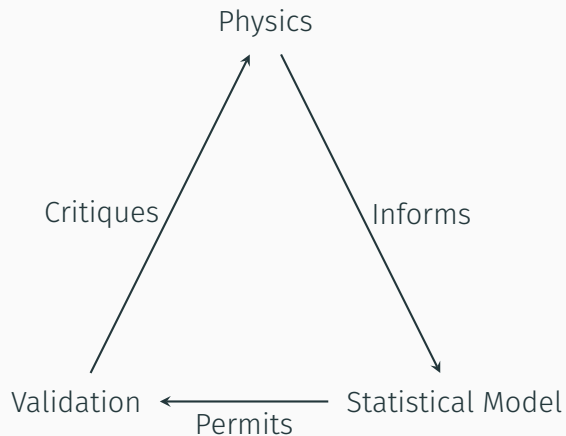
¹The Ohio State University

²Ohio University

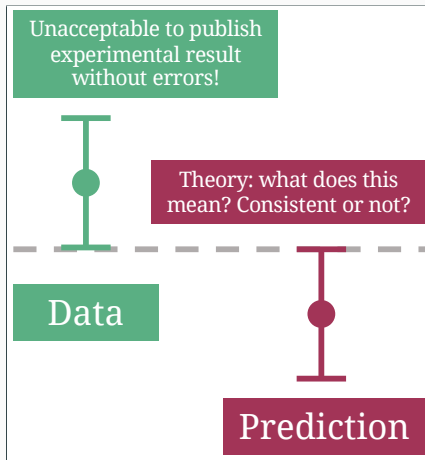
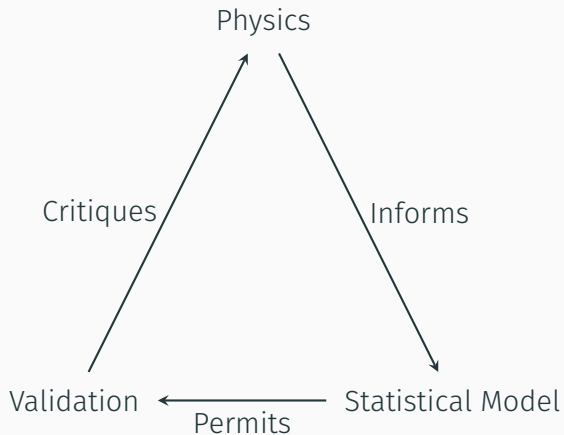
³Salisbury University



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



Why Bayesian?



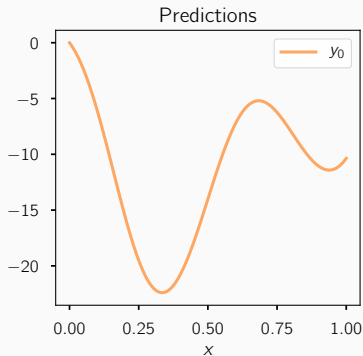
- More intuitive
 - Confidence intervals \rightarrow credible intervals
 - p -values \rightarrow posterior probabilities
- Conventional results often recovered as a special case
- Assumptions are made **explicit**
- Well suited for incorporating theoretical error

Physical Motivation

Chiral EFT in One Slide

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

$\{y_0\}$

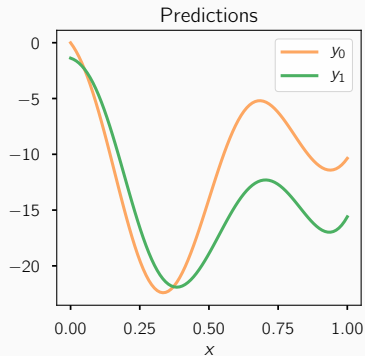


$y_0 \rightarrow \text{LO}$

Chiral EFT in One Slide

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$\{y_0, y_1\}$



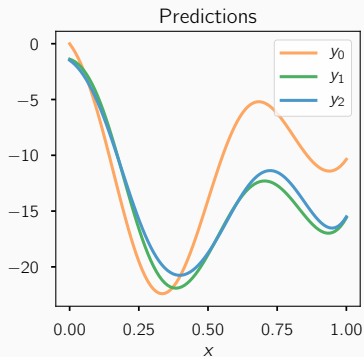
$y_0 \rightarrow \text{LO}$

$y_1 \rightarrow \text{NLO}$

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

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



$$y_0 \rightarrow \text{LO}$$

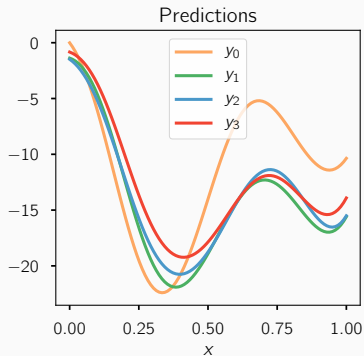
$$y_1 \rightarrow \text{NLO}$$

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

Chiral EFT in One Slide

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



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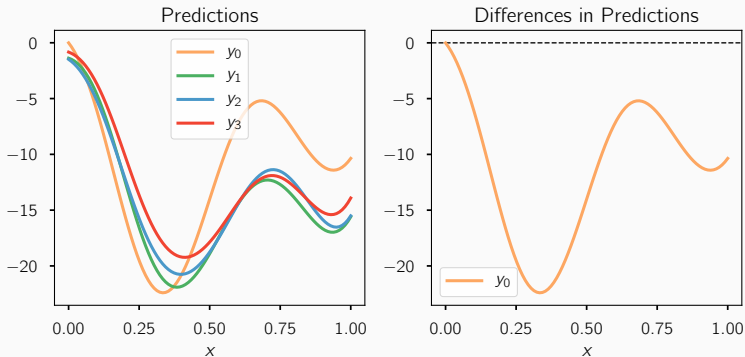
⋮

