MODELING EFT TRUNCATION ERRORS USING GAUSSIAN PROCESSES

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for the BUQEYE collaboration
(Bayesian Uncertainty Quantification: Errors for Your EFT)

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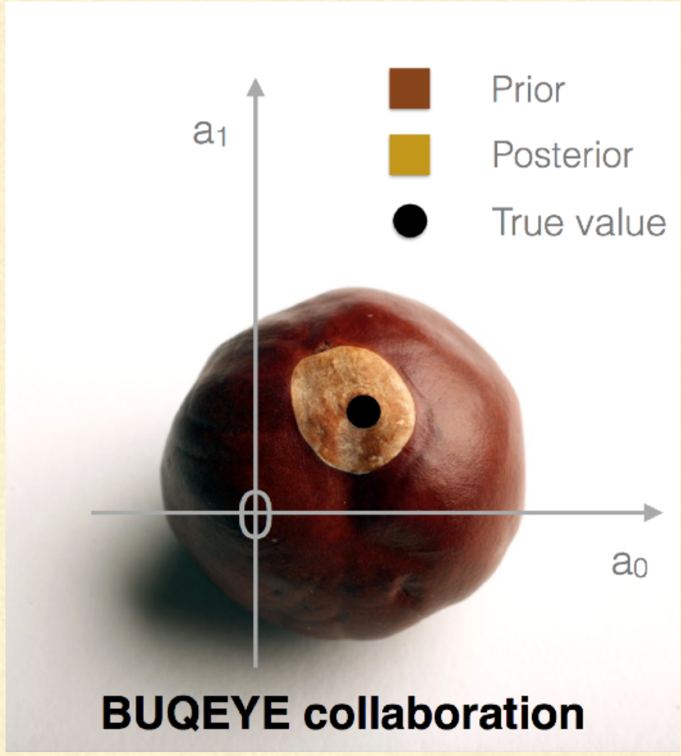
S. Wesolowski (Salisbury University)



RESEARCH SUPPORTED BY THE US DOE AND NSF AND EMMI

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Check two different aspects of “model”

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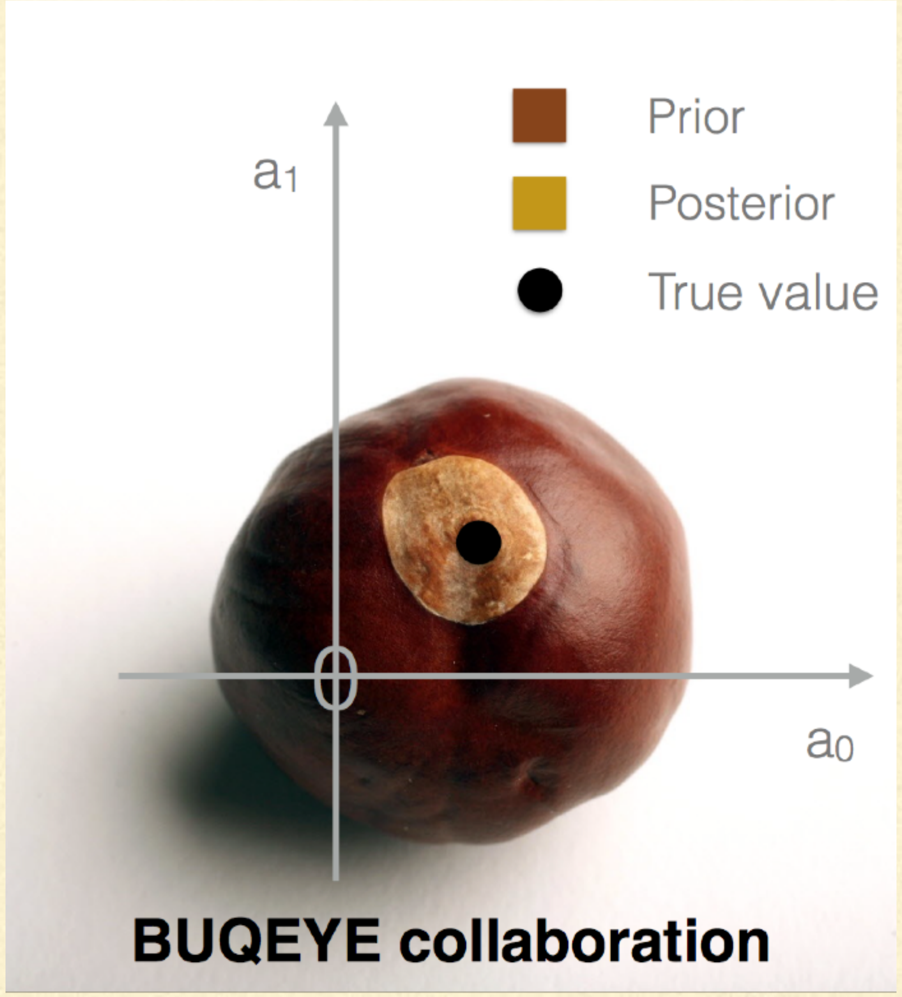
Outline

- Calculating rigorous truncation errors
- Diagnosing ChiEFT NN expansions
- Gaussian processes for truncation errors
- Preliminary results from analysis of ChiEFT NN potentials with GP truncation errors
- Summary



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S. Wesolowski, N. Klco, R. J. Furnstahl, DP, and A. Thapaliya, J. Phys. G. **43,** 074001 (2016)

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S. Wesolowski, R. Furnstahl, J. Melendez, DP, J. Phys. G **46**, 045102 (2019)

An EFT expansion in pictures

- General EFT series for observable to order k: $y = y_{\rm ref} \sum_{n=0}^{k} c_n Q^n$
- In ChiEFT $Q = \dfrac{(p, m_\pi)}{\Lambda_b}; \quad \Lambda_b \approx 600 \text{ MeV}$

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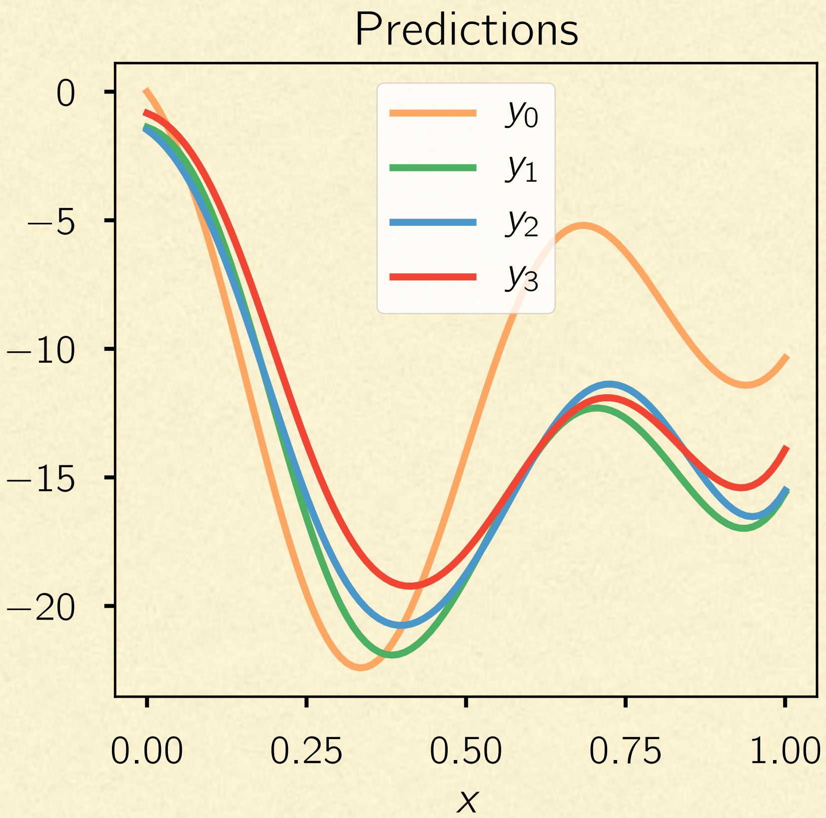

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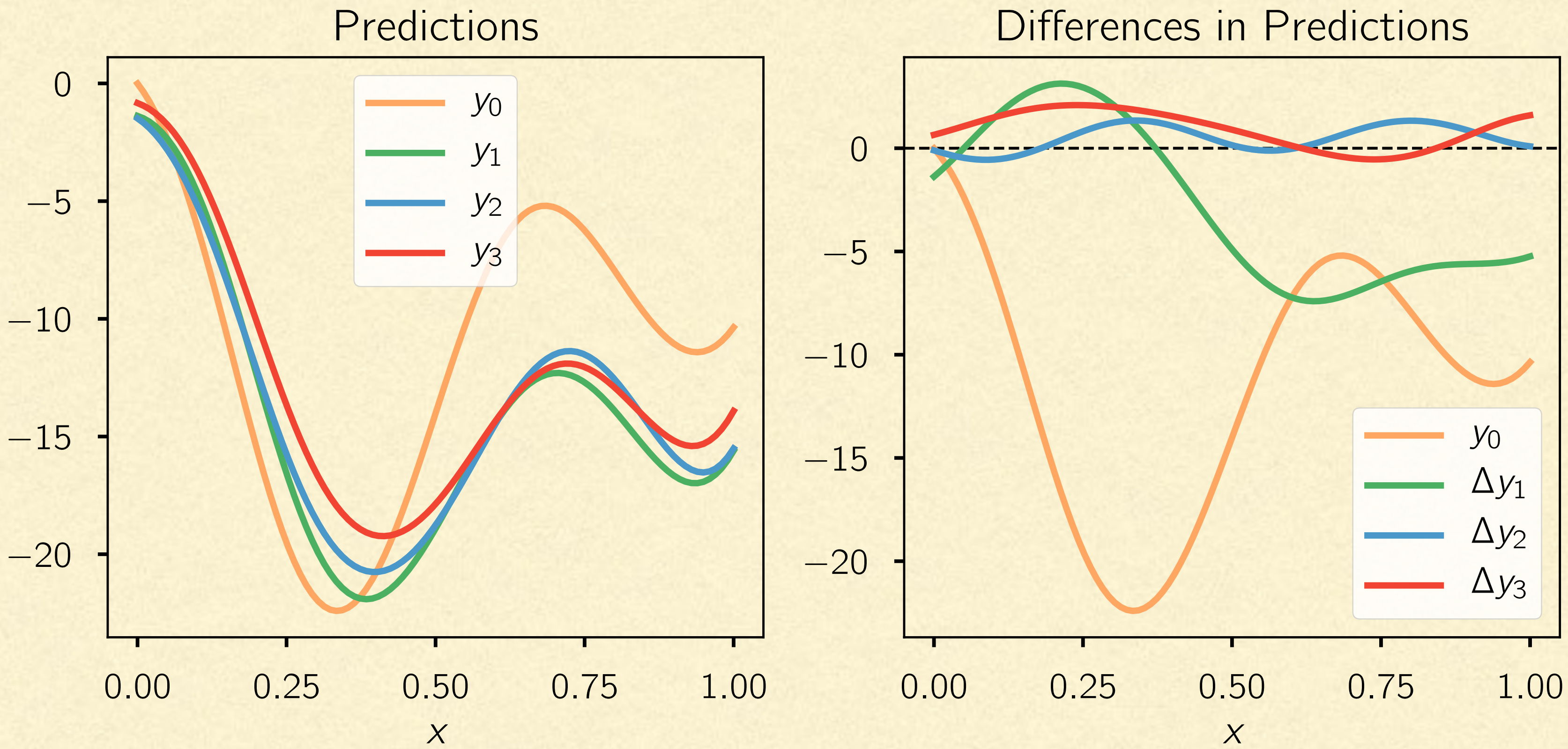

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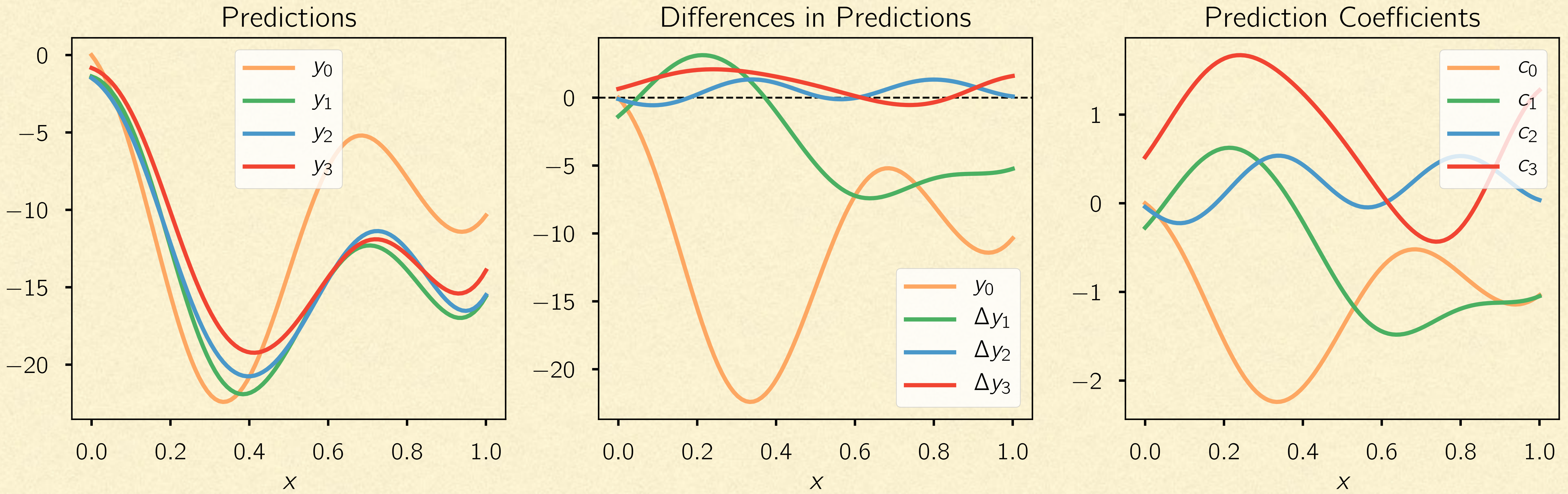

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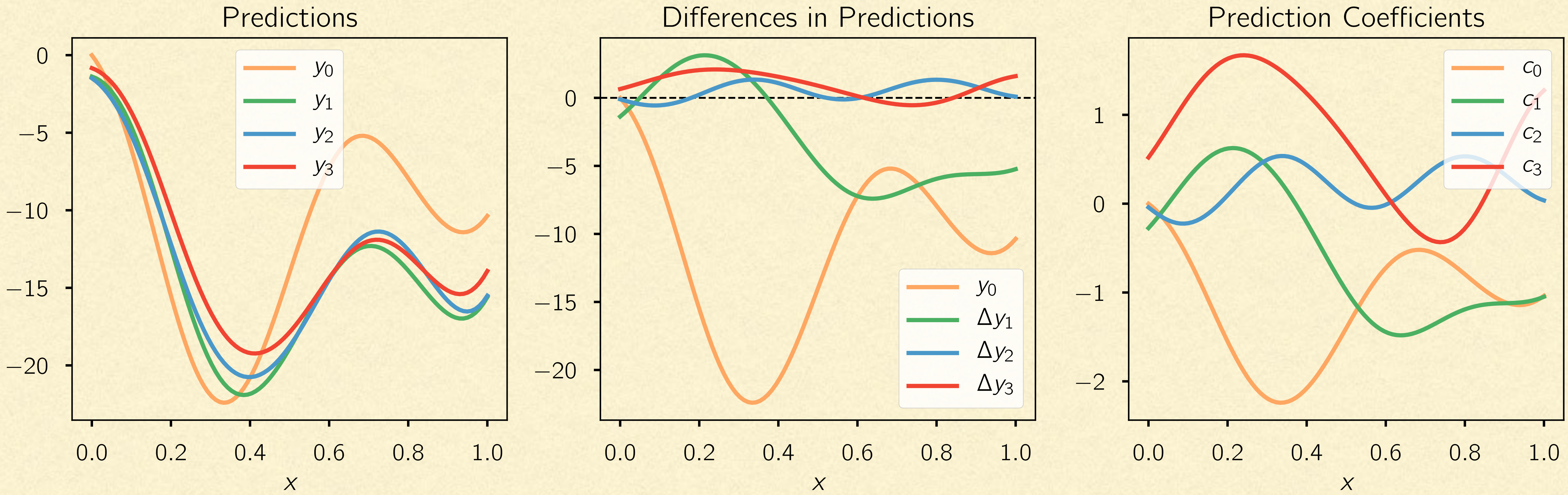

This is what a healthy observable expansion looks like: bounded coefficients, that do not grow or shrink with order.

Probability for EFT coefficients

Furnstahl, Klco, DP, Wesolowski, PRC, 2015 after Cacciari and Houdeau, JHEP, 2011

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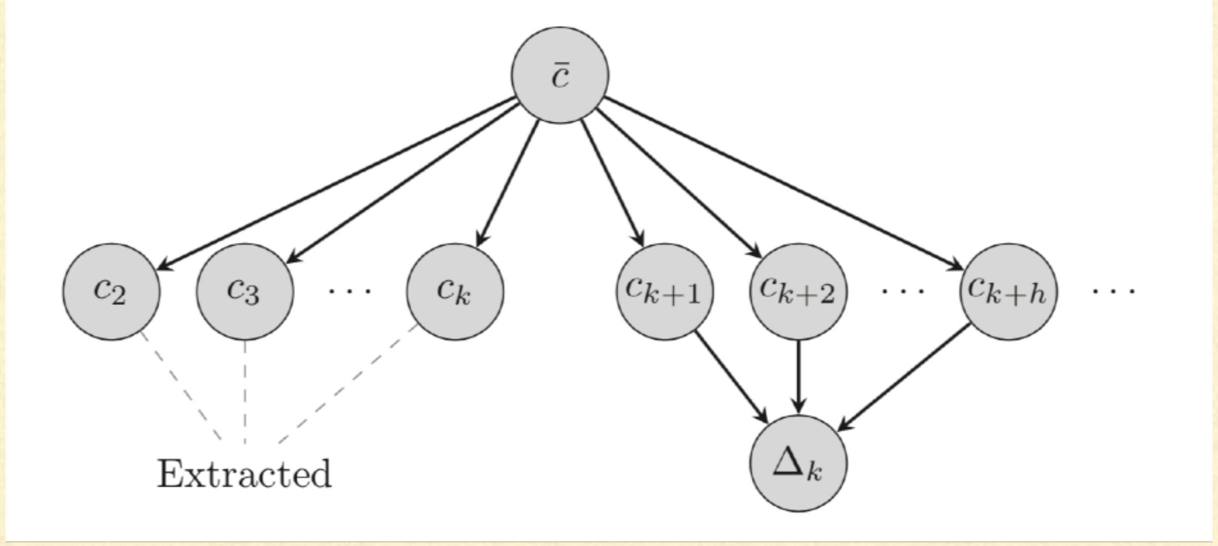
- Bayesian model:



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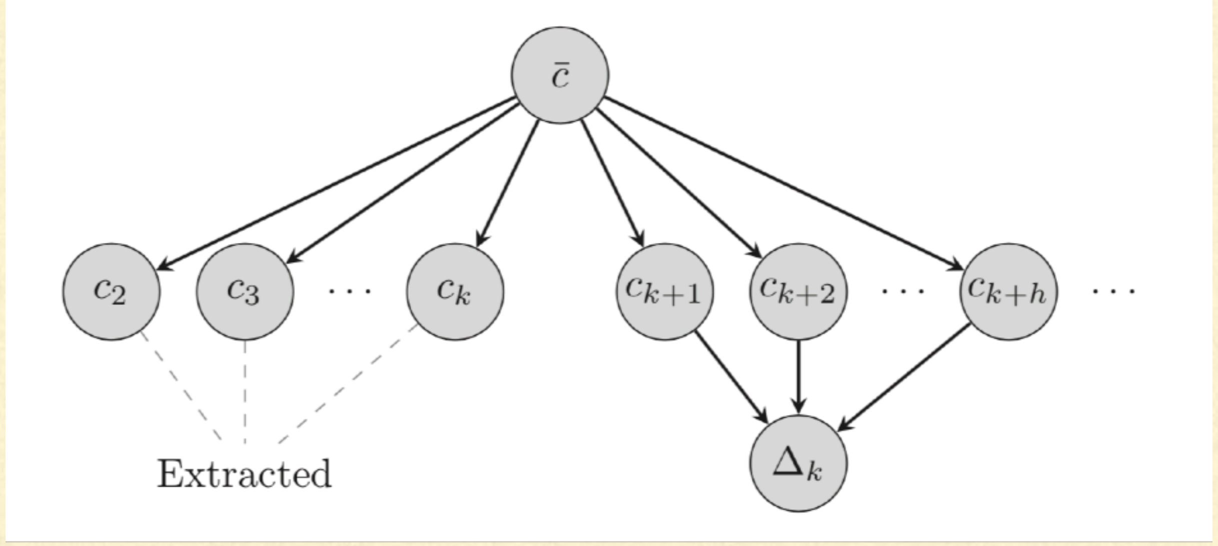
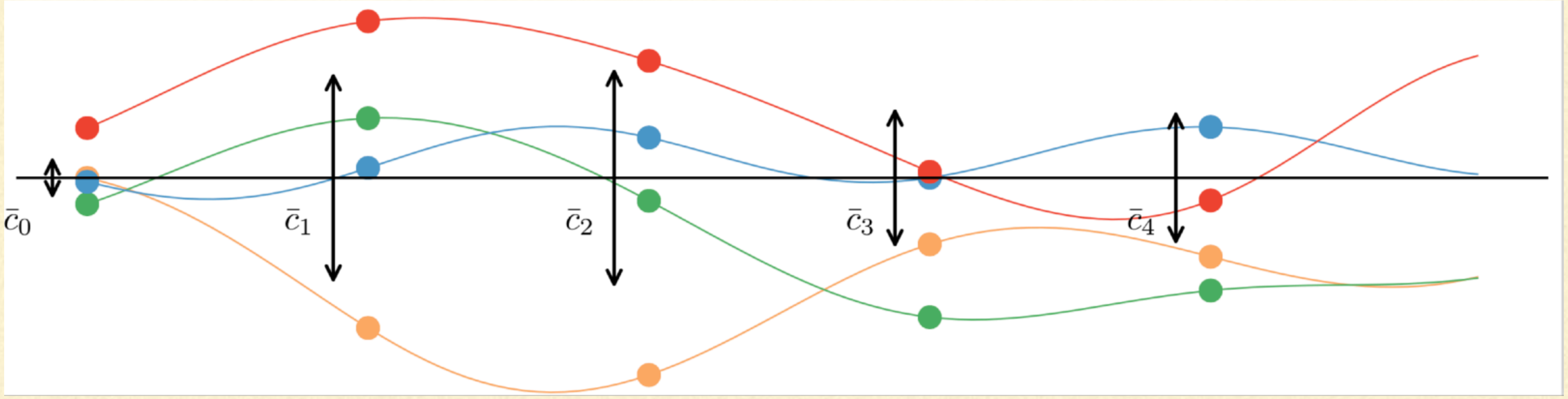




First shot: cbar can be different at different kinematic points: "uncorrelated model"

Normal naturalness

Furnstahl, Klco, DP, Wesolowski, PRC, 2015; Melendez, Furnstahl, Wesolowski, PRC, 2017

- c_n's are normally distributed, with mean 0 and standard deviation cbar. that is a) fixed or b) distributed uniformly in its logarithm

$$\mathrm{pr}(c_n|\bar{c}) = \frac{1}{\sqrt{2\pi}\bar{c}} e^{-c_n^2/2\bar{c}^2};\ \mathrm{pr}(\bar{c}) \propto \frac{1}{\bar{c}}\theta(\bar{c}-\bar{c}_<)\theta(\bar{c}_> - \bar{c})$$

- Marginalization:

$$\mathrm{pr}(c_{k+1}|c_0, c_1, \ldots, c_k) = \int_0^\infty d\bar{c}\, \mathrm{pr}(c_{k+1}|\bar{c})\mathrm{pr}(\bar{c}|c_0, c_1, \ldots c_k)$$

$$= \int_0^\infty \frac{d\bar{c}}{\bar{c}^{k+3}} \exp\left(-\frac{c_{k+1}^2}{2\bar{c}^2}\right) \exp\left(-\frac{(k+1)\langle c^2\rangle}{2\bar{c}^2}\right)$$

- Student's t-distribution results:

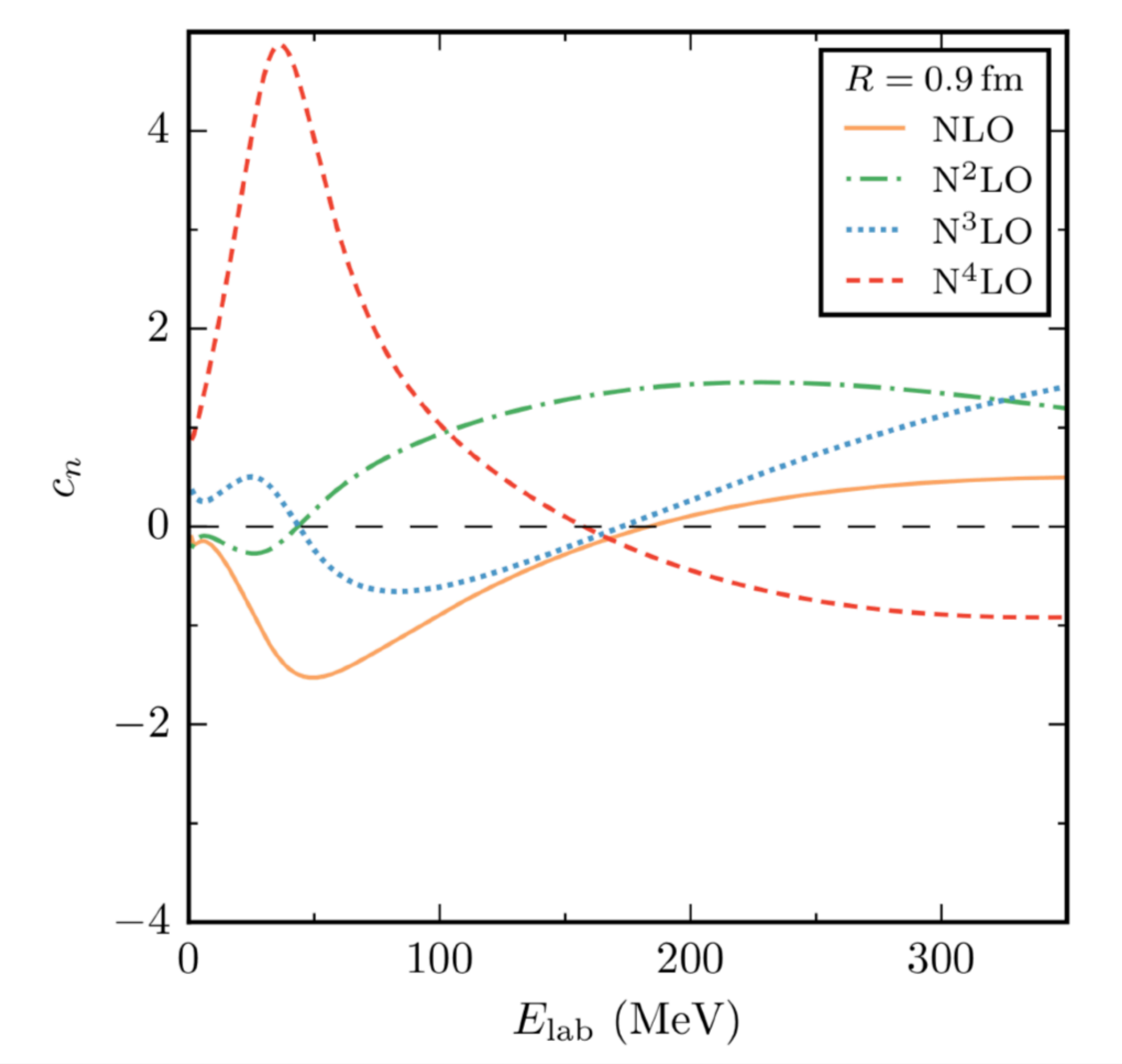
$$\mathrm{pr}(c_{k+1}|c_0, c_1, \ldots, c_k) \propto \frac{\Gamma\left(\frac{k+2}{2}\right)}{\Gamma\left(\frac{k+1}{2}\right)} \left(\frac{(k+1)\langle c^2\rangle}{(k+1)\langle c^2\rangle + c_{k+1}^2}\right)^{(k+2)/2}$$

- DoB intervals computed using known results for this distribution. Size of error bar set by $\langle c^2 \rangle$, k, Q^{k+1}, and y_{ref}.

Error bands for NN observables

Melendez, Furnstahl, Wesolowski, PRC, 2017

EKM R=0.9 fm potential



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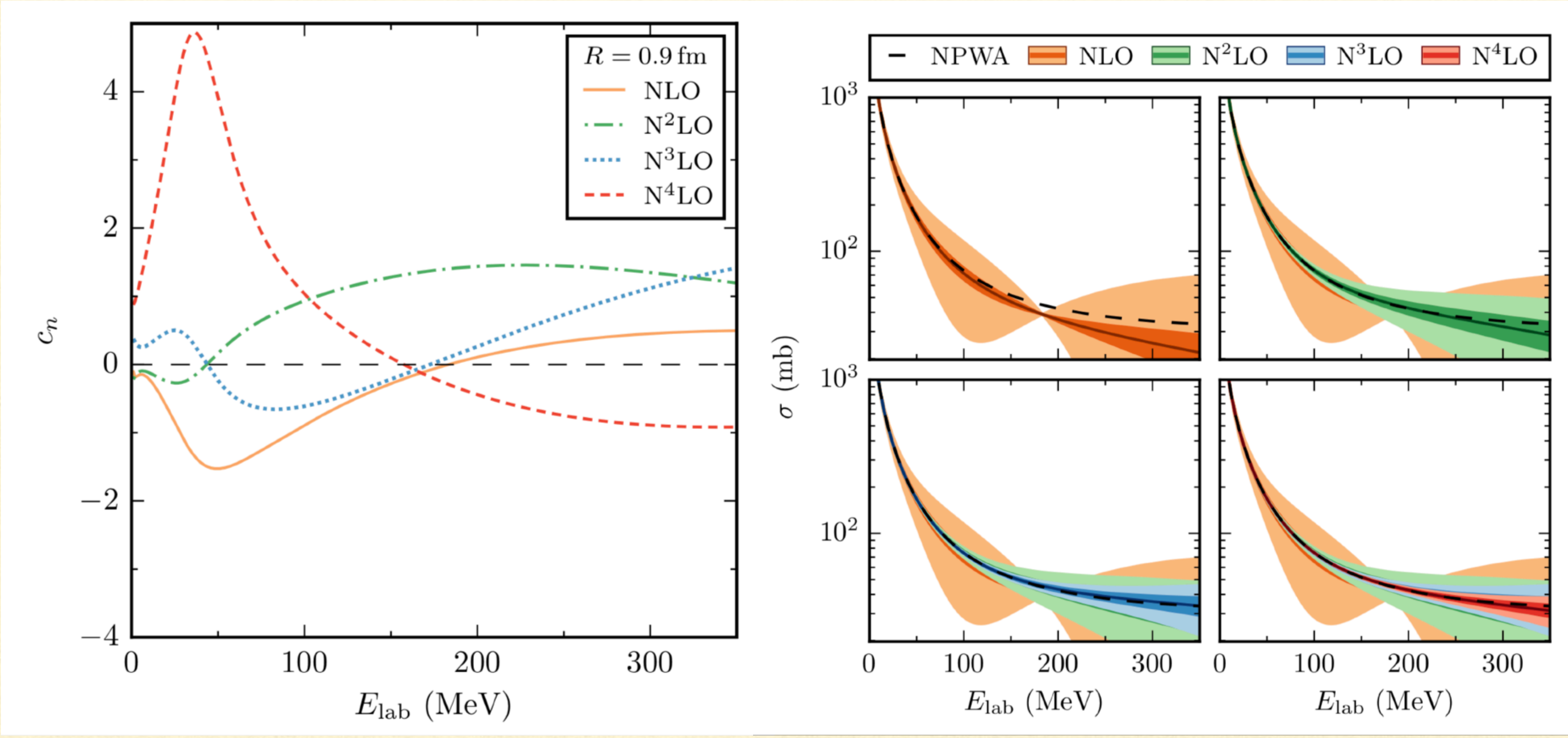

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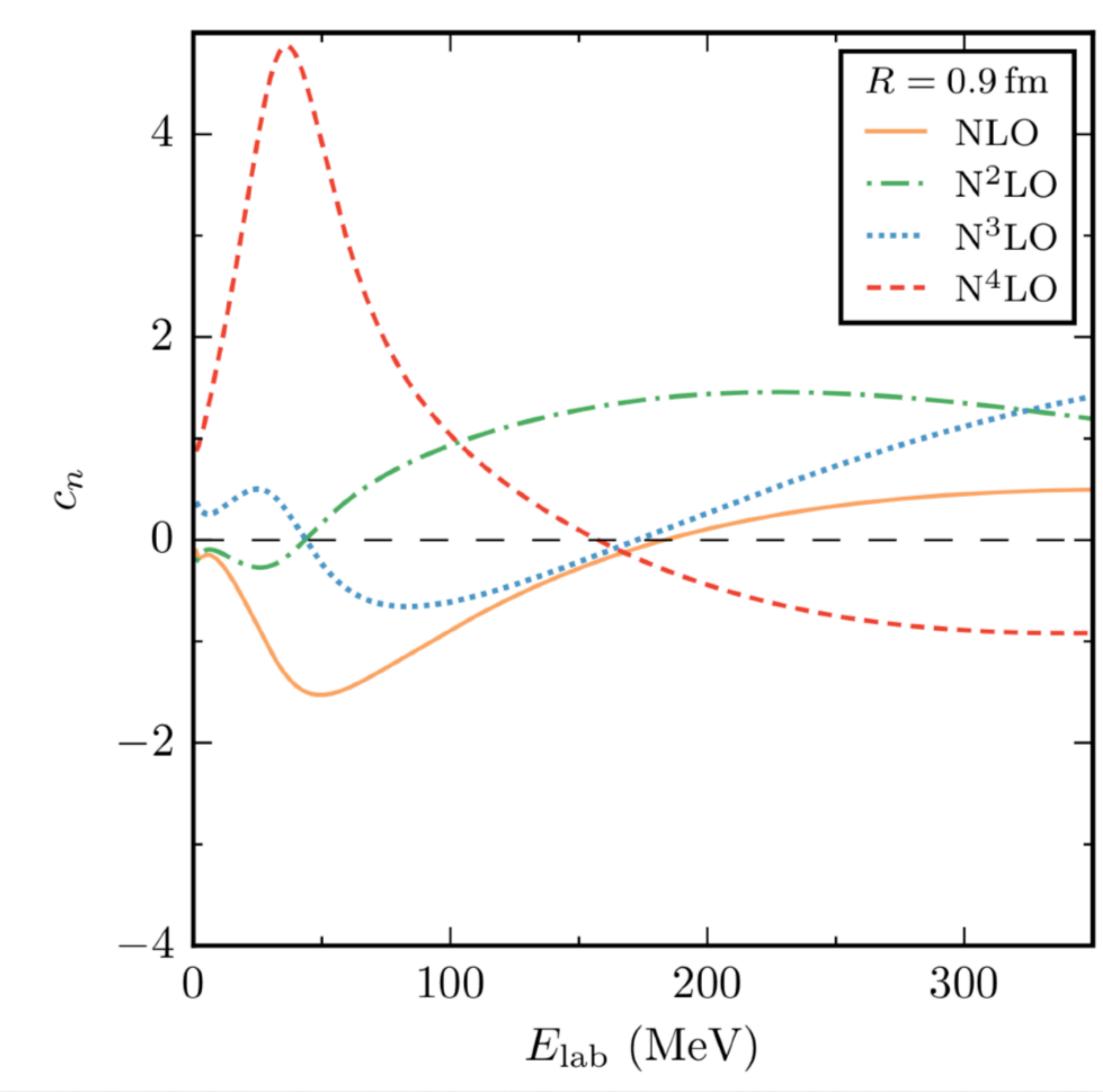