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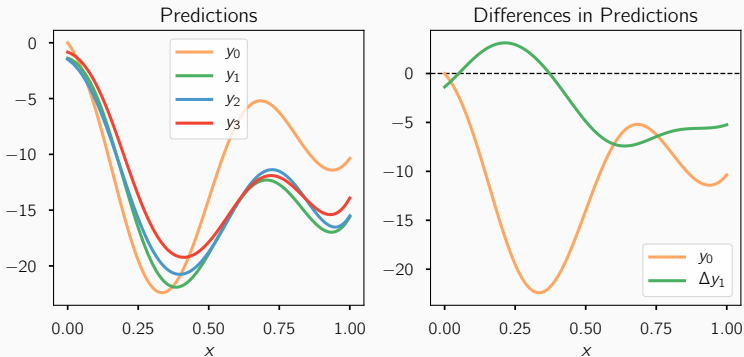
$$y_0 = y_0$$



Chiral EFT in One Slide

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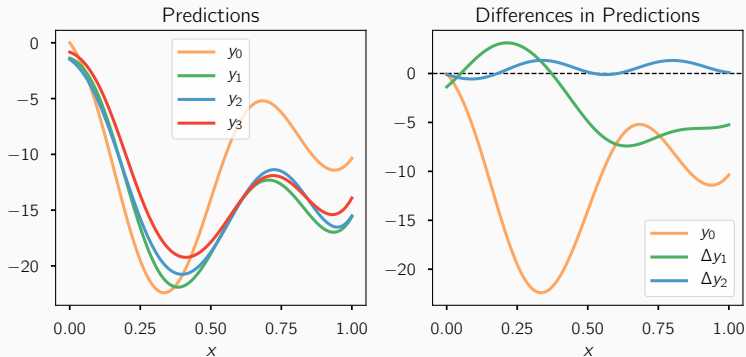
$$y_1 = y_0 + \Delta y_1$$



Chiral EFT in One Slide

- $V_{NN}(\vec{a}) = V_{LO} + V_{NLO} + \dots + V_{N^kLO} \implies \boxed{\text{Schrödinger Eq.}} \implies y_k(x; \vec{a})$
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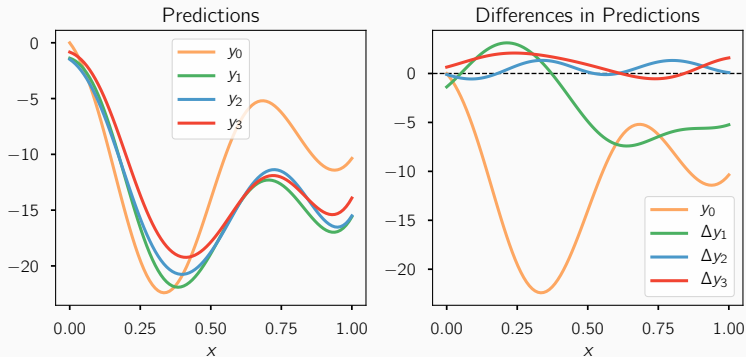
$$y_2 = y_0 + \Delta y_1 + \Delta y_2$$



Chiral EFT in One Slide

- $V_{NN}(\vec{a}) = V_{LO} + V_{NLO} + \dots + V_{N^kLO} \implies \boxed{\text{Schrödinger Eq.}} \implies y_k(x; \vec{a})$
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- $\Delta y_n = y_{\text{ref}} c_n Q^n$

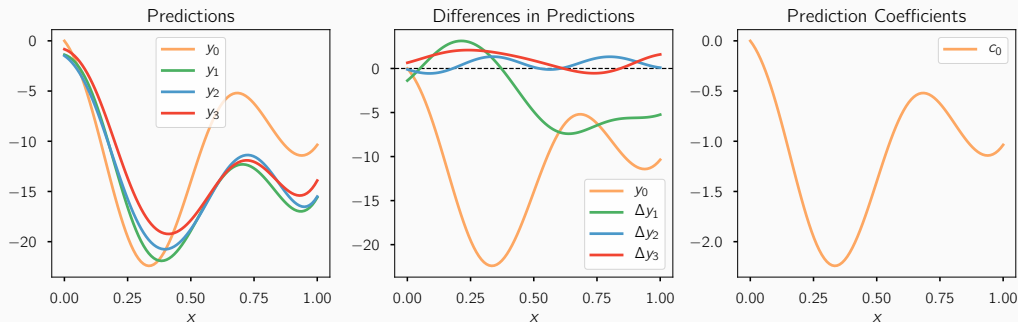
$$y_3 = y_0 + \Delta y_1 + \Delta y_2 + \Delta y_3$$



Chiral EFT in One Slide

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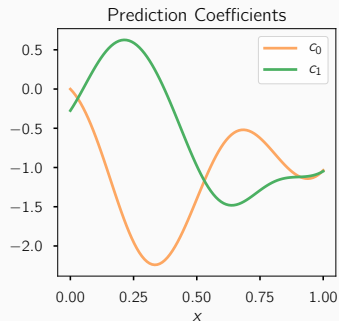
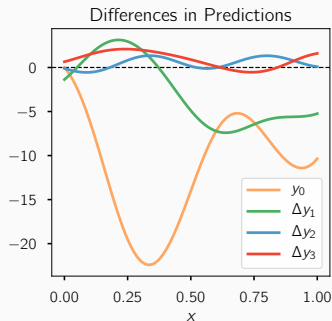
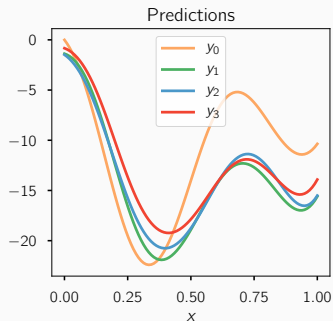
$$y_0 = y_{\text{ref}} [c_0 Q^0]$$