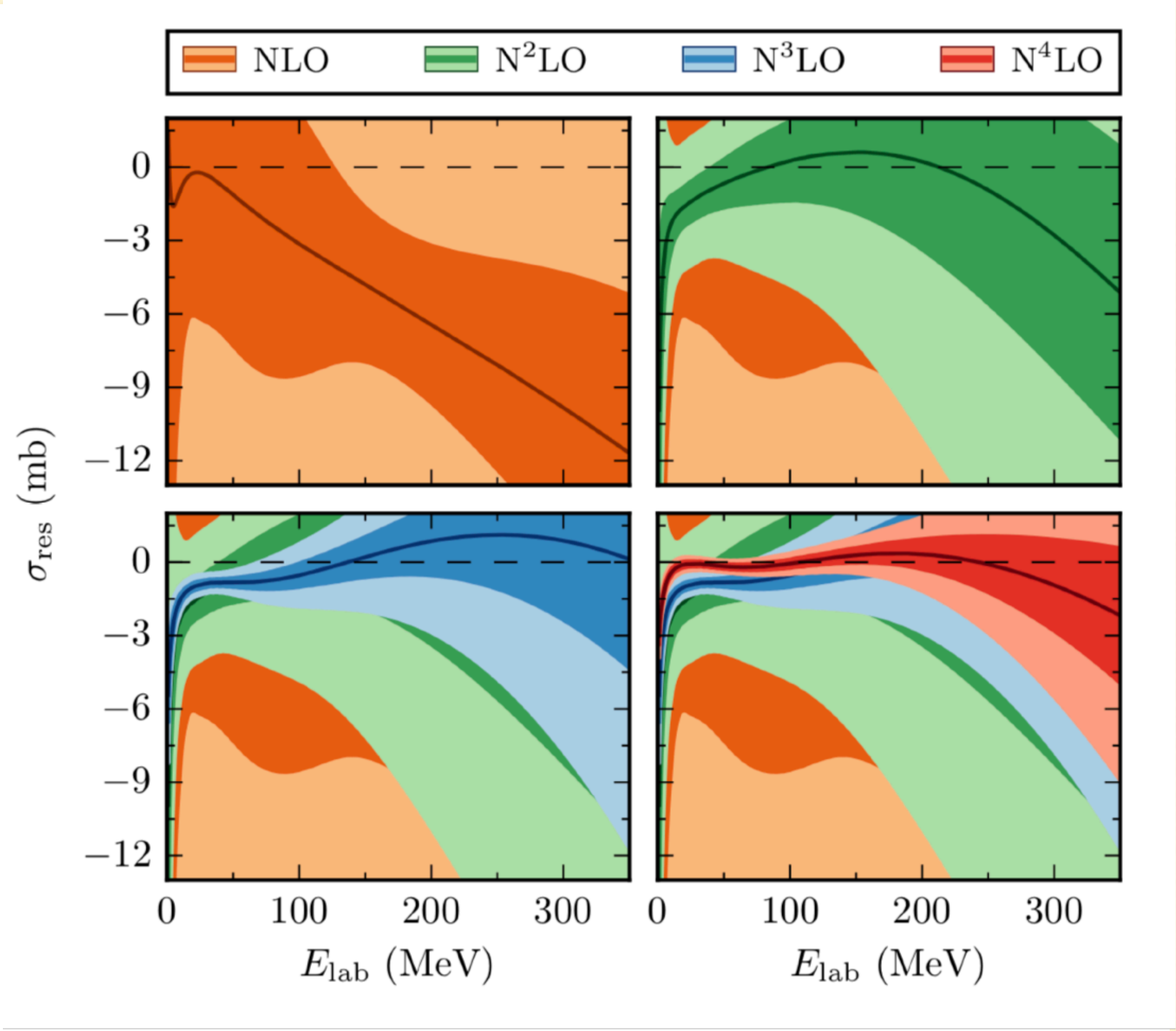

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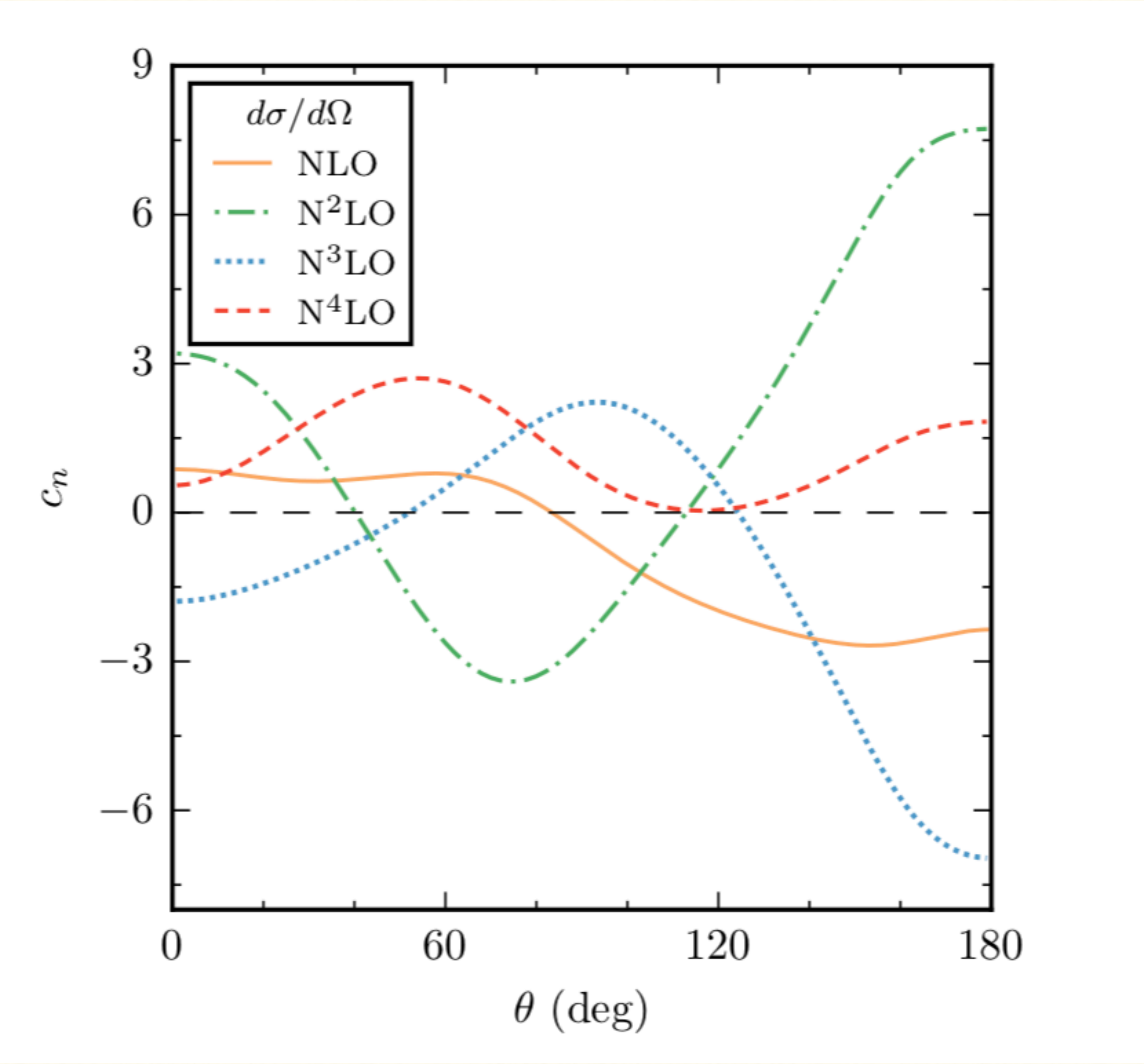

E_{lab}=96 MeV

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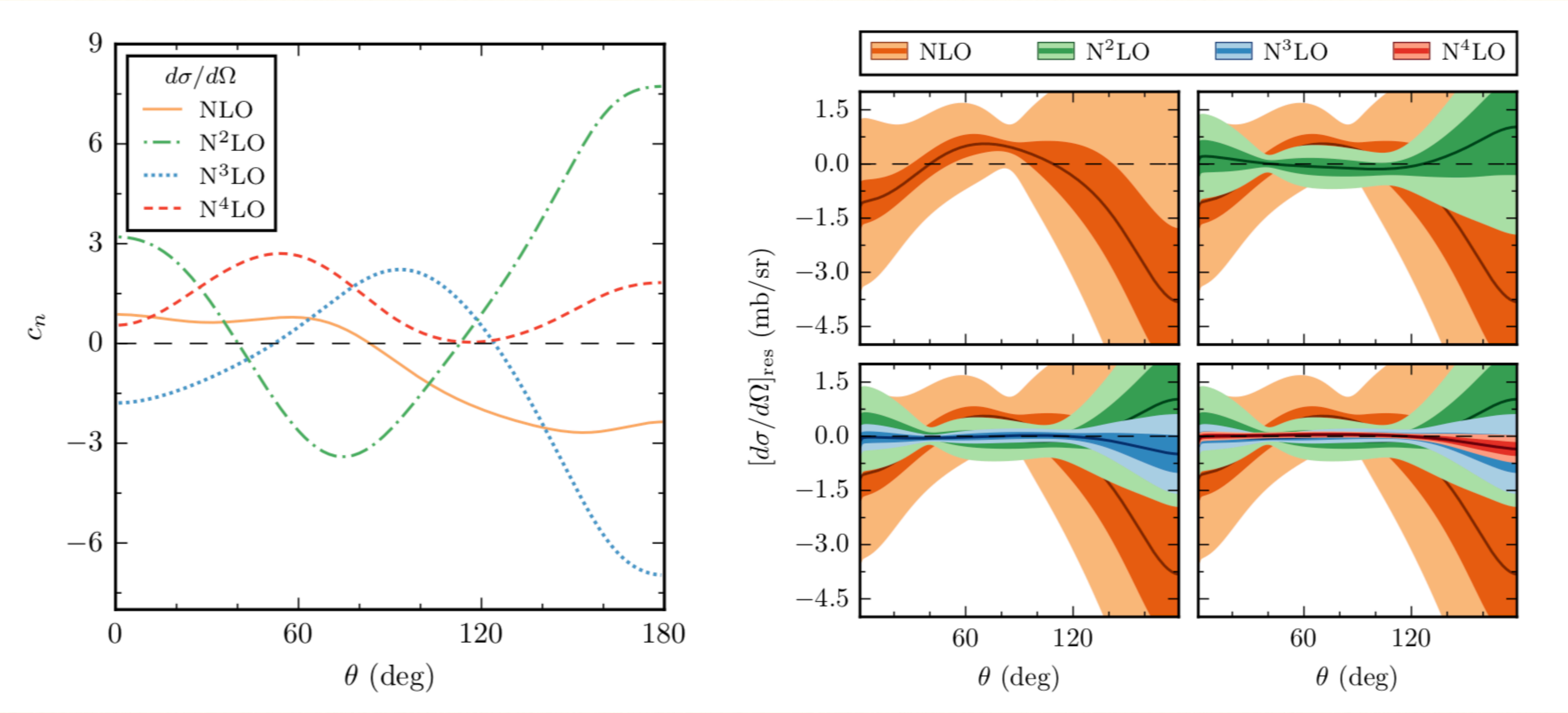

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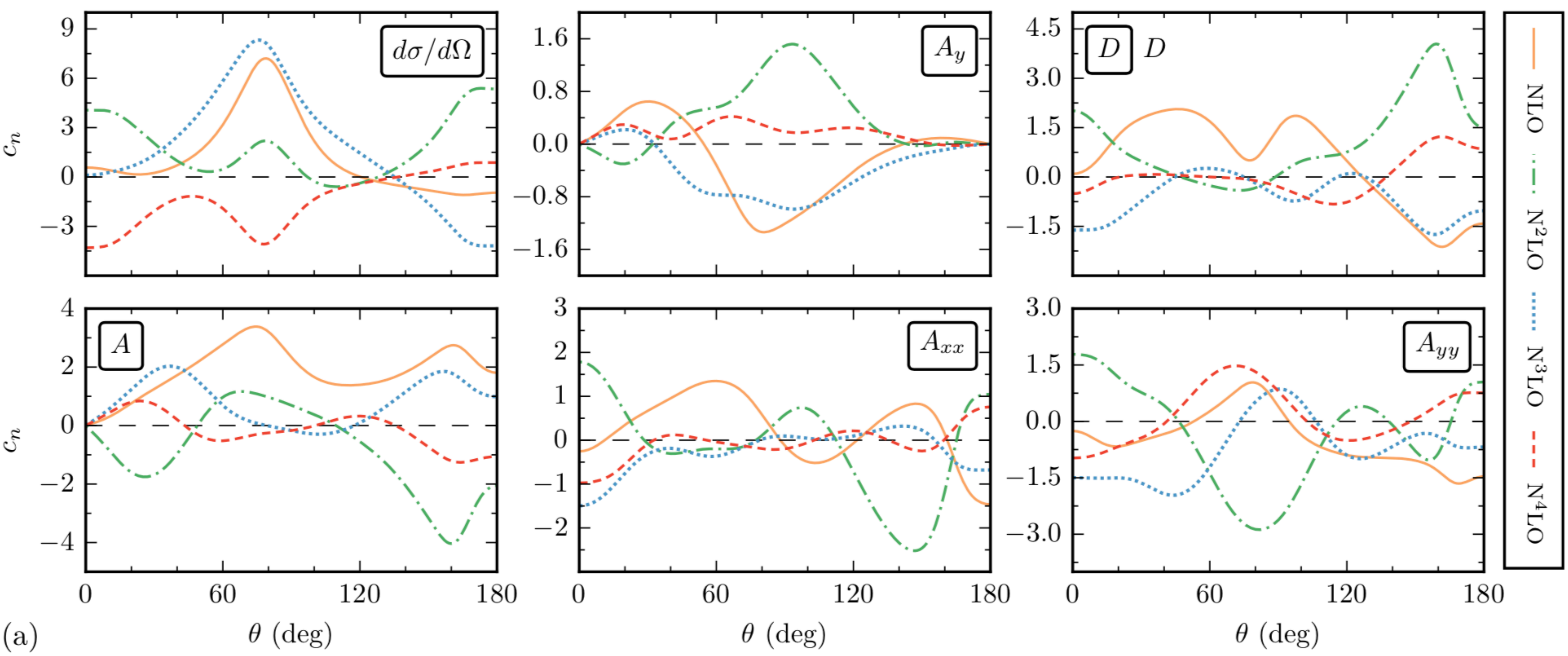

E_{lab}=250 MeV

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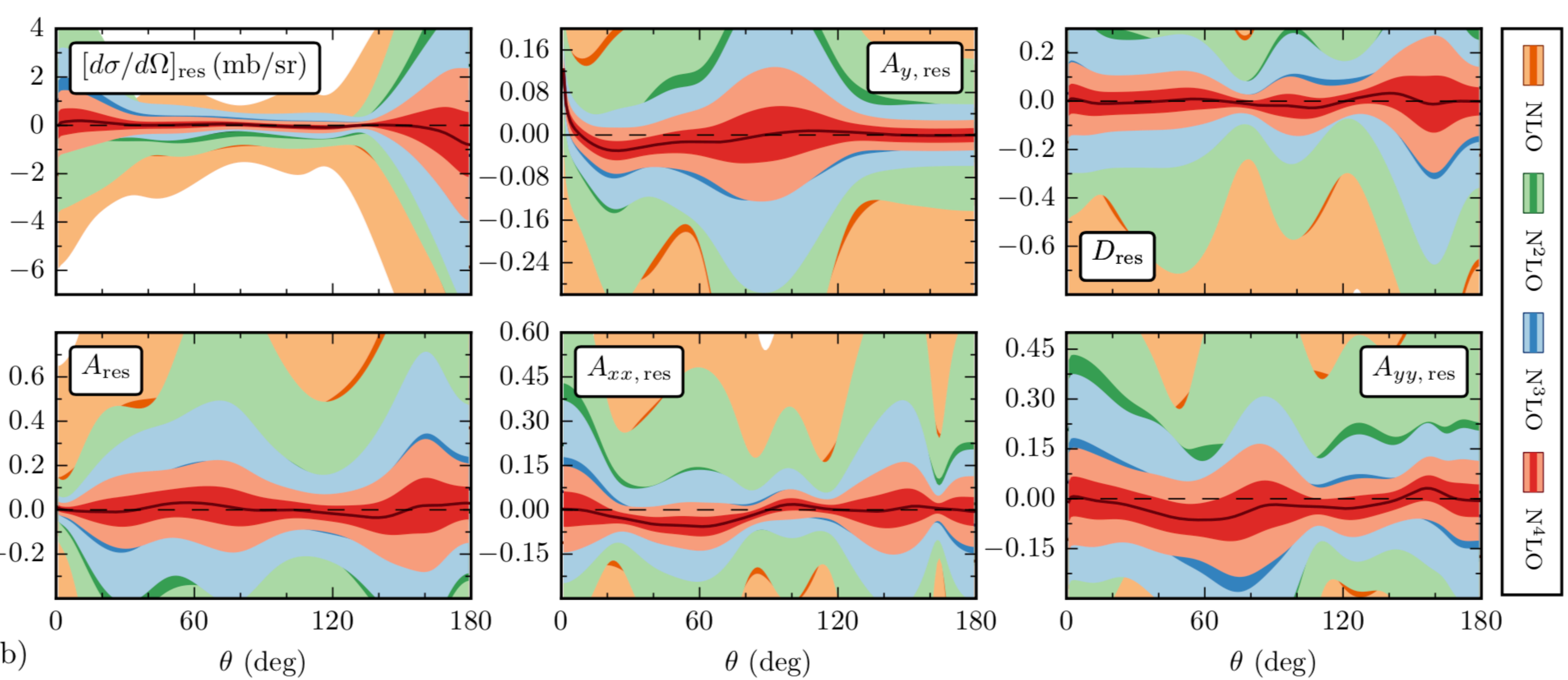

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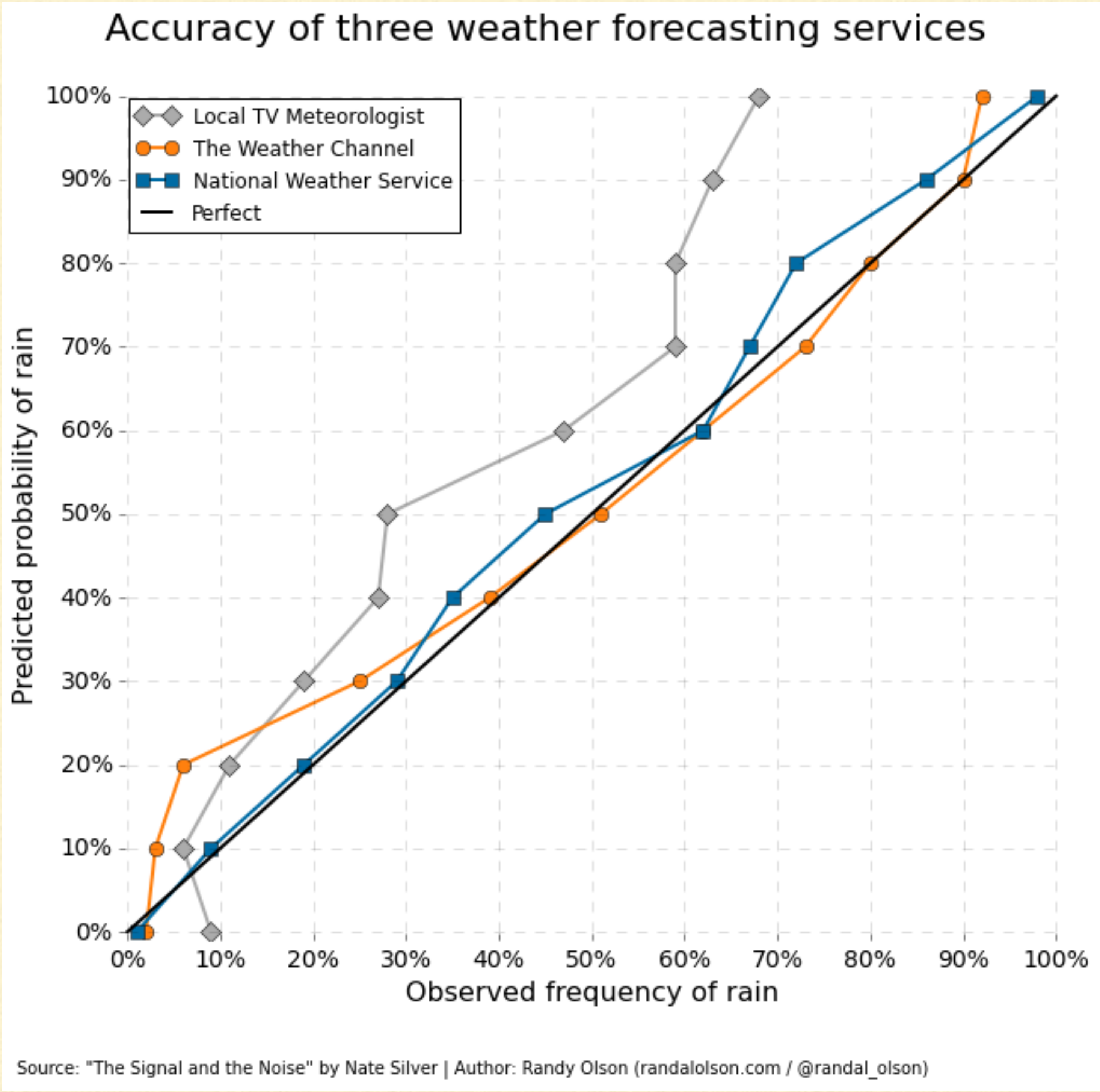

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- Fix a given DOB interval: compute success ratio, compare

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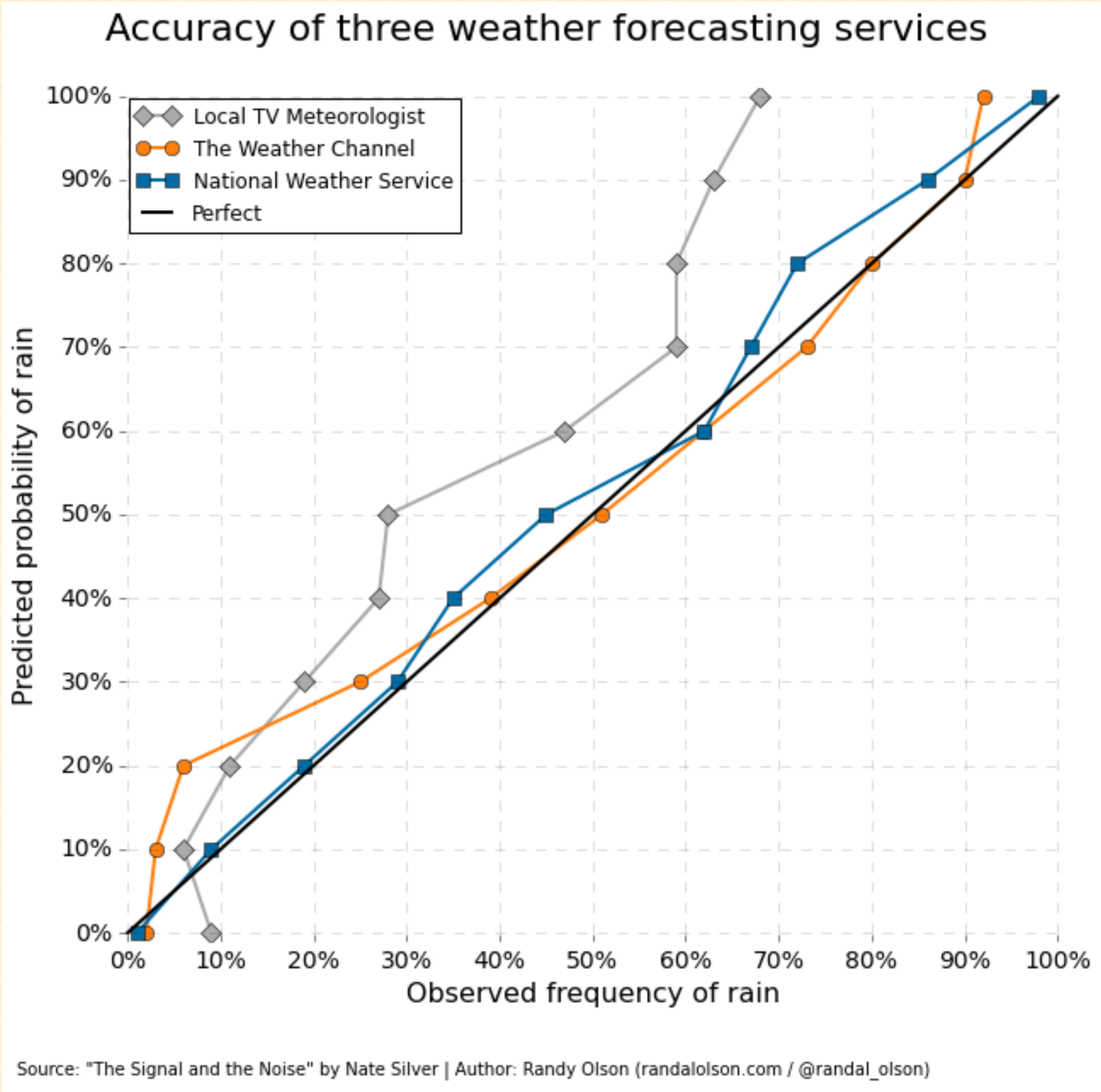