Chiral EFT in One Slide

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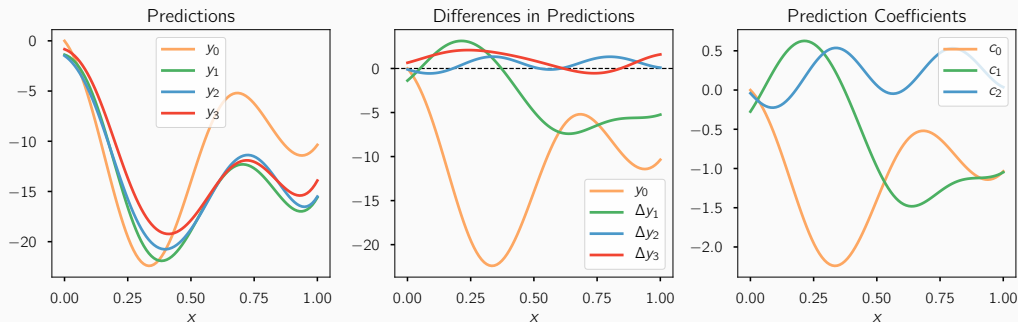
$$y_1 = y_{\text{ref}} [c_0 Q^0 + c_1 Q^1]$$



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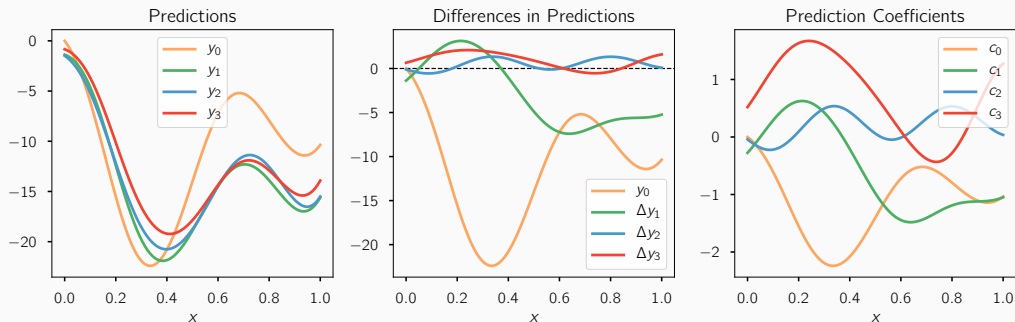
$$y_2 = y_{\text{ref}} [c_0 Q^0 + c_1 Q^1 + c_2 Q^2]$$



Chiral EFT in One Slide

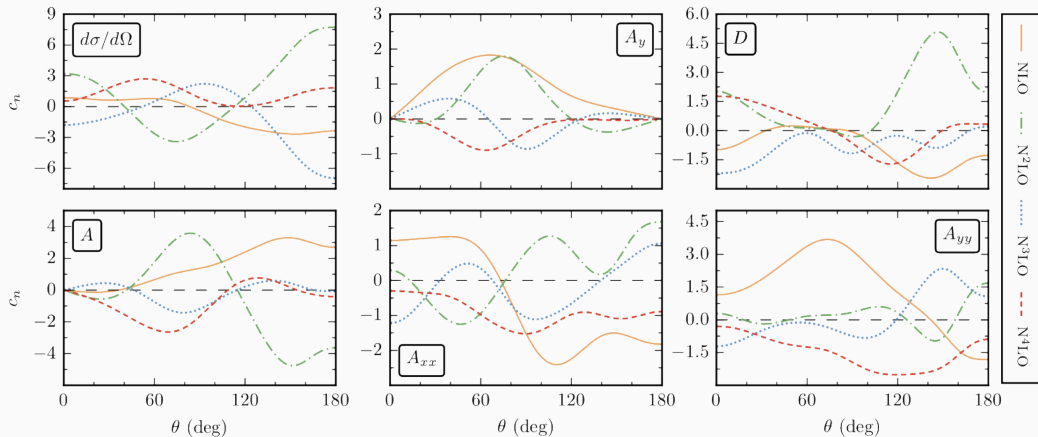
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$$y_3 = y_{\text{ref}} [c_0 Q^0 + c_1 Q^1 + c_2 Q^2 + c_3 Q^3]$$



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

The diagram illustrates the decomposition of experimental data into theoretical components and their uncertainties. At the top, the text "To theorists, magic" has two arrows pointing down to the equation $y_{\text{exp}}(x) = y_{\text{th}}(x, \vec{a}) + \delta y_{\text{th}}(x) + \delta y_{\text{exp}}$. Below the equation, the word "Parameters" has an arrow pointing up to the vector \vec{a} . The word "Discrepancy" has an arrow pointing up to the term $\delta y_{\text{th}}(x)$.


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

Parameters

Discrepancy

$$\begin{array}{c} \chi^2 \text{ fit} \\ \curvearrowright \\ y_{\text{exp}}(x) = y_{\text{th}}(x, \vec{a}) \end{array} \quad + \delta y_{\text{exp}}$$

rigorous fit


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

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

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

How do we design this?

How does it affect fitting \vec{a} ?

- Decompose prediction

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



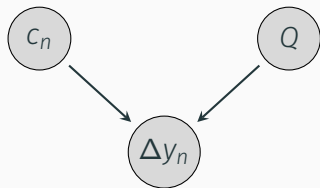
Data

The Hierarchical Model

- Decompose prediction

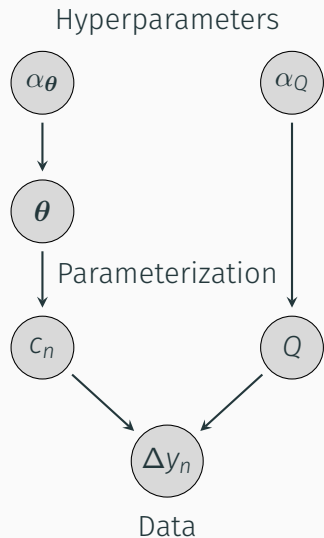
$$\left. \begin{aligned} y_k &= y_0 + \sum_{n=1}^k \Delta y_n \\ &= y_{\text{ref}} \sum_{n=0}^k c_n Q^n \end{aligned} \right\}$$

Parameterization



Data

The Hierarchical Model



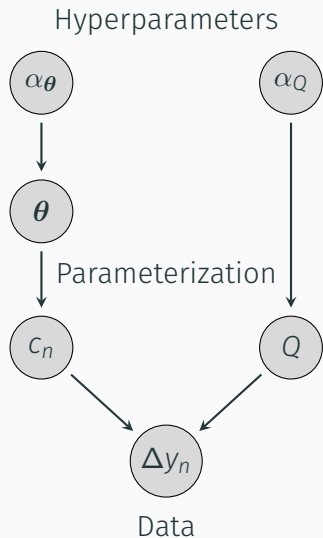
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- Promote c_n (and Q) to random variables

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

The Hierarchical Model



- Decompose prediction

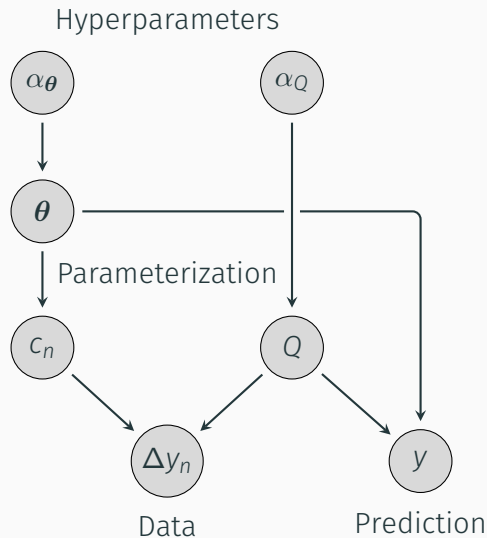
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- Train statistical parameters ($\boldsymbol{\theta}$ and Q) and LECs \vec{a} on data