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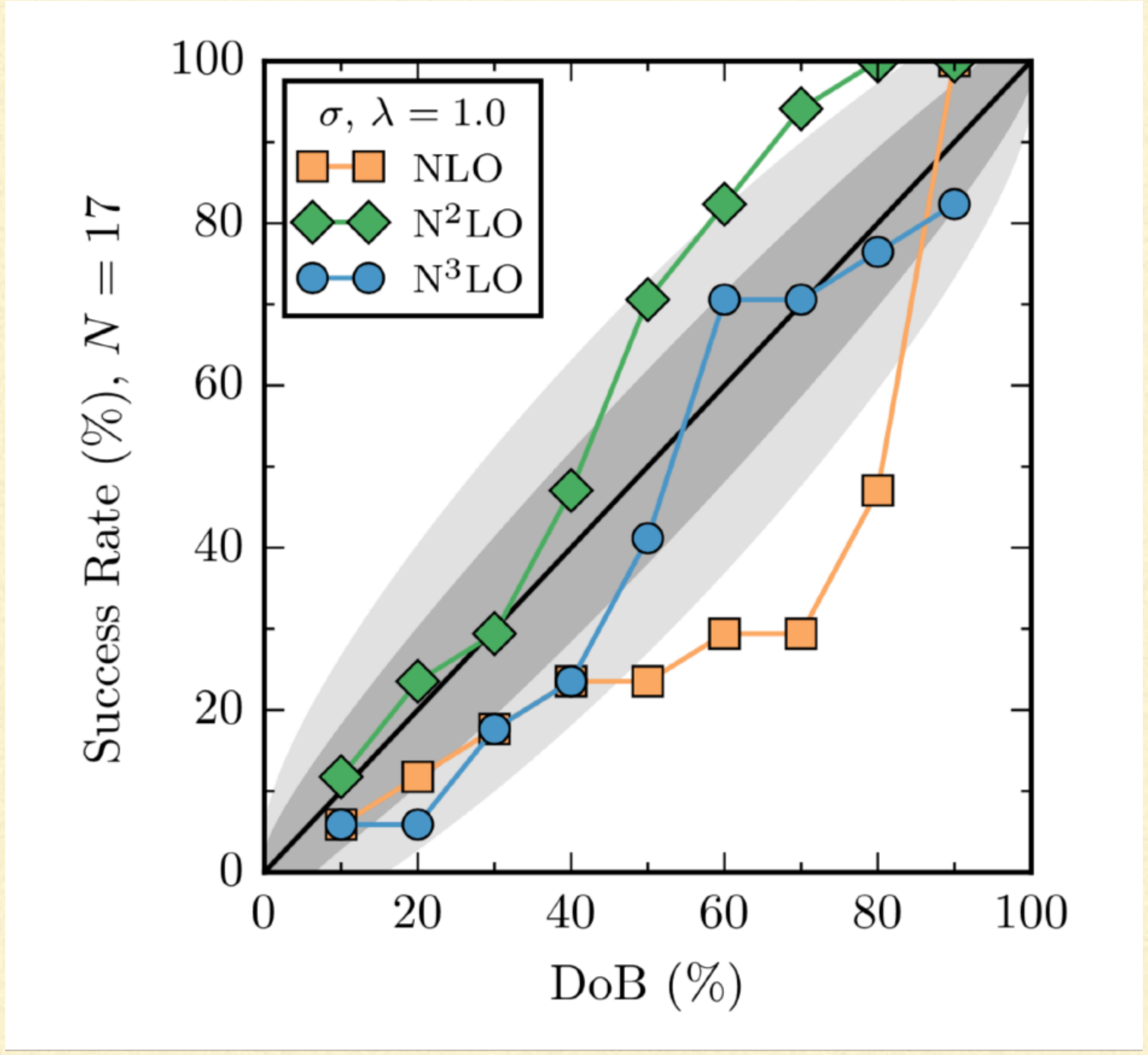
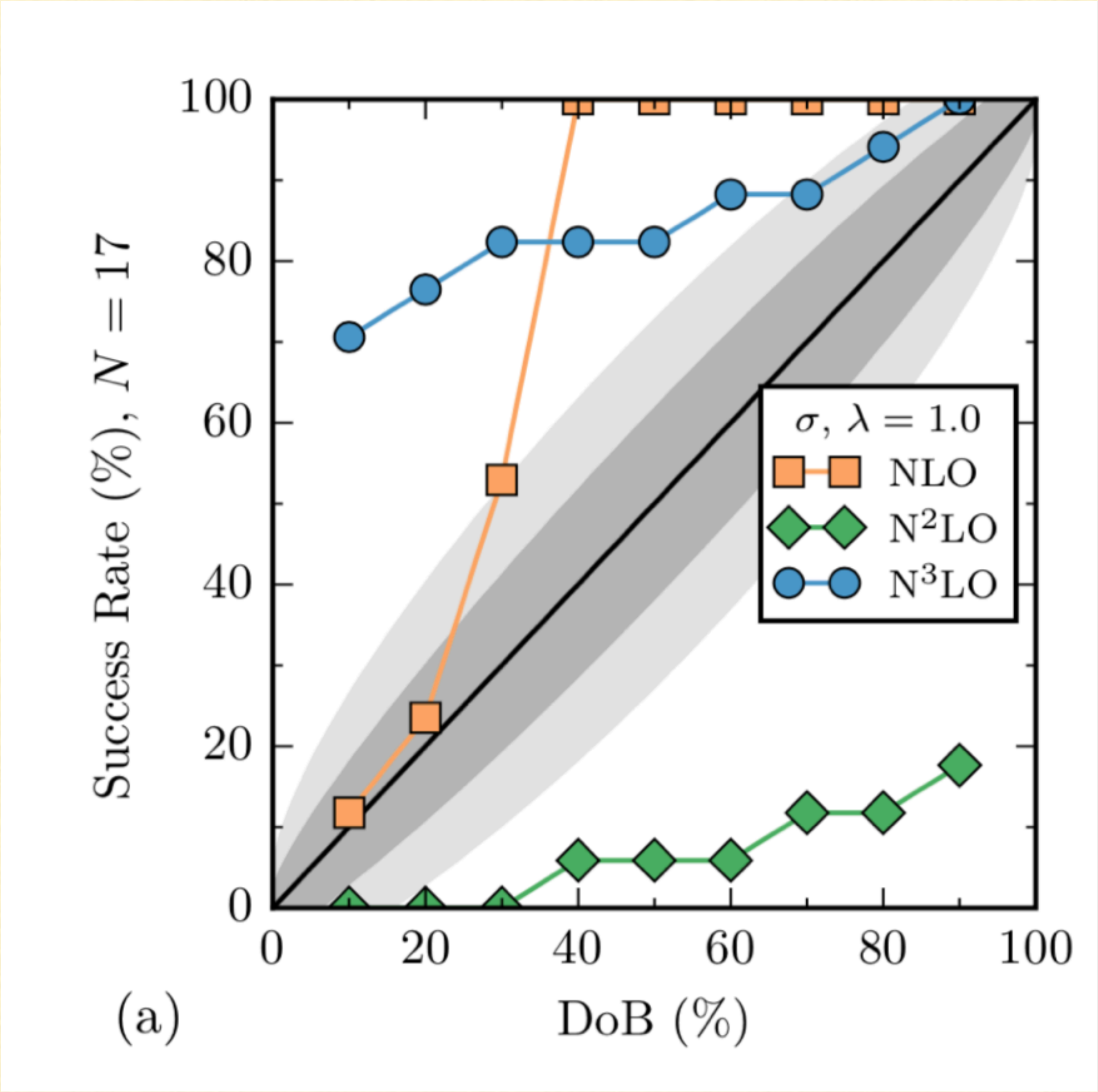
- Consider predictions at each order, with their error bars, as data and test them to see if the procedure is consistent
- Fix a given DOB interval: compute success ratio, compare
- Look at this for EKM predictions
- Should be near diagonal, with fluctuations described by Poisson statistics

Physics from calibration plots

R=0.9 fm



R=1.2 fm



- Allows assessment of order-by-order convergence
- Can look at differential cross section and spin observables too

Breakdown-scale Inference

- Λ_b determines the size of the c_n's. Choose it too big, and they'll be too big. Choose it too small, they'll be too small. And progressively so as one moves to higher and higher order.

- We have a theory for $pr(c_n|c_0, c_1, \ldots, c_k)$: now use Bayes' theorem to see how (im)probable are the c_n's that dimensionful EFT coefficients (b_n's) produce for a given Λ_b.

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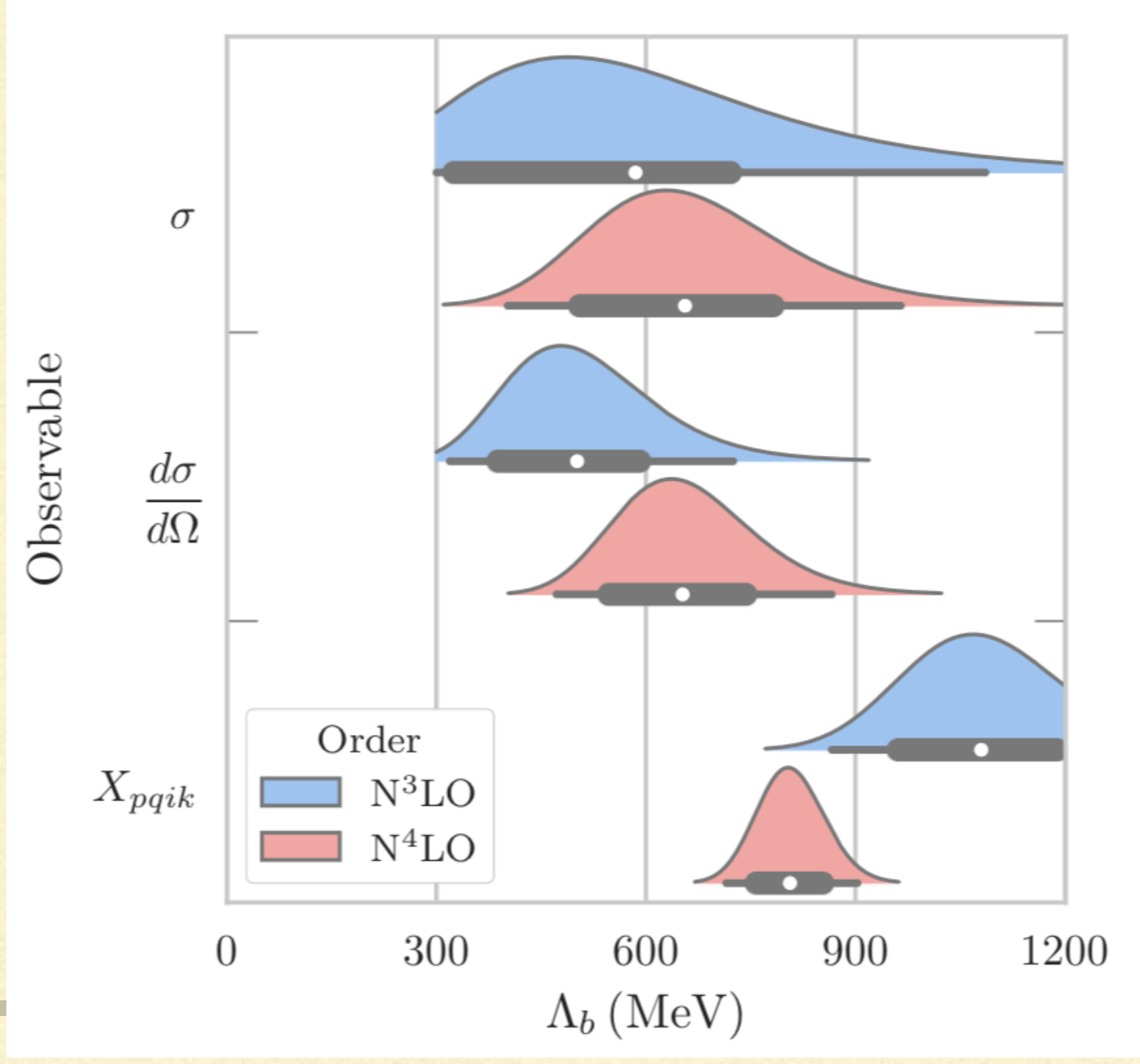
Using 5 energies (and 2 angles):



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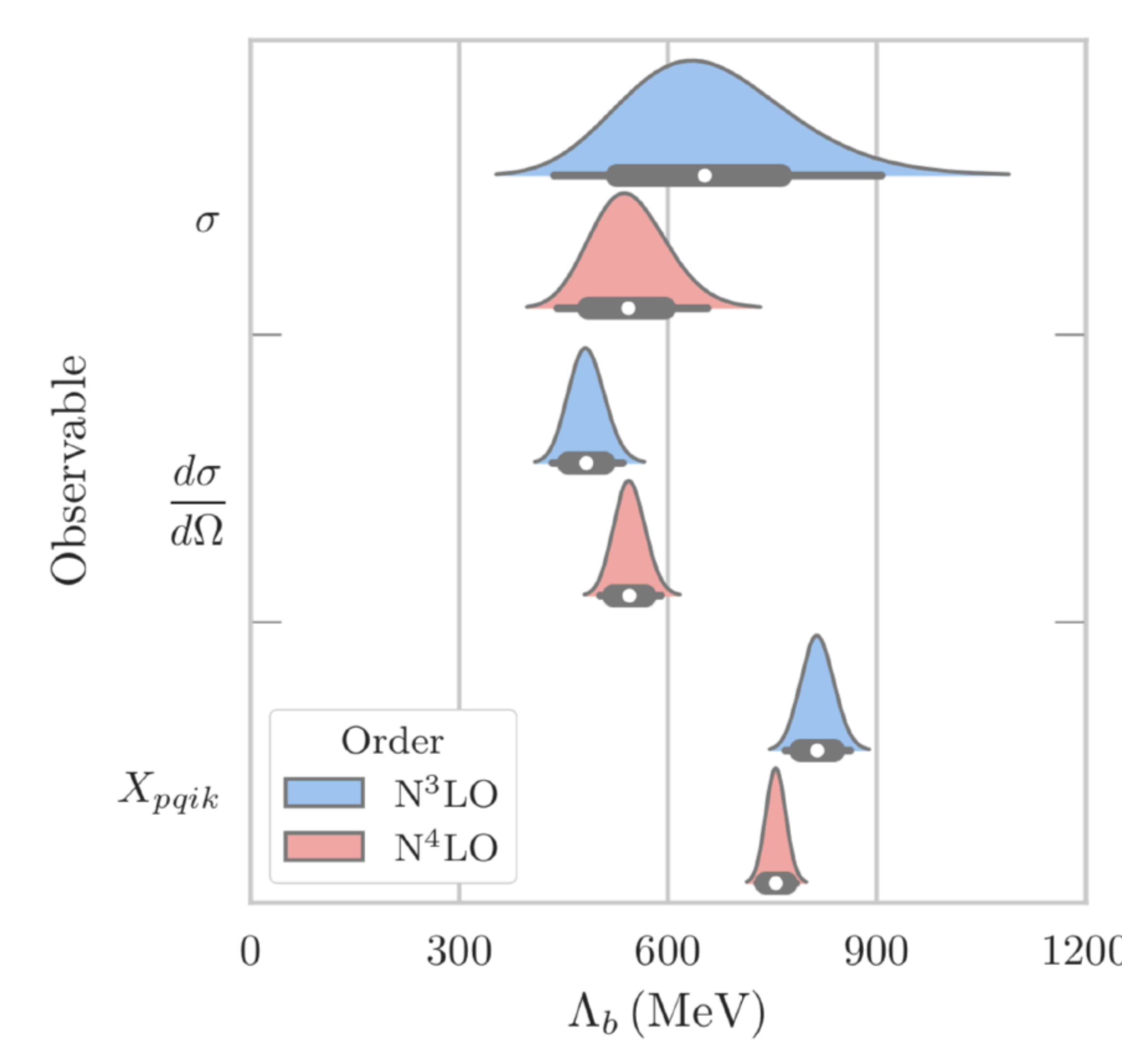
Using 17 energies (and 7 angles):