The Hierarchical Model



- Decompose prediction

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

```

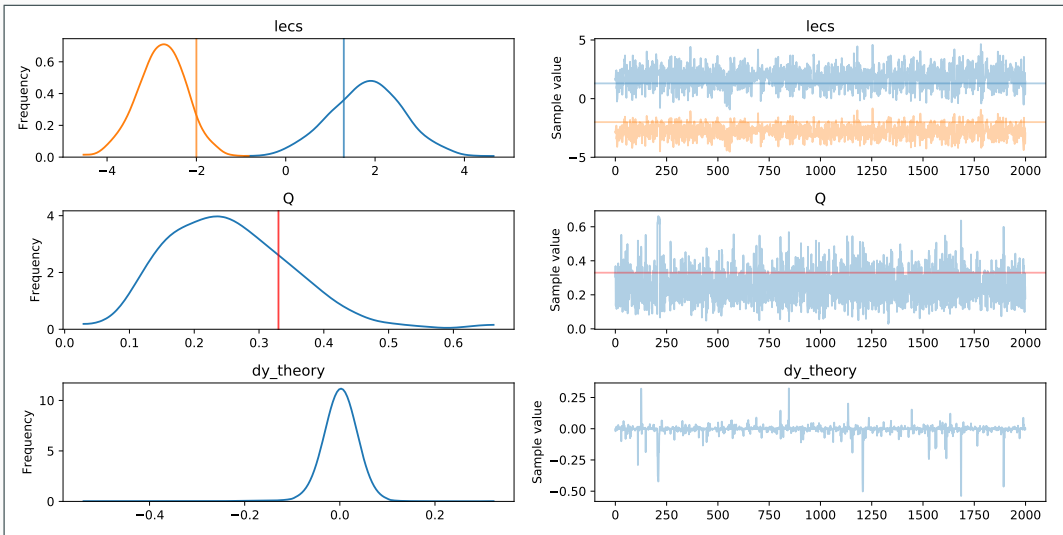
# Setup code goes up here ...
with Model() as model: # Build statistical model with PyMC3
    Q = Beta('Q', alpha=5, beta=15) # Priors
    sigma = Lognormal('sigma', mu=0, sd=1)
    c_n = Normal('c_n', mu=0, sd=sigma, shape=(n_high_orde, 1))
    dy_theory = Deterministic('dy_theory',
        tt.sum(c_n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

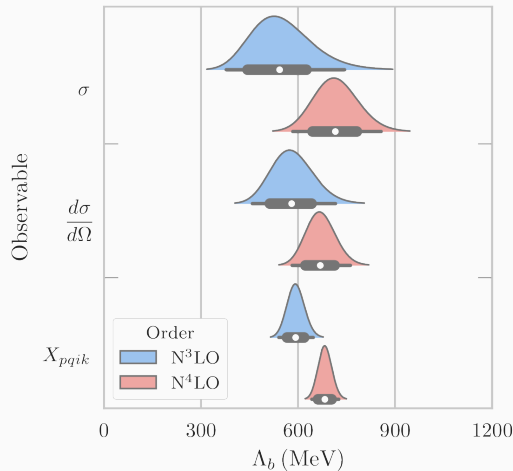
So what?

Rigorous Estimation of Unknown Quantities

- The breakdown scale of the EFT Λ_b :

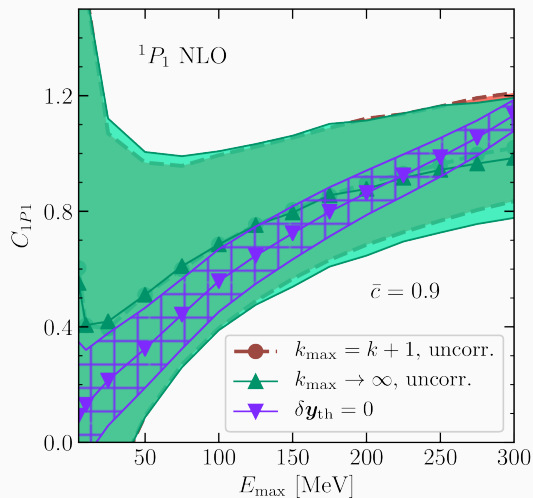
$$Q \approx \frac{f(p, m_\pi)}{\Lambda_b}$$

- 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

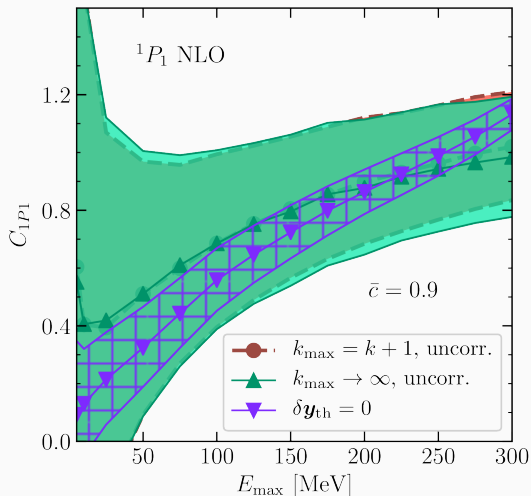


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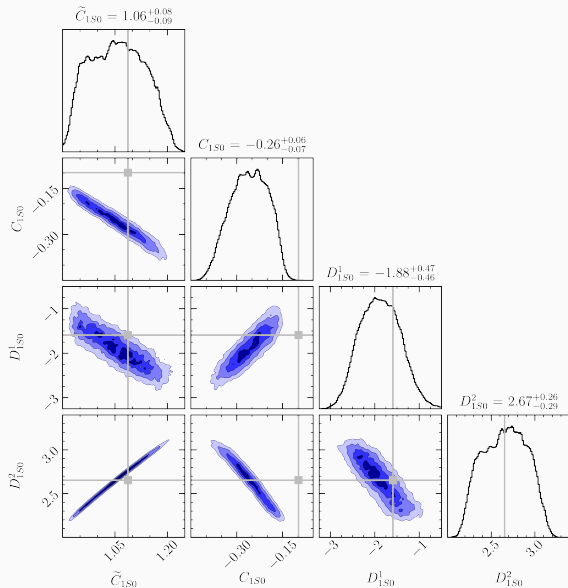
- y axis: posterior median $\pm 1\sigma$
- x axis: max energy of data in fit
- Q , and hence δy_{th} , grows with energy

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

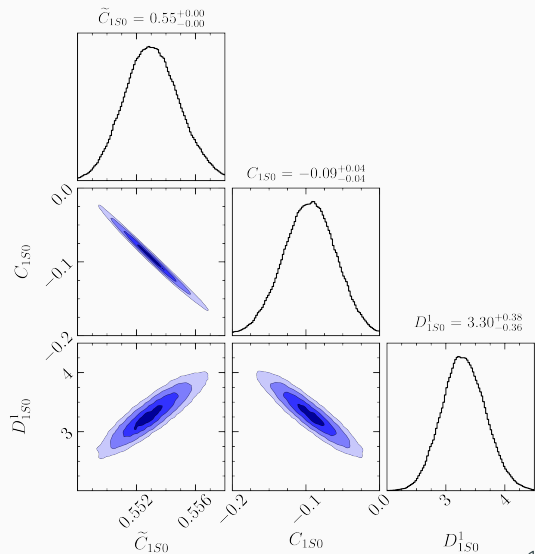
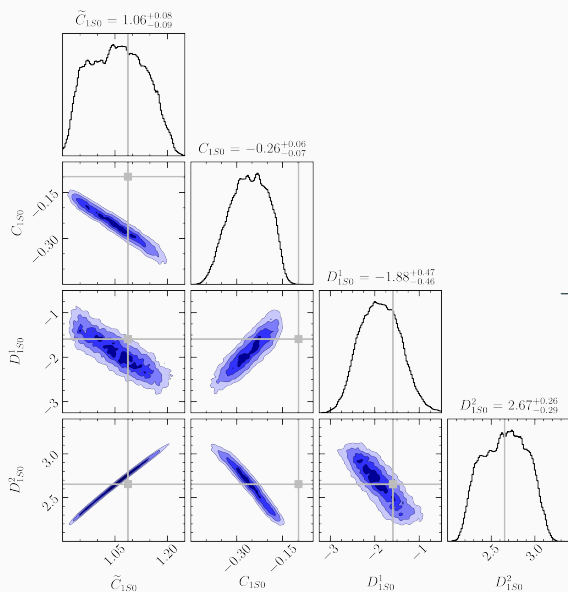
- This weights high energy data less!
- Stabilizes LEC fit as a function of E
- LEC uncertainty is more realistic



Discovering Physics (Redundant LECs)



Discovering Physics (Redundant LECs)



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

Model Validation

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and as far as they are certain, they do not refer to reality.*

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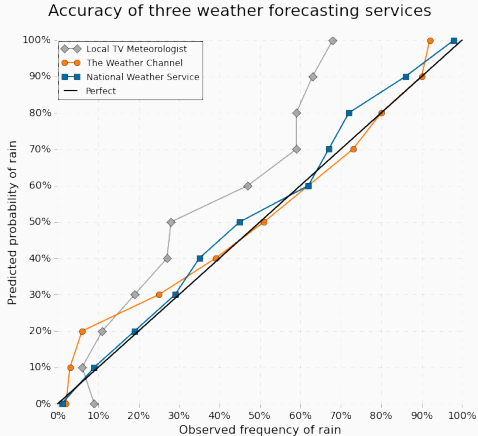
1. Are the theory error bands actually working?
2. Are the EFT parameters sufficient? Are they overfitting?

Bayesian Solution

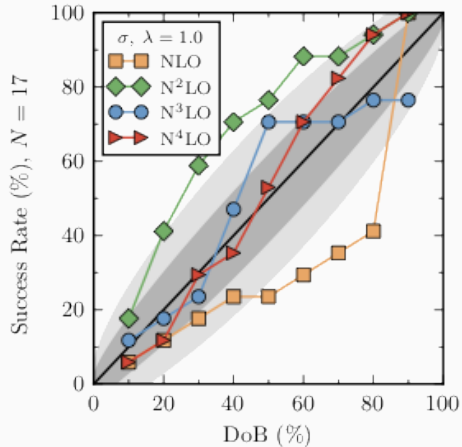
1. Use the posterior predictive $\text{pr}(y | M)$ to generate fake data
2. Can assign probabilities to **models**

Credible Interval Diagnostics

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



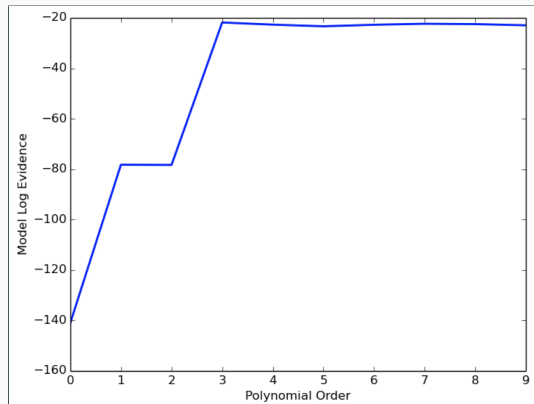
Source: "The Signal and the Noise" by Nate Silver | Author: Randy Olson (randalolson.com / @randal_olson)



Model Selection: Bayes Factors

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

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

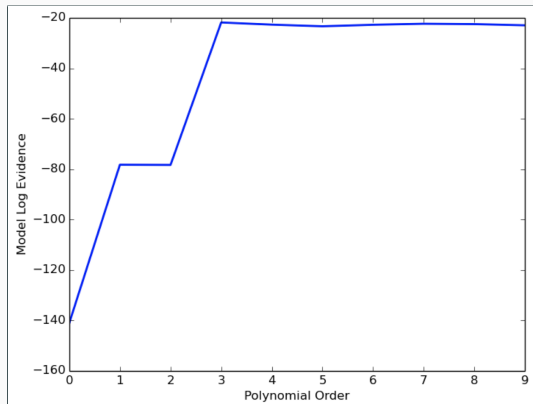


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- Requires computation of evidence $\text{pr}(\mathcal{D} | M)$ which can be tricky
- But can be used to prevent overfitting, and to choose between competing models!





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

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

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What is Gained

- Full accounting of uncertainty (keeps experimentalists happy)

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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

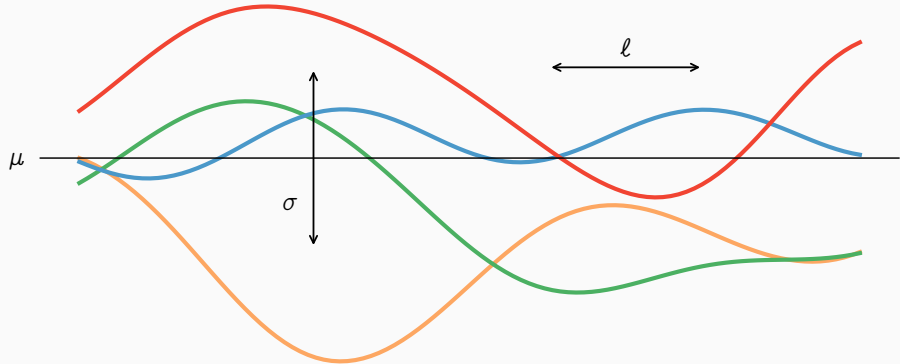
arXiv:1808.08211

arXiv:1704.03308



Gaussian Process Priors on Observable Coefficients