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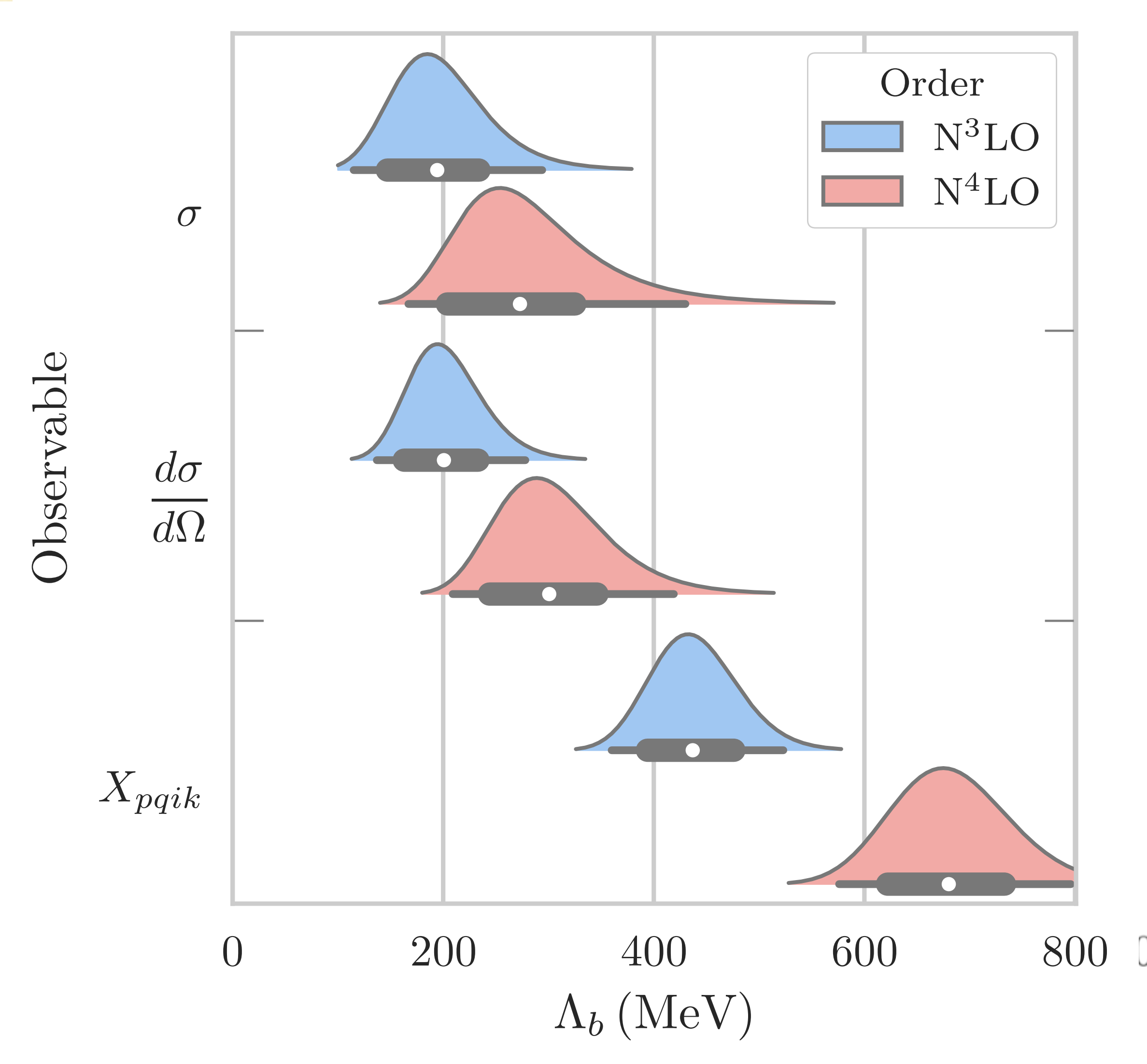
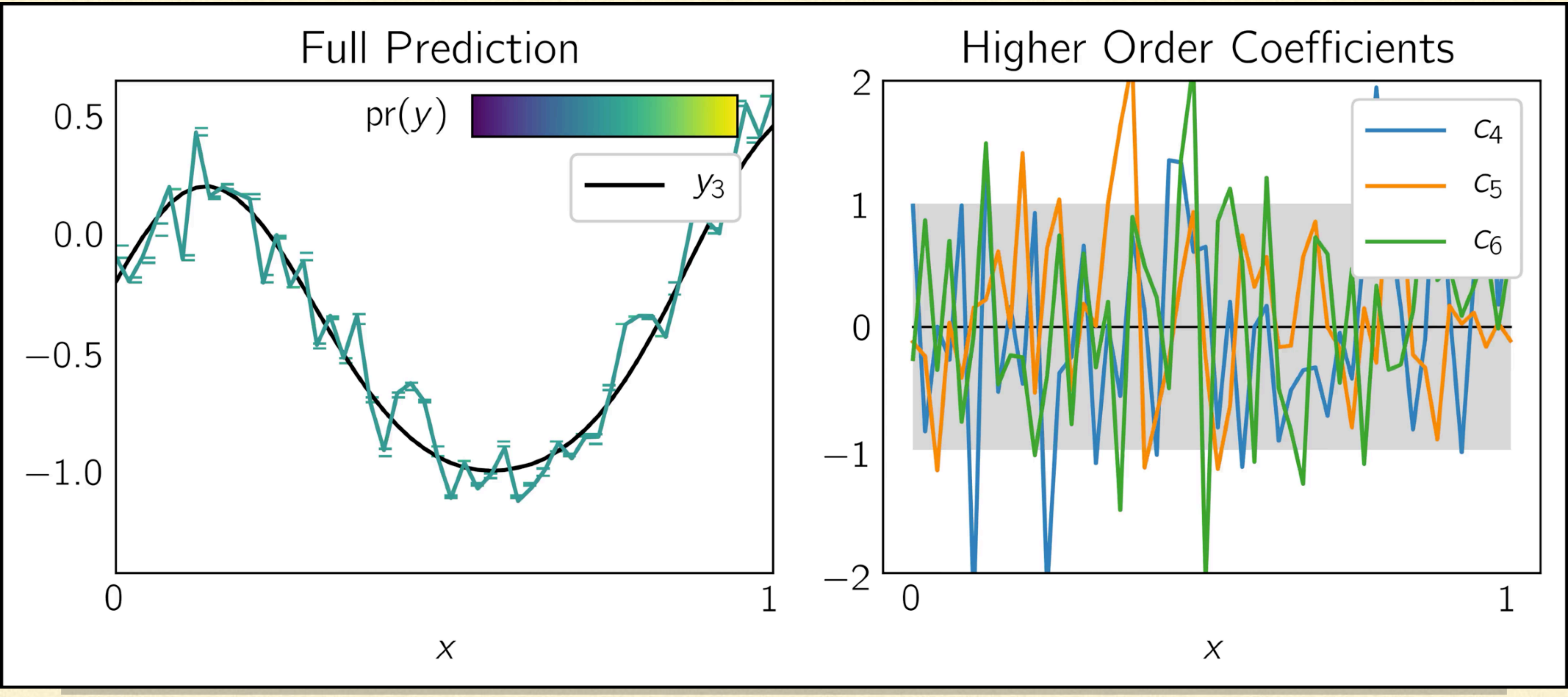


Why GPs?

Assumptions about correlation structure have significant impact on parameter estimation, NN model assessments, physics extraction, ….



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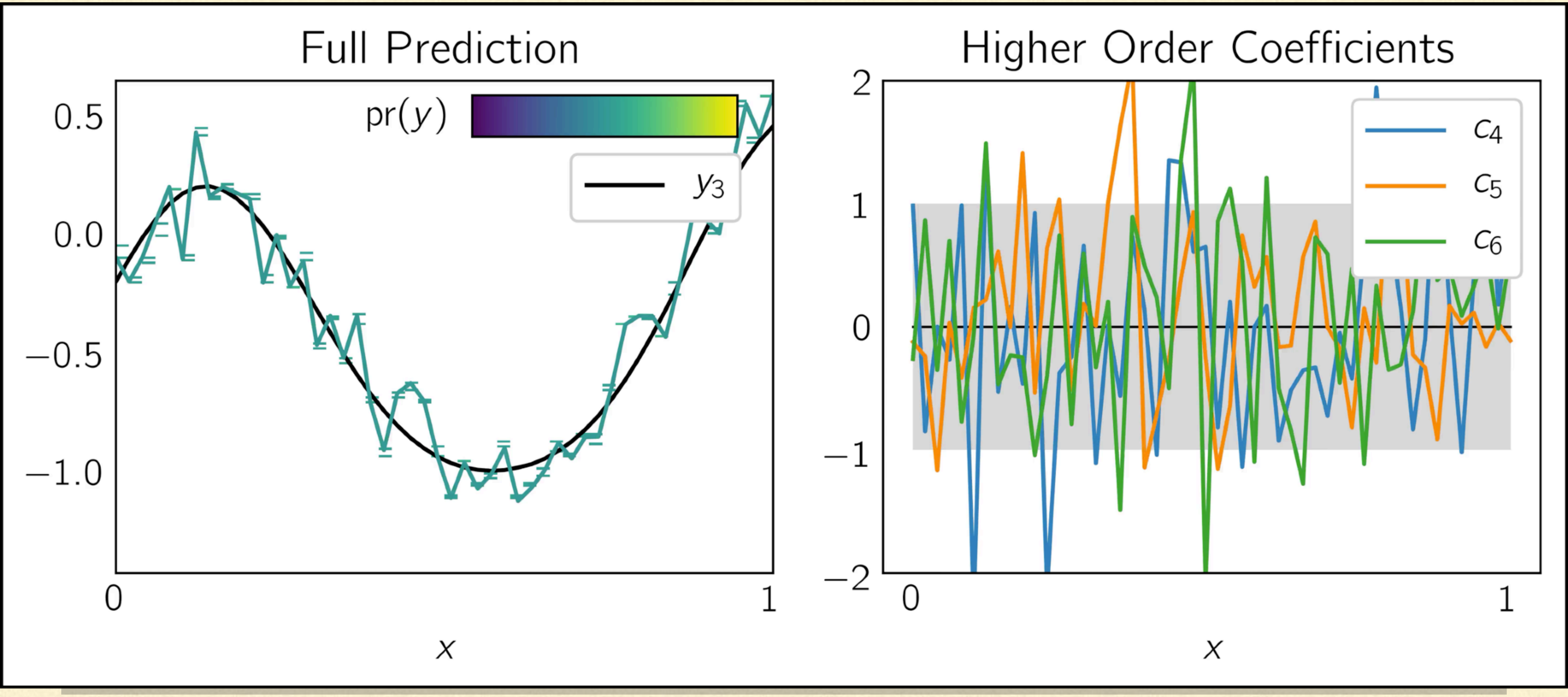

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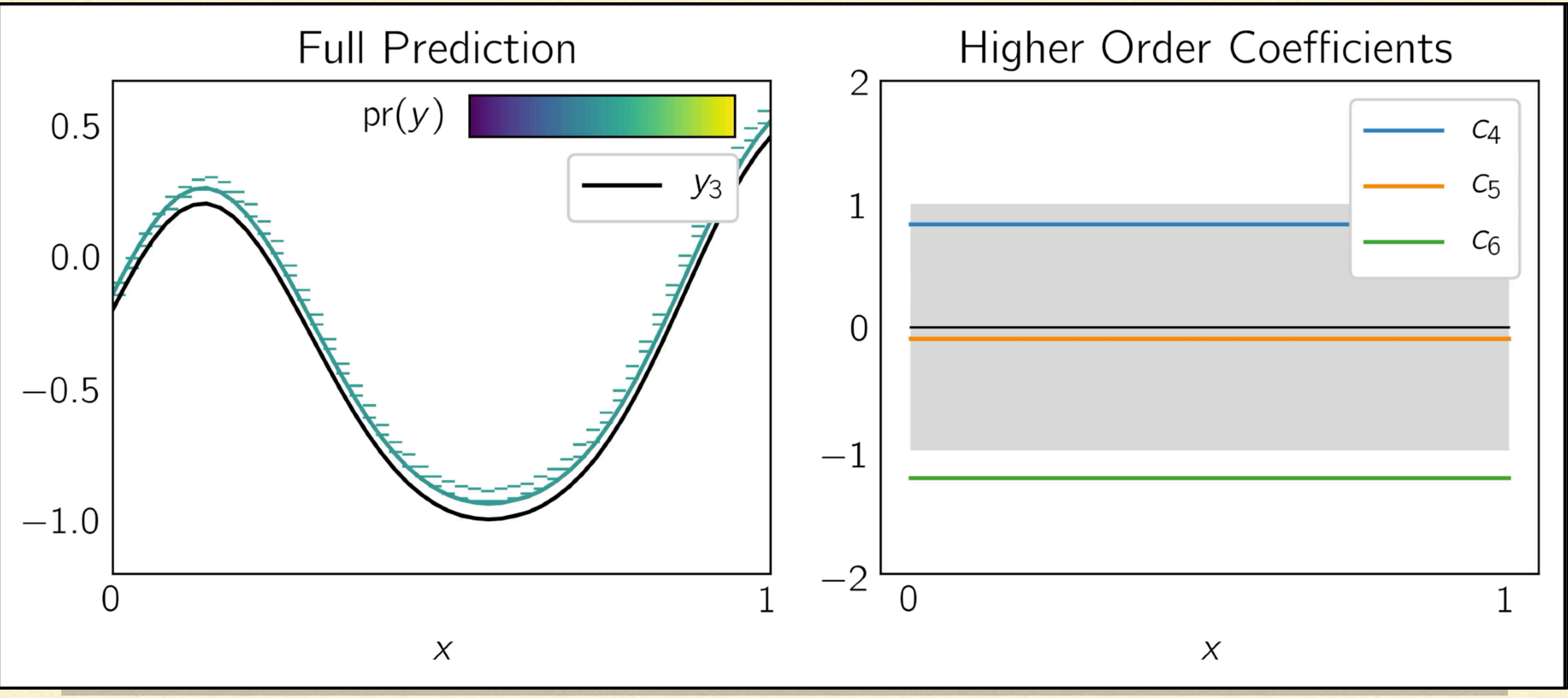

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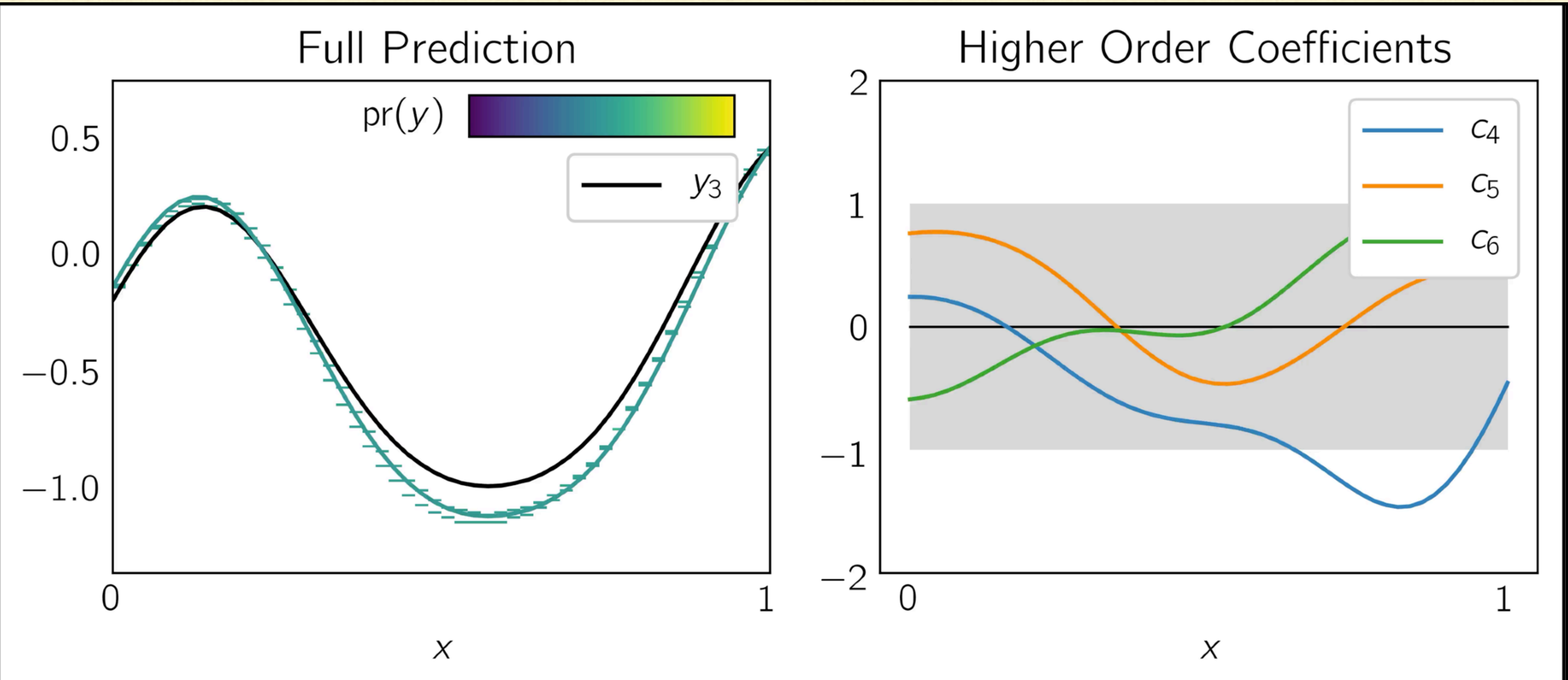

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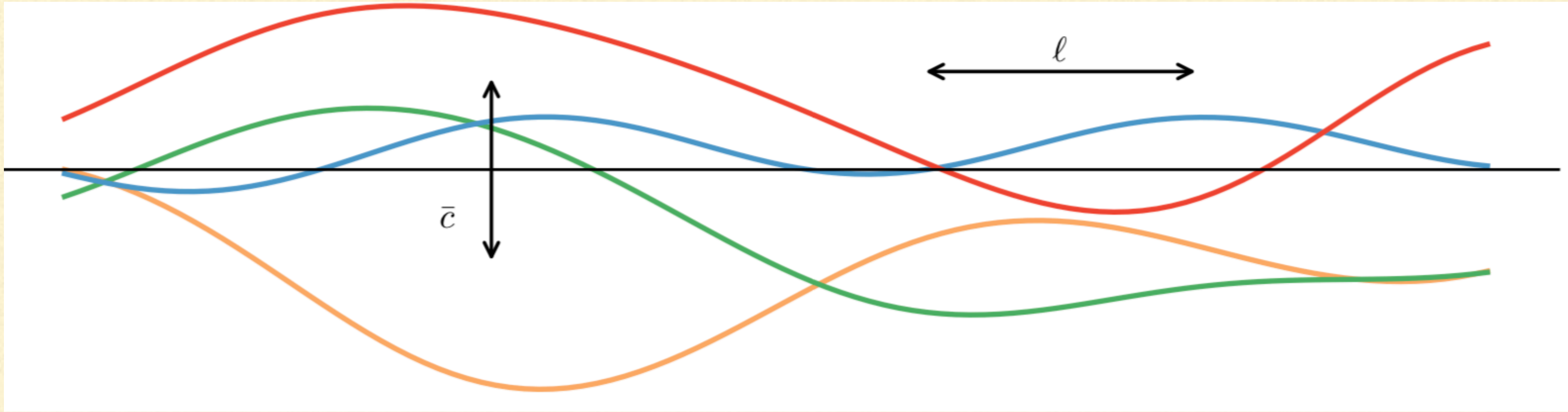

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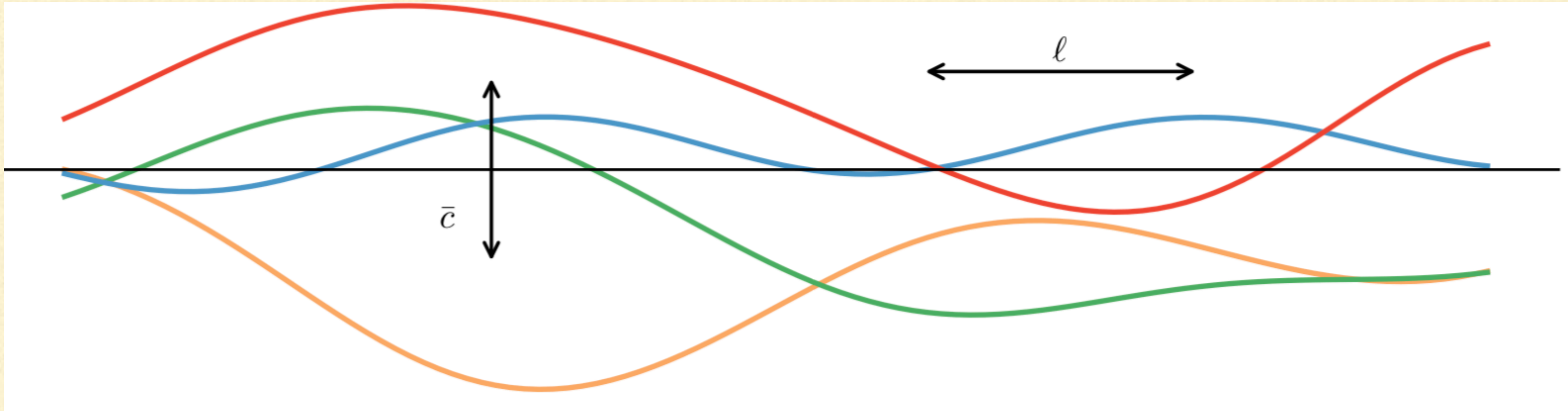

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Our hypothesis:

EFT coefficients at different orders can be modeled as:

- independent but identical realizations of one Gaussian Process;
- with a correlation structure; here we use a "squared exponential" (Gaussian) kernel, but we test it

A bit more on Gaussian Processes

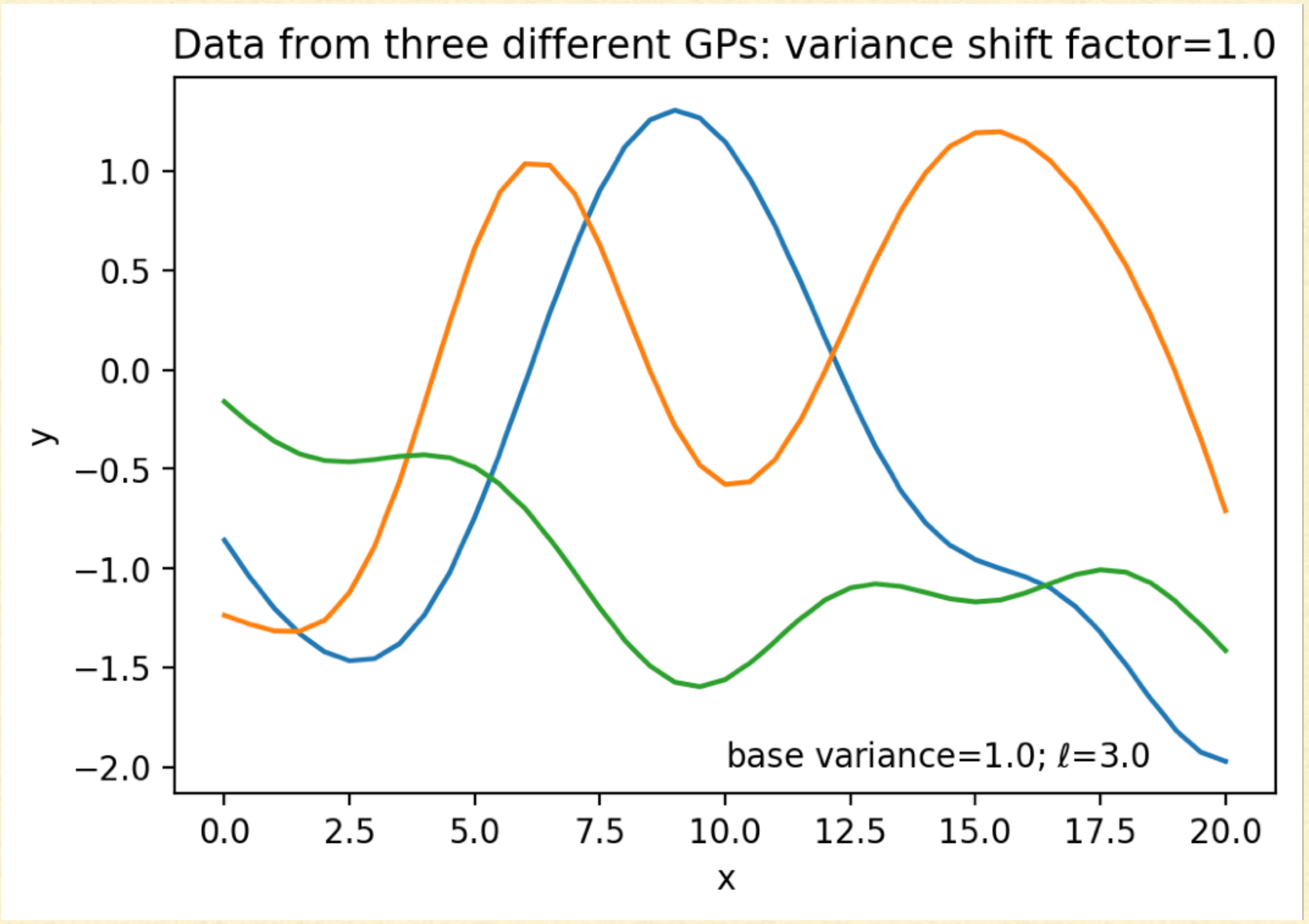
- Non-parametric, probabilistic model for a function
- Suppose we already know f at $x_1, x_2, x_3, \ldots, x_n$.
- Specify how f(y) is correlated with $f(x_1)$, $f(x_2)$, …..; don't specify underlying functional form.
- But value of f(y) is not deterministic: it's given by a (Gaussian) probability distribution.
- Correlation decreases as points get further away from each other.
- Specify correlation matrix of f at x and y, e.g.:

$$k(f(x), f(y)) = \bar{c}^2 \exp\left(-\frac{(x-y)^2}{2\ell^2}\right)$$

- Two parameters cbar and ℓ

Learning cbar and ℓ: Toy Example

- Generate three data sets from an underlying GP with mean 0, variance 1 and length scale 3.



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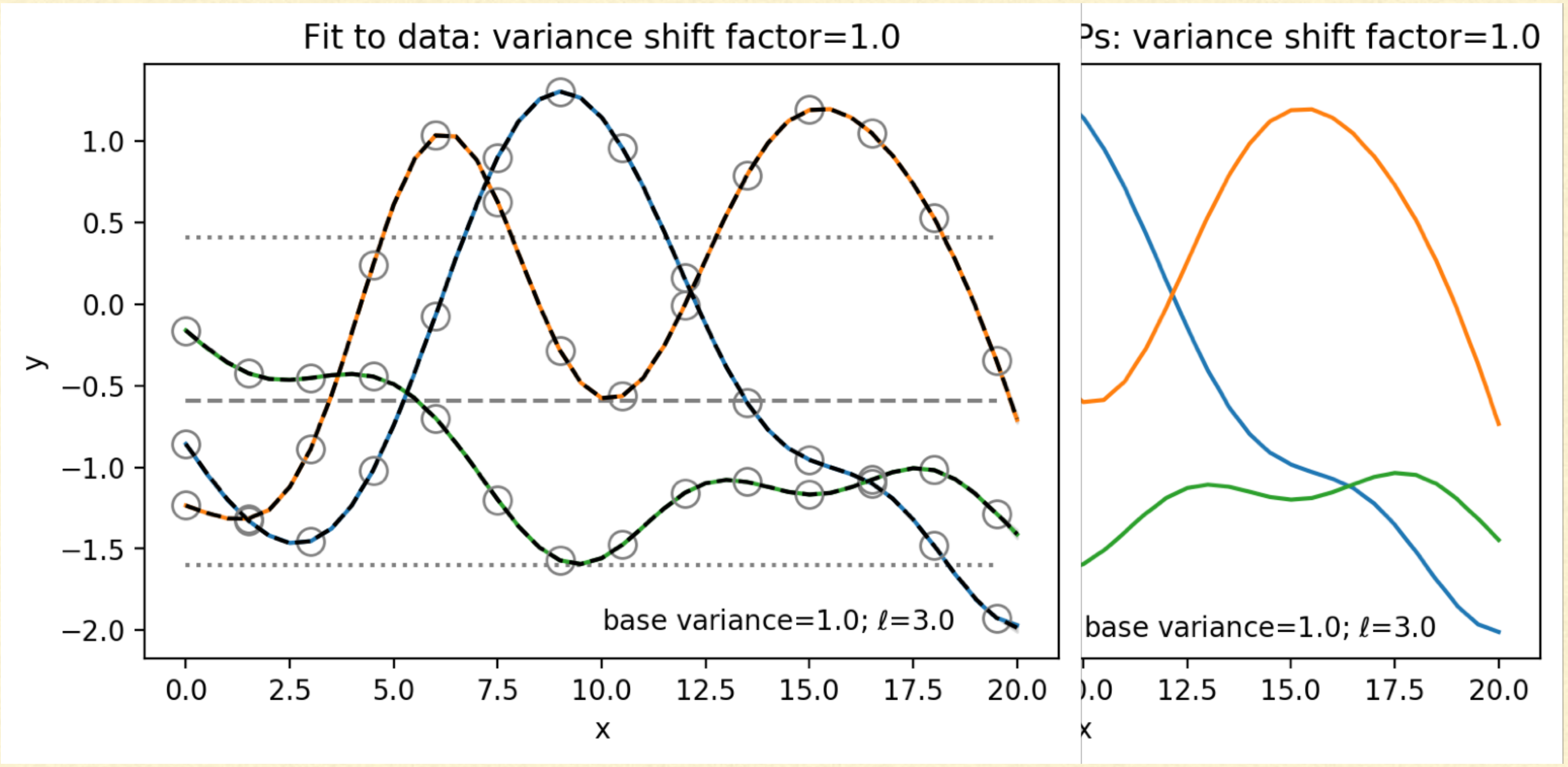

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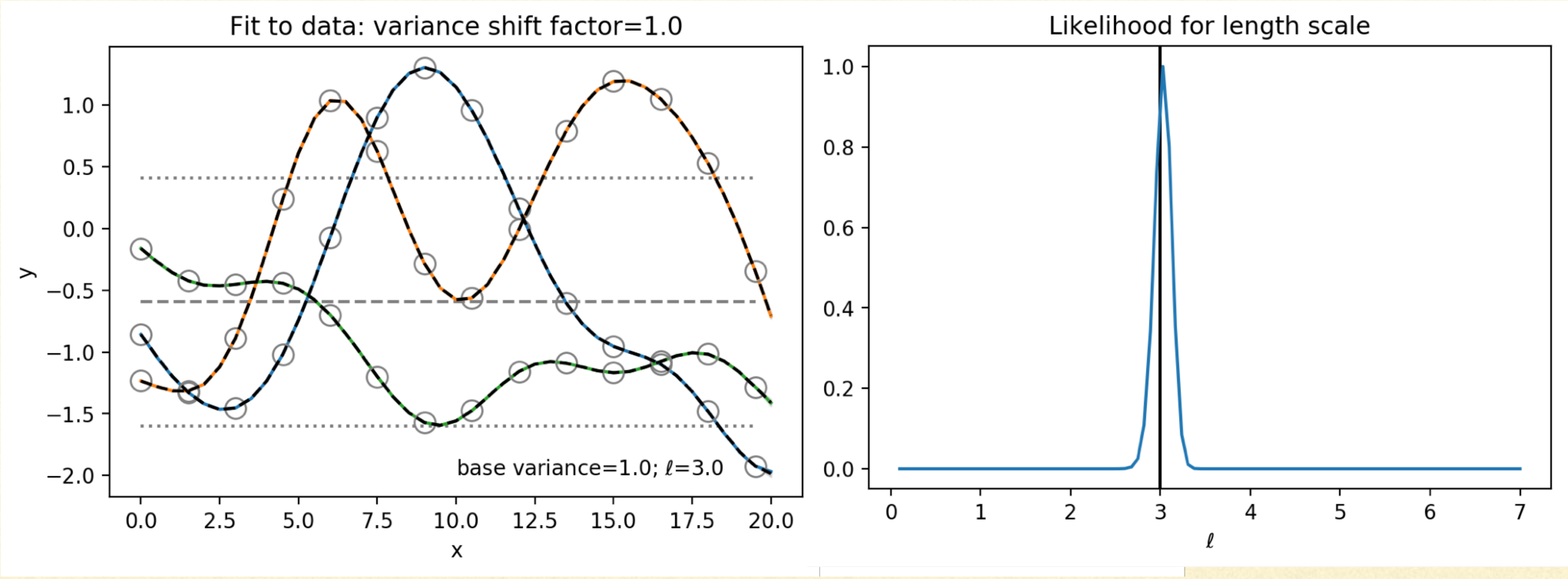

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- Assess performance of fitted GP on "testing data" set.
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- Define Mahalanobis distance, which does account for correlations

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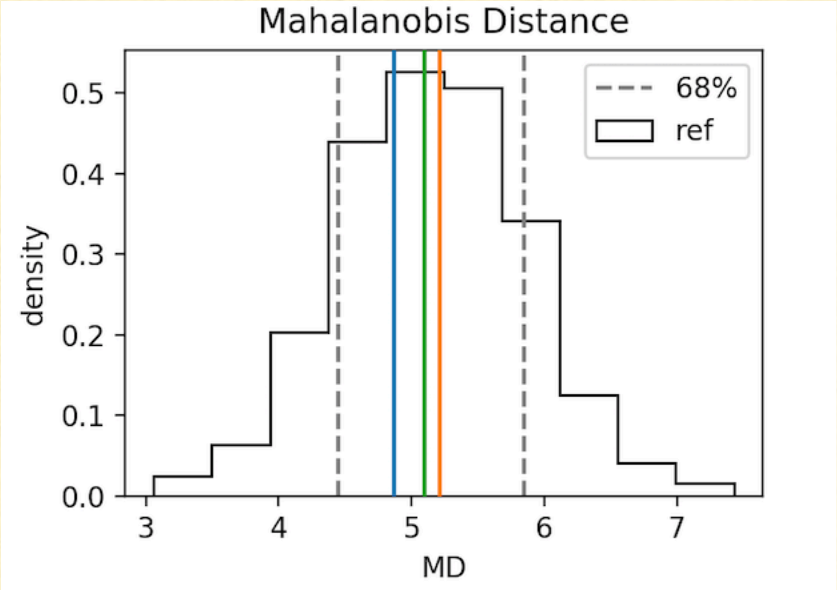

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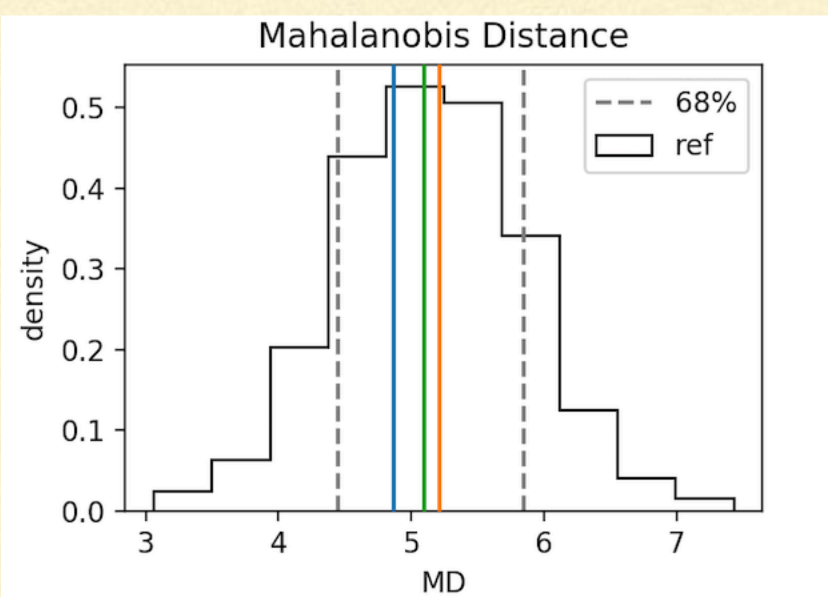

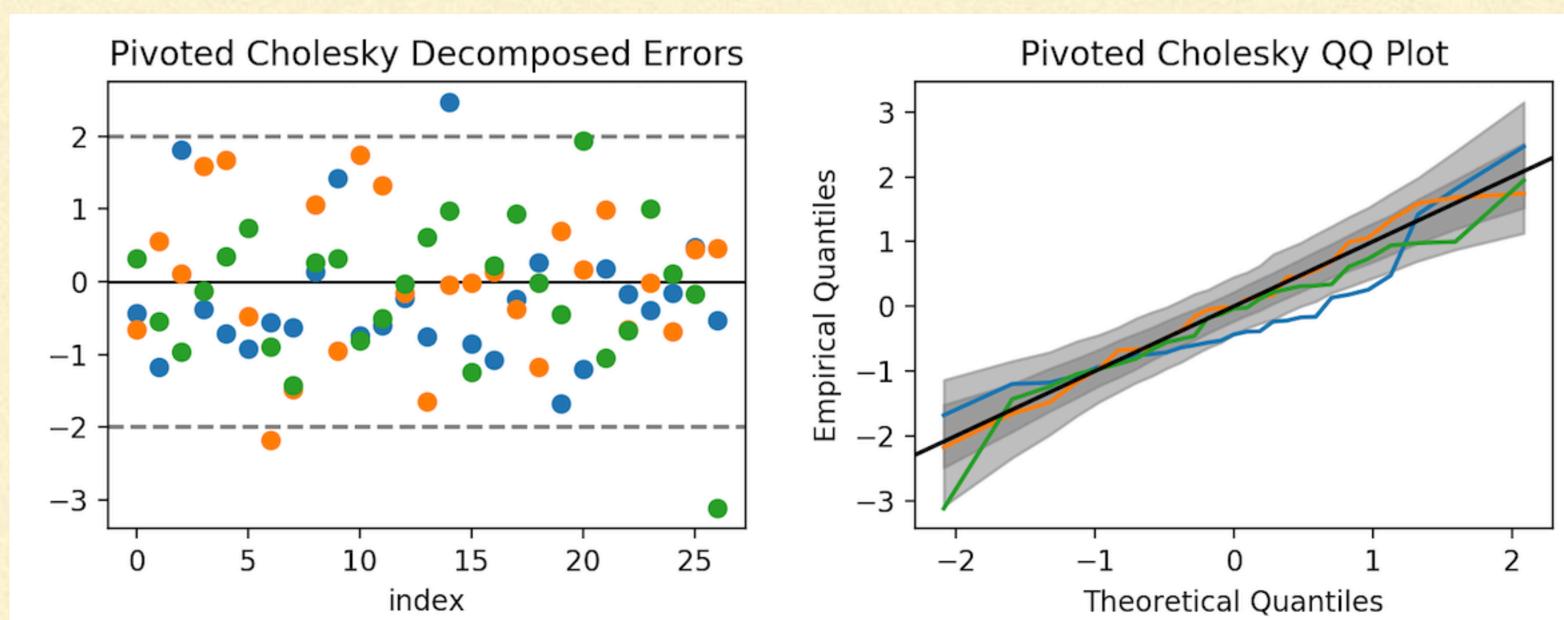

What can go wrong 1: different cbar's

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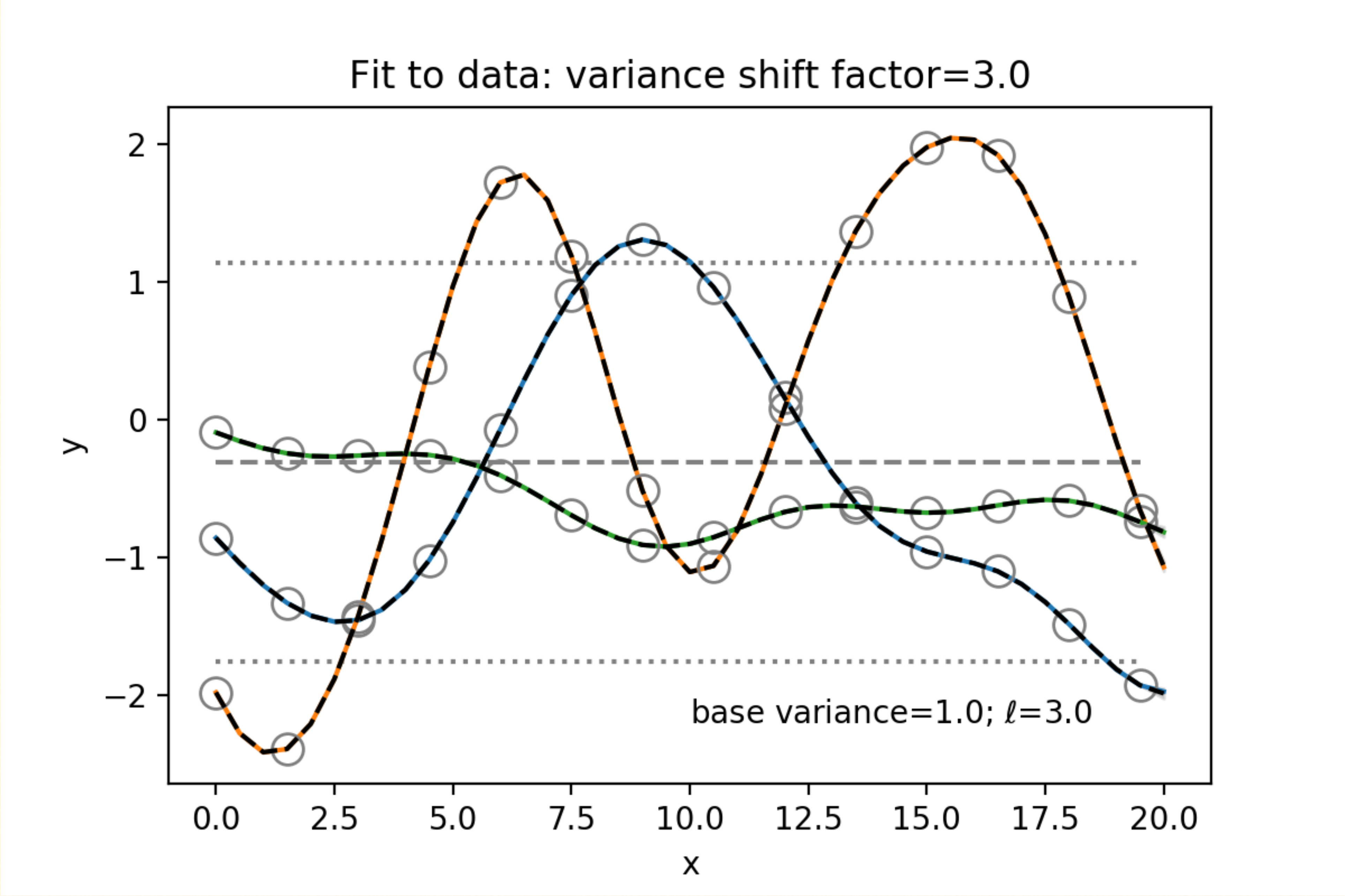