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



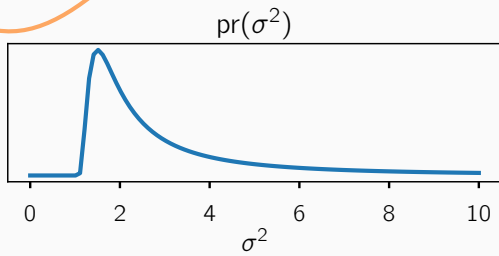
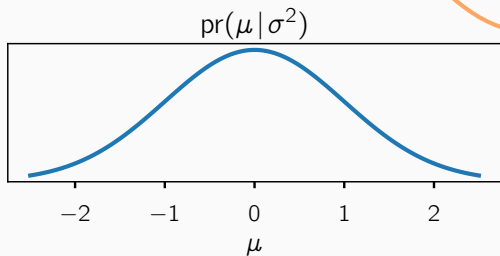
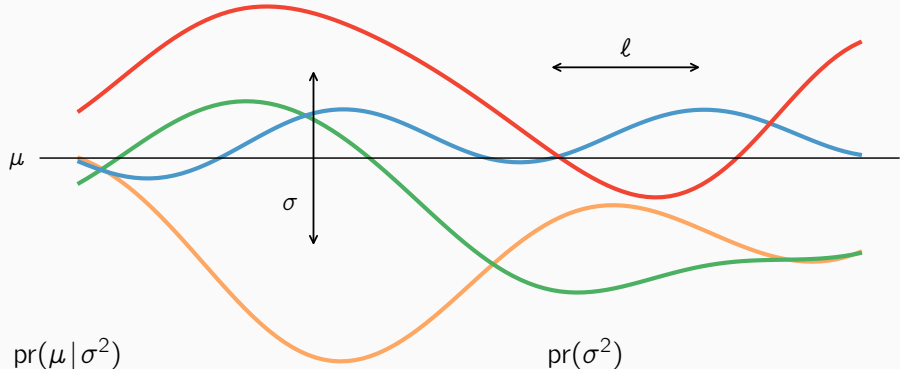
Gaussian Process Priors on Observable Coefficients

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Conjugate priors:

$$\mu | \sigma^2 \sim \mathcal{N}(m, \sigma^2 V)$$

$$\sigma^2 \sim \text{IG}(a, b)$$

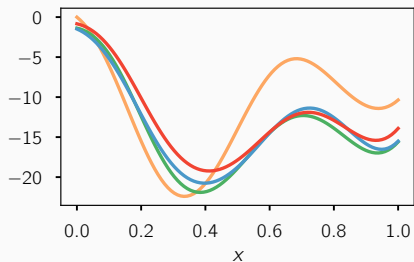


Main equation

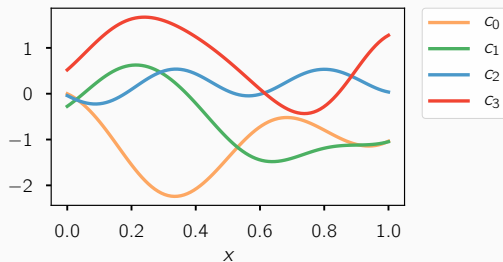
$$y_k = y_{\text{ref}} \sum_{n=0}^k c_n Q^n$$

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

Predictions



Prediction Coefficients



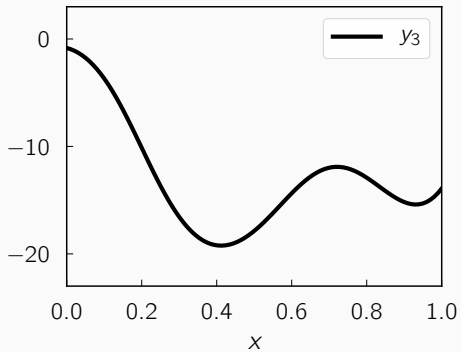
Model Building

Main equation

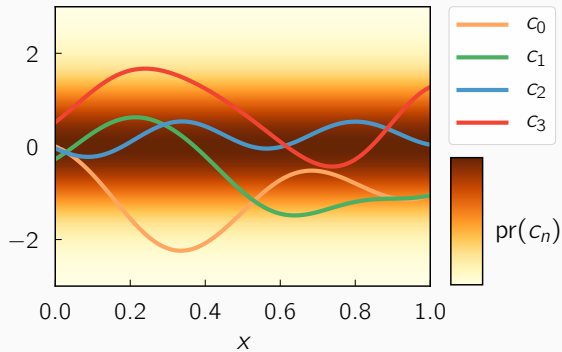
$$y_k = y_{\text{ref}} \sum_{n=0}^k c_n Q^n$$

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

Best Prediction



Prediction Coefficients

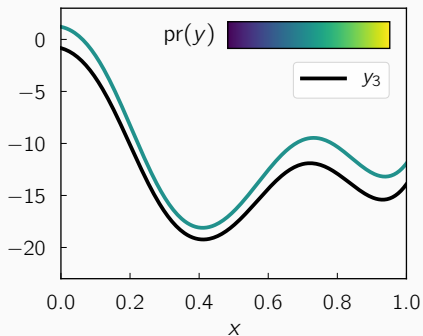


Main equation

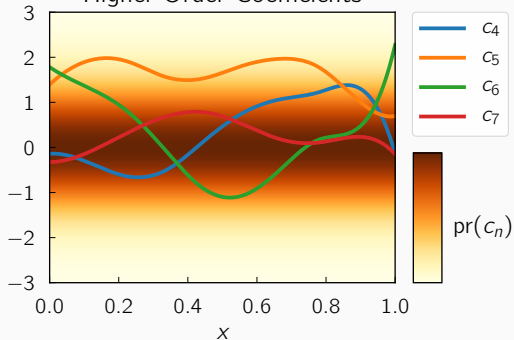
$$y = y_{\text{ref}} \sum_{n=0}^{\infty} c_n Q^n$$

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Full Prediction



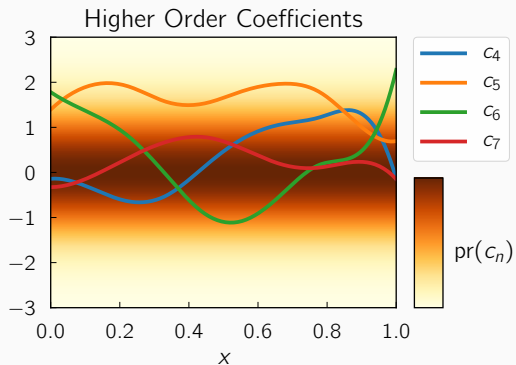
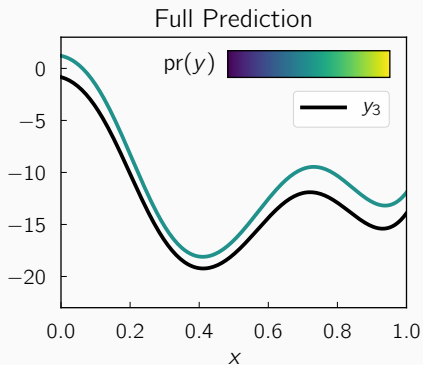
Higher Order Coefficients



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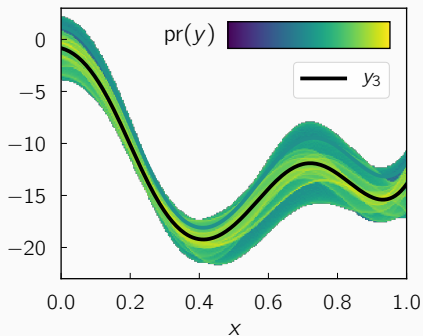


Main equation

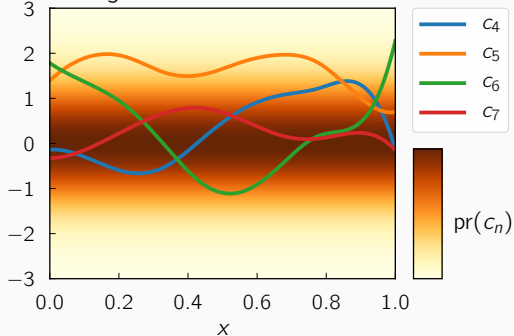
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Higher Order Coefficients



Discrepancy Distribution

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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Gaussian sum rules