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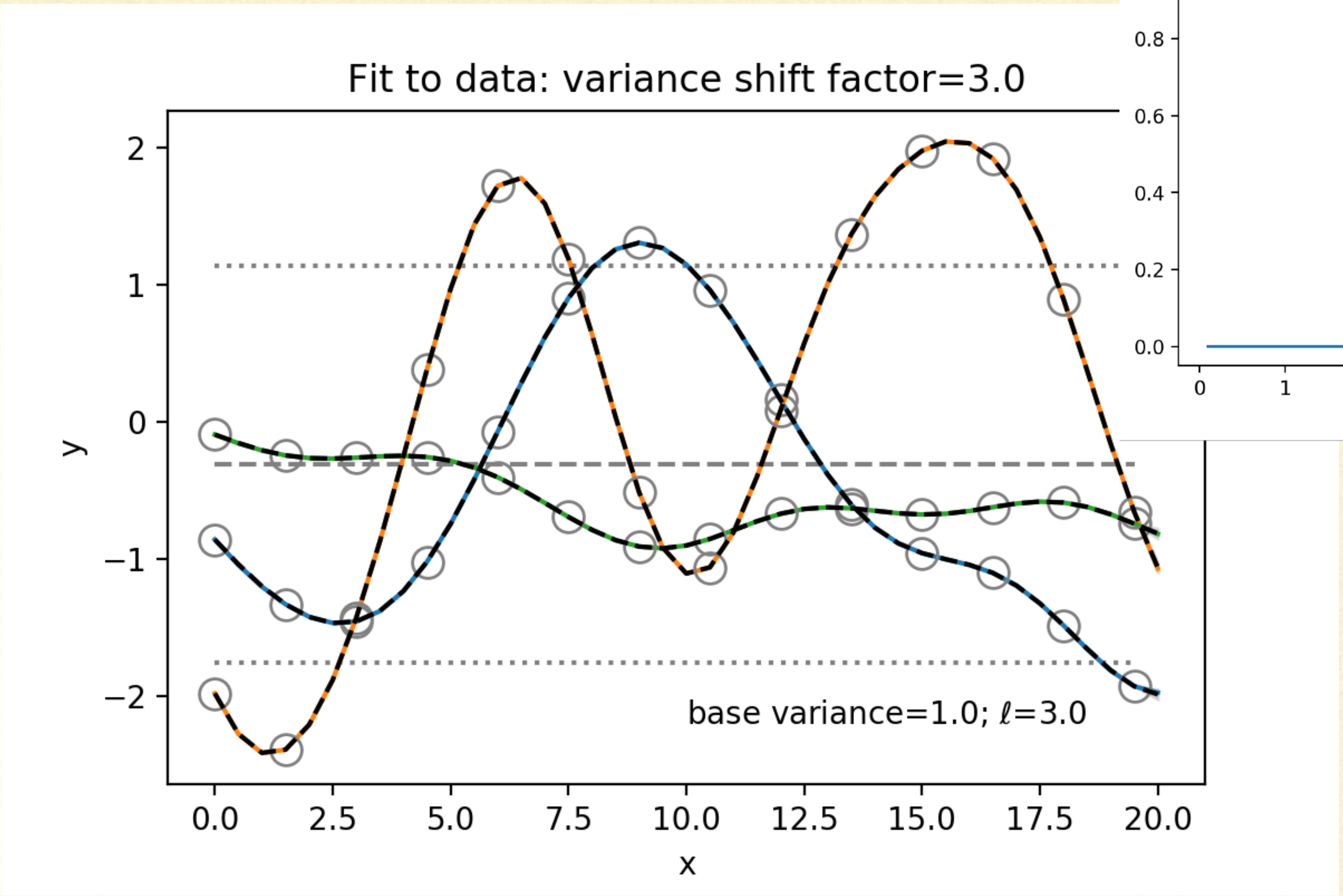

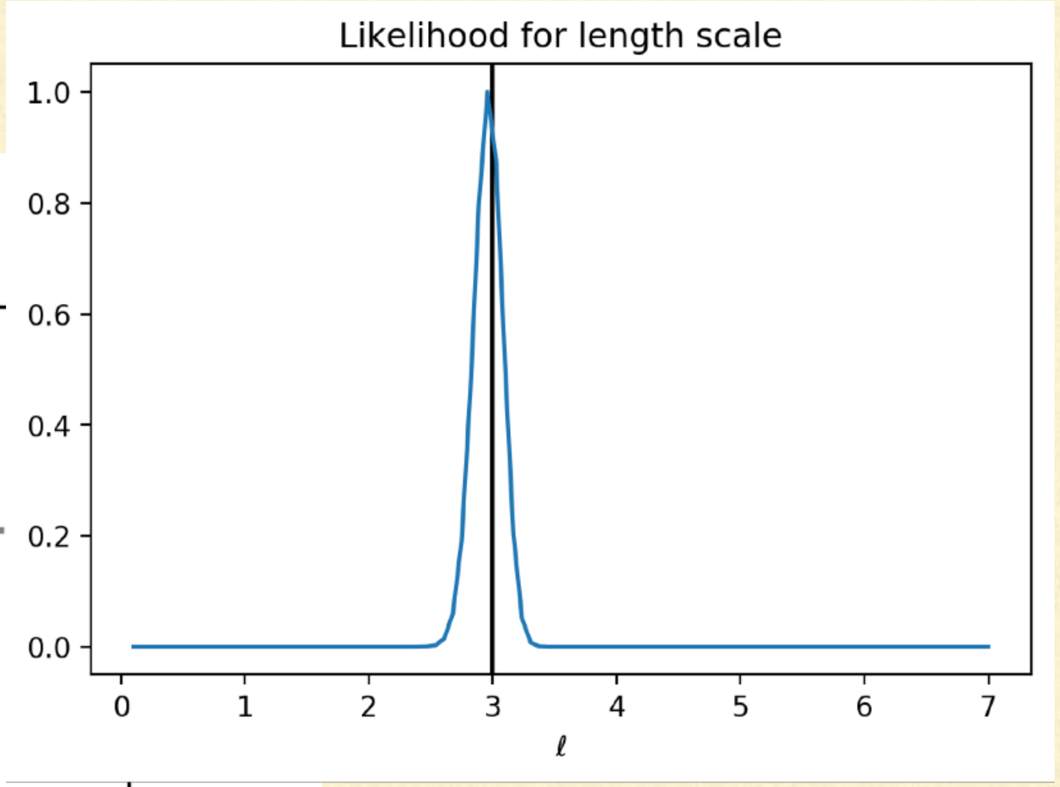

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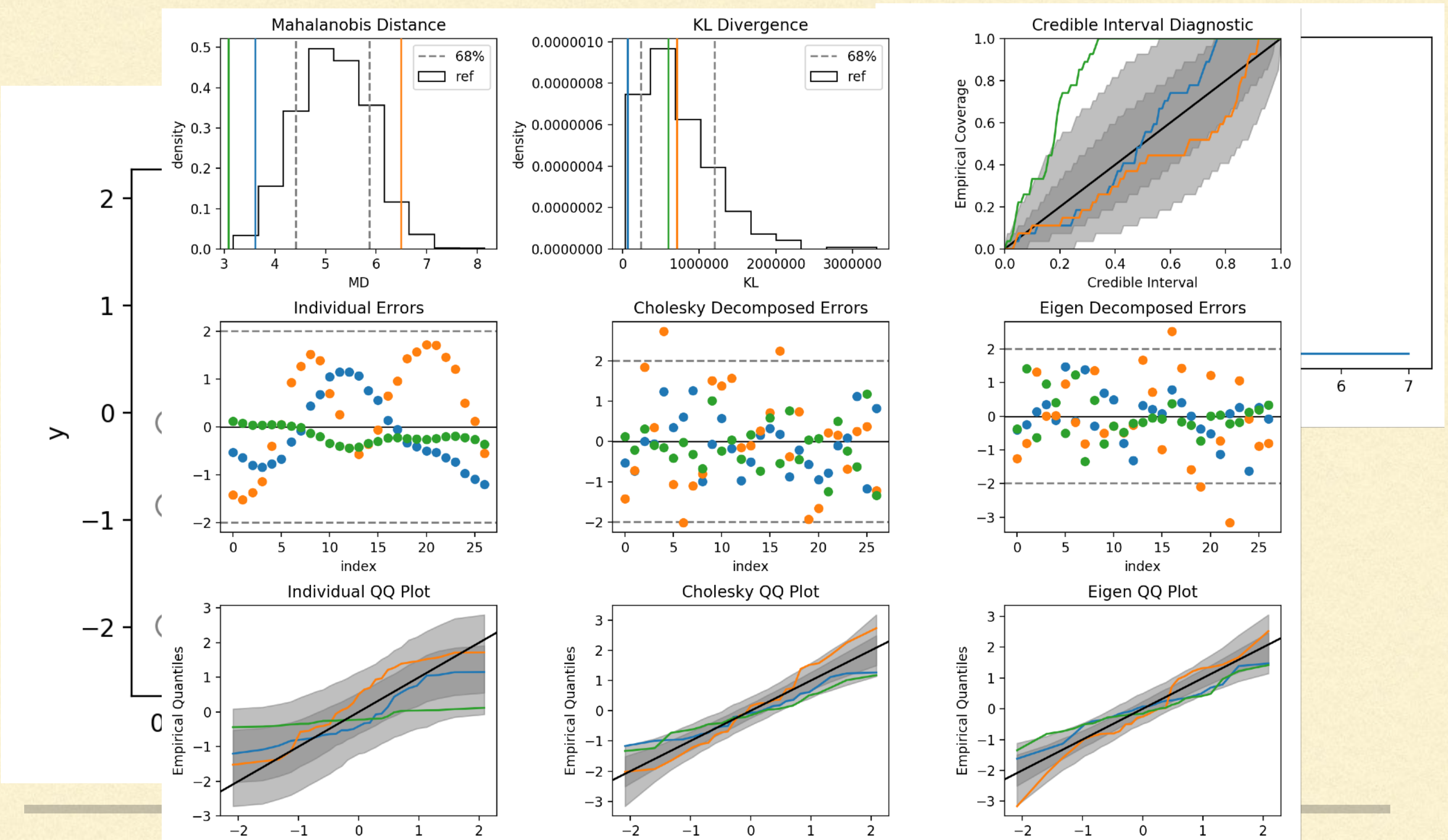
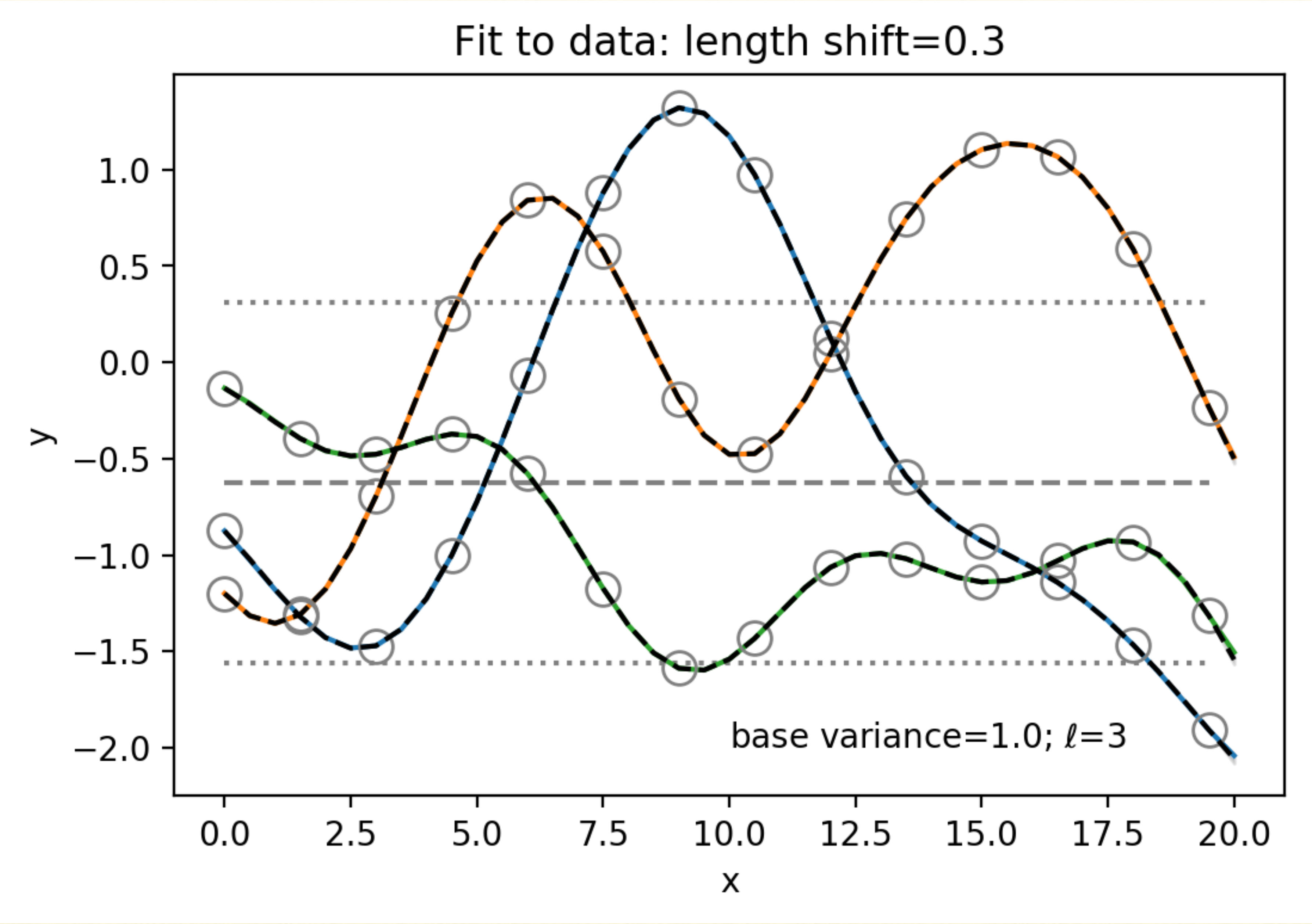


What can go wrong II: different ℓs

- Try to fit single GP to data with different ℓs



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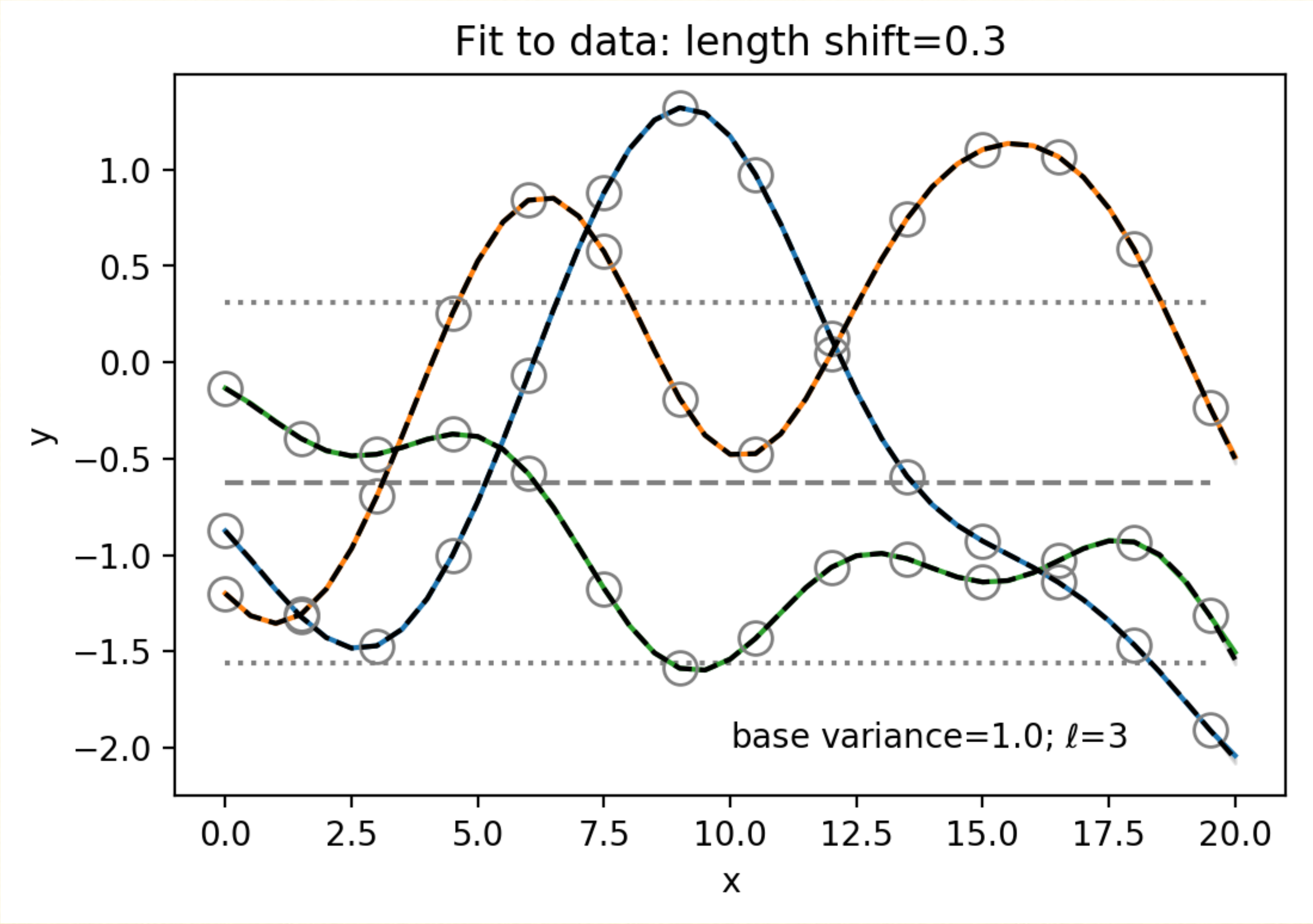