$$a\mathcal{N}(\mu_1, \Sigma_1) + b\mathcal{N}(\mu_2, \Sigma_2) = \mathcal{N}(a\mu_1 + b\mu_2, a^2\Sigma_1 + b^2\Sigma_2)$$

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Discrepancy Distribution

$$\text{pr}(\delta y_{\text{th}} | \boldsymbol{\theta}) = \mathcal{GP}(\mu_{\text{th}}, \Sigma_{\text{th}}) = \mathcal{GP}\left(\frac{\mu Q^{k+1}}{1-Q}, y_{\text{ref}}^2 \frac{\sigma^2 Q^{2(k+1)}}{1-Q^2} R_\ell\right)$$

Standard χ^2

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

Implications for EFT Fitters

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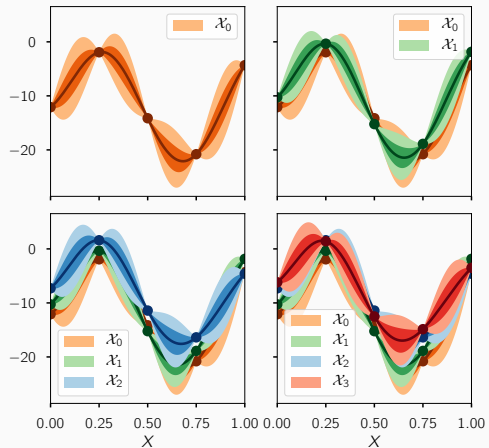
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- Different correlation assumptions \rightarrow different results!

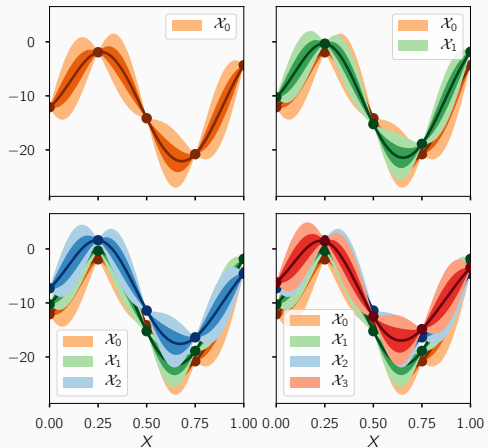
Quantifying Truncation Uncertainty

Conditional Distributions

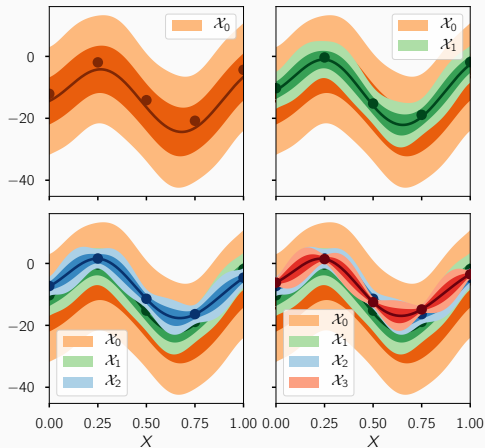


Quantifying Truncation Uncertainty

Conditional Distributions



Conditional + Error



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

This model permits mostly analytic calculation of evidence

$$\text{pr}(\mathcal{D} | \ell, Q) = \frac{\Gamma(a^*)}{\Gamma(a)} \frac{b^a}{(b^*)^{a^*}} \sqrt{\frac{|V^*|}{|V|}} \frac{|2\pi R_\ell|^{-(k+1)/2}}{|Q|^{k(k+1)/2}}$$

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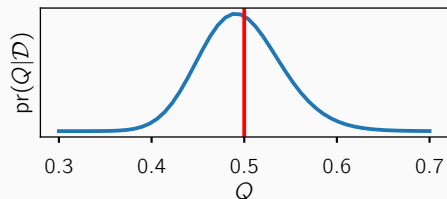
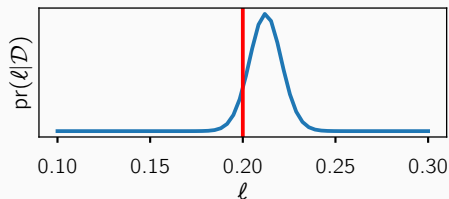
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$$\text{Here, } Q \propto \frac{1}{\Lambda_b}$$