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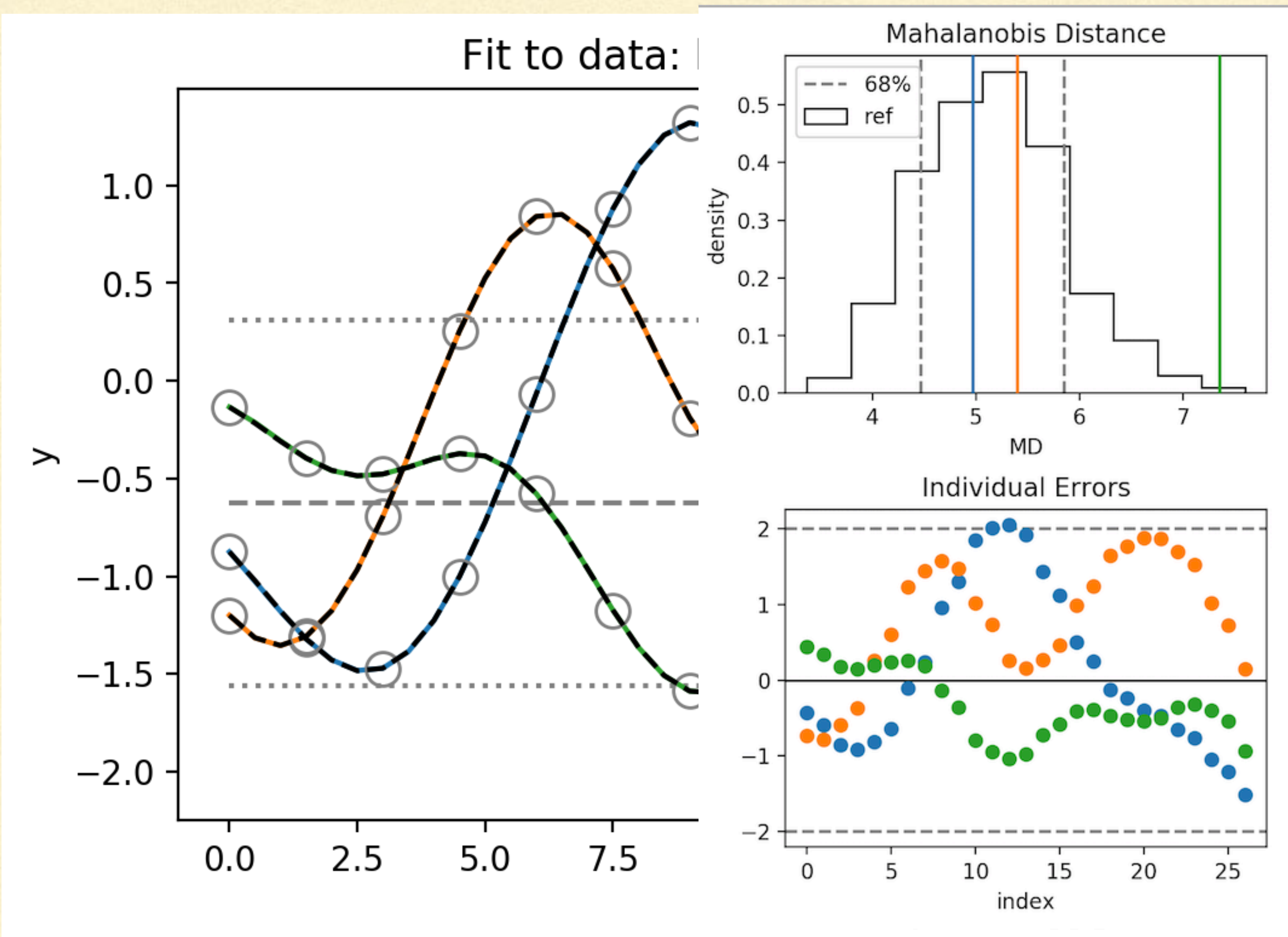
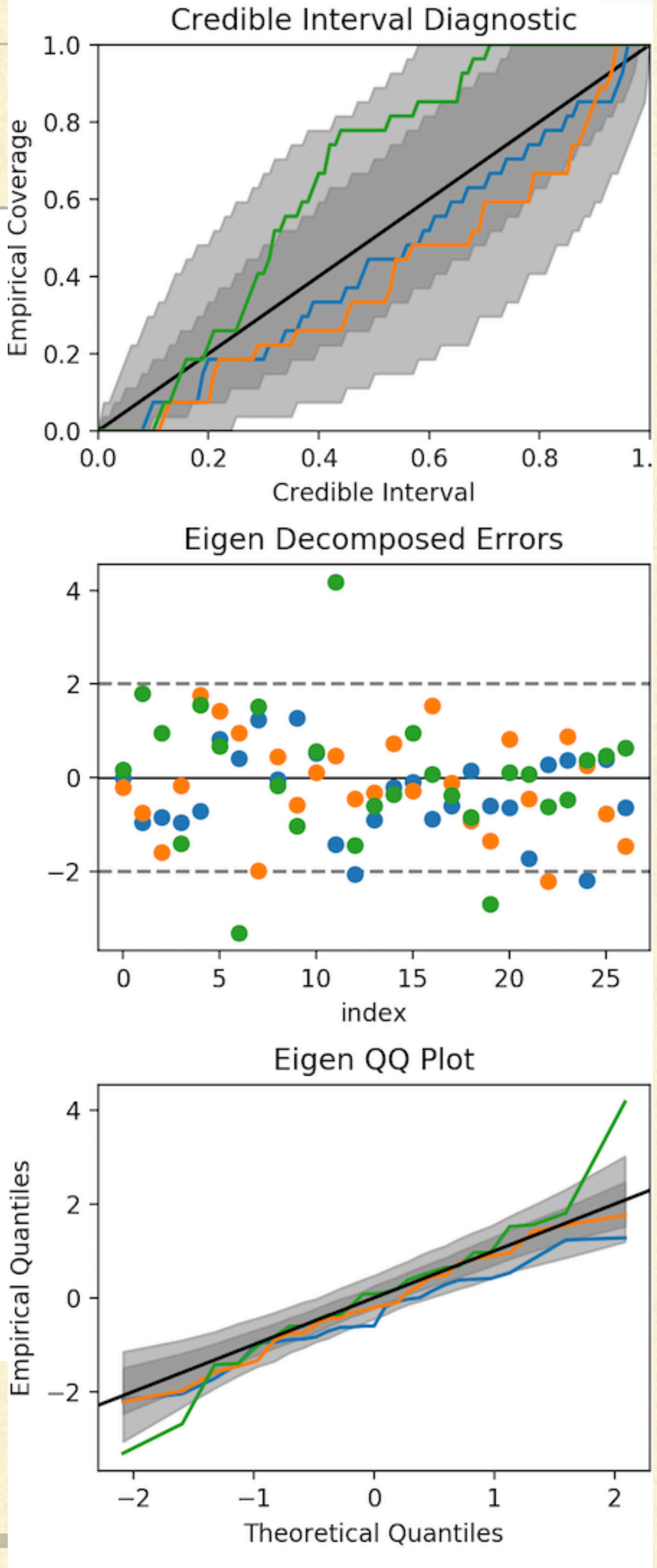
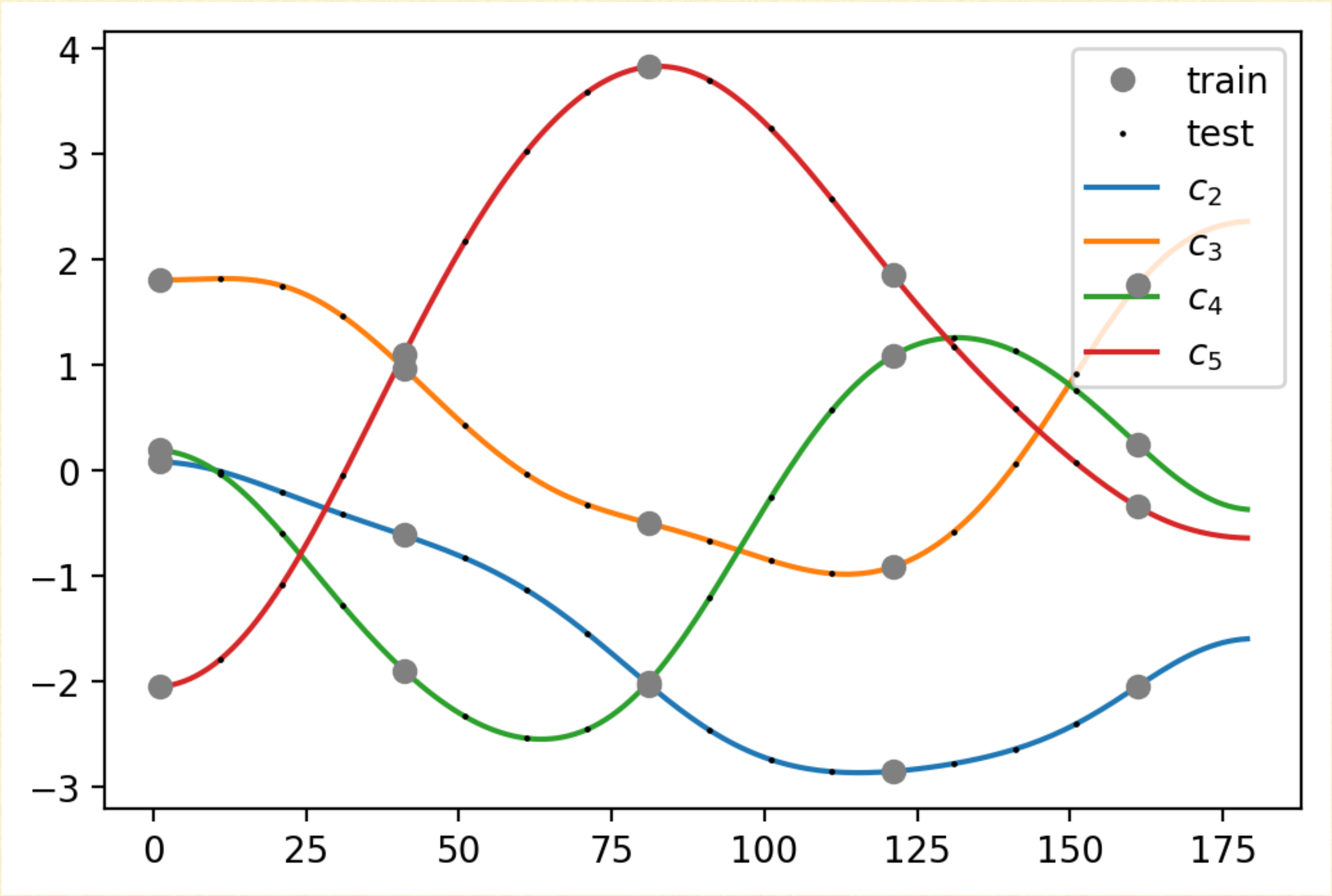




Differential cross section vs. angle

$\frac{d\sigma}{d\Omega}$ E_{lab}=96 MeV **PRELIMINARY**



RKE potential; Λ=500 MeV

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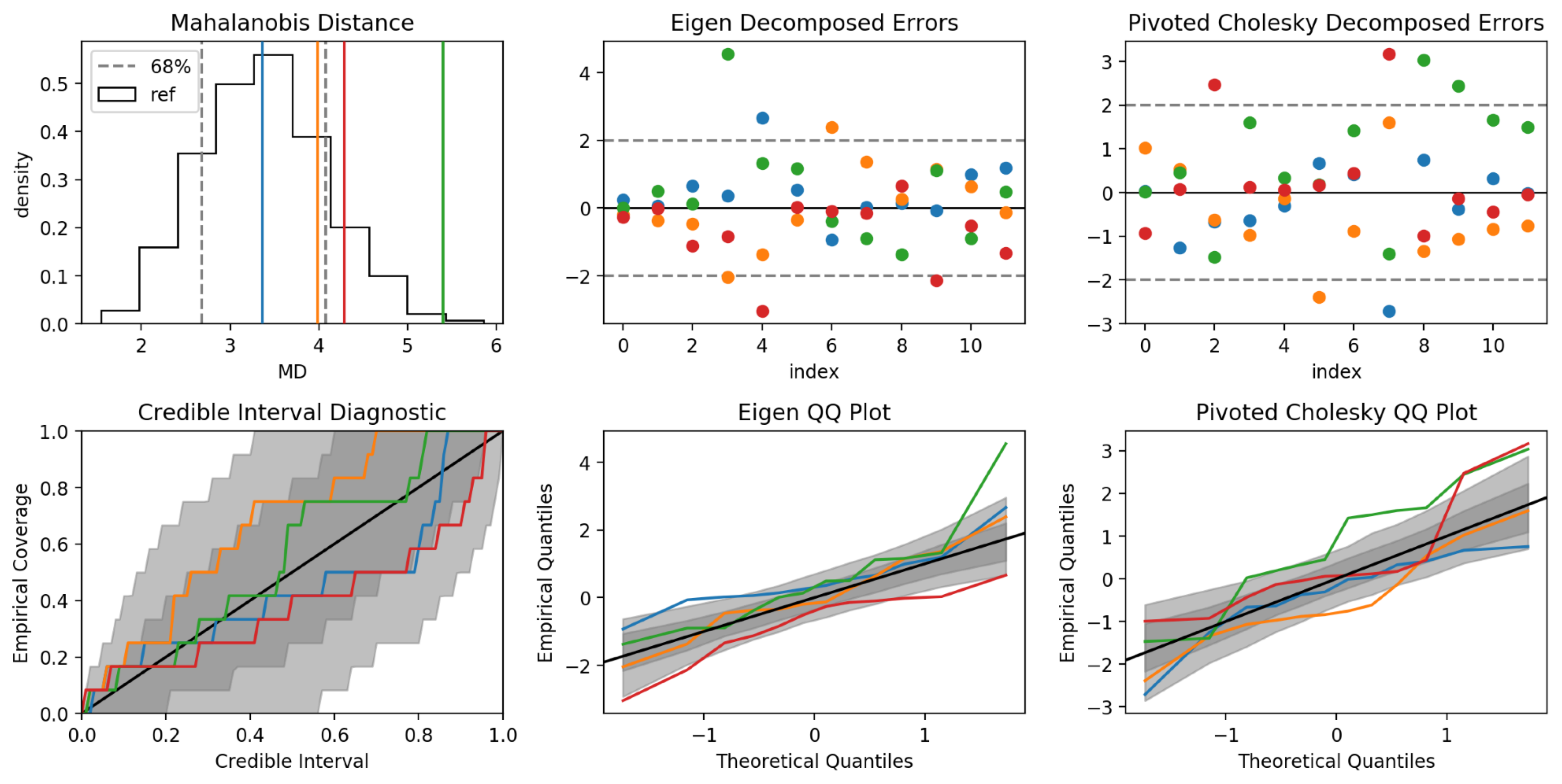

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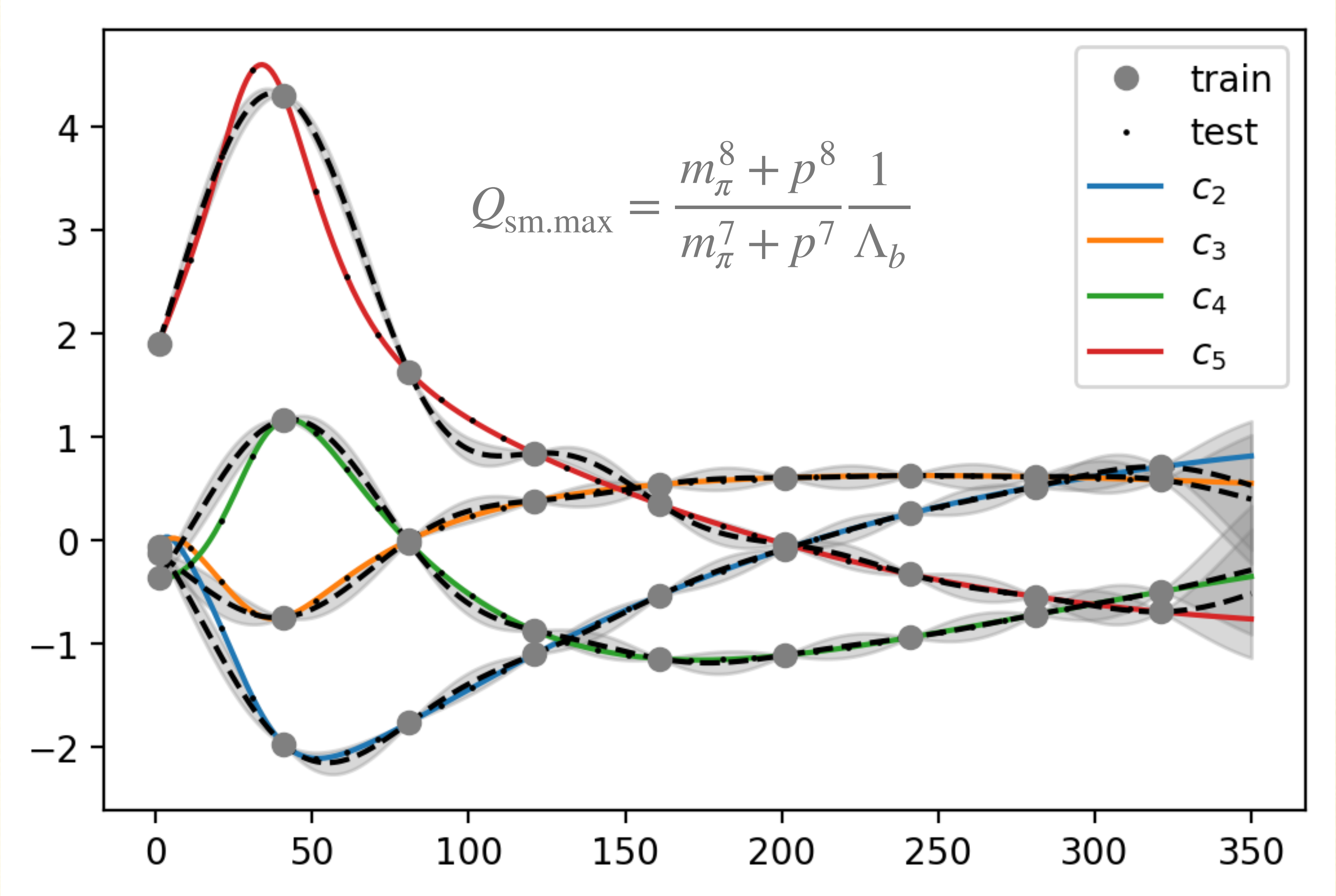

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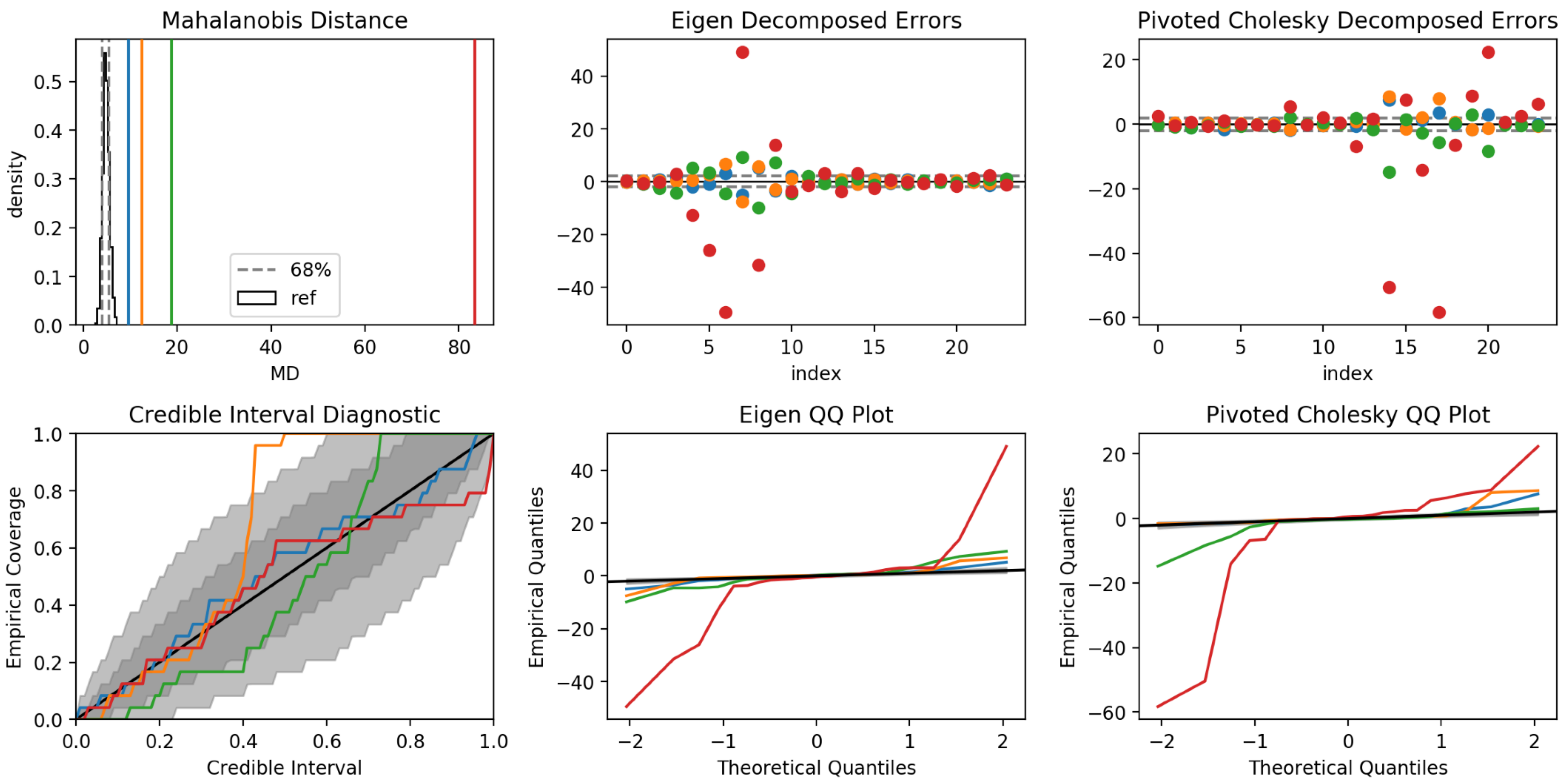

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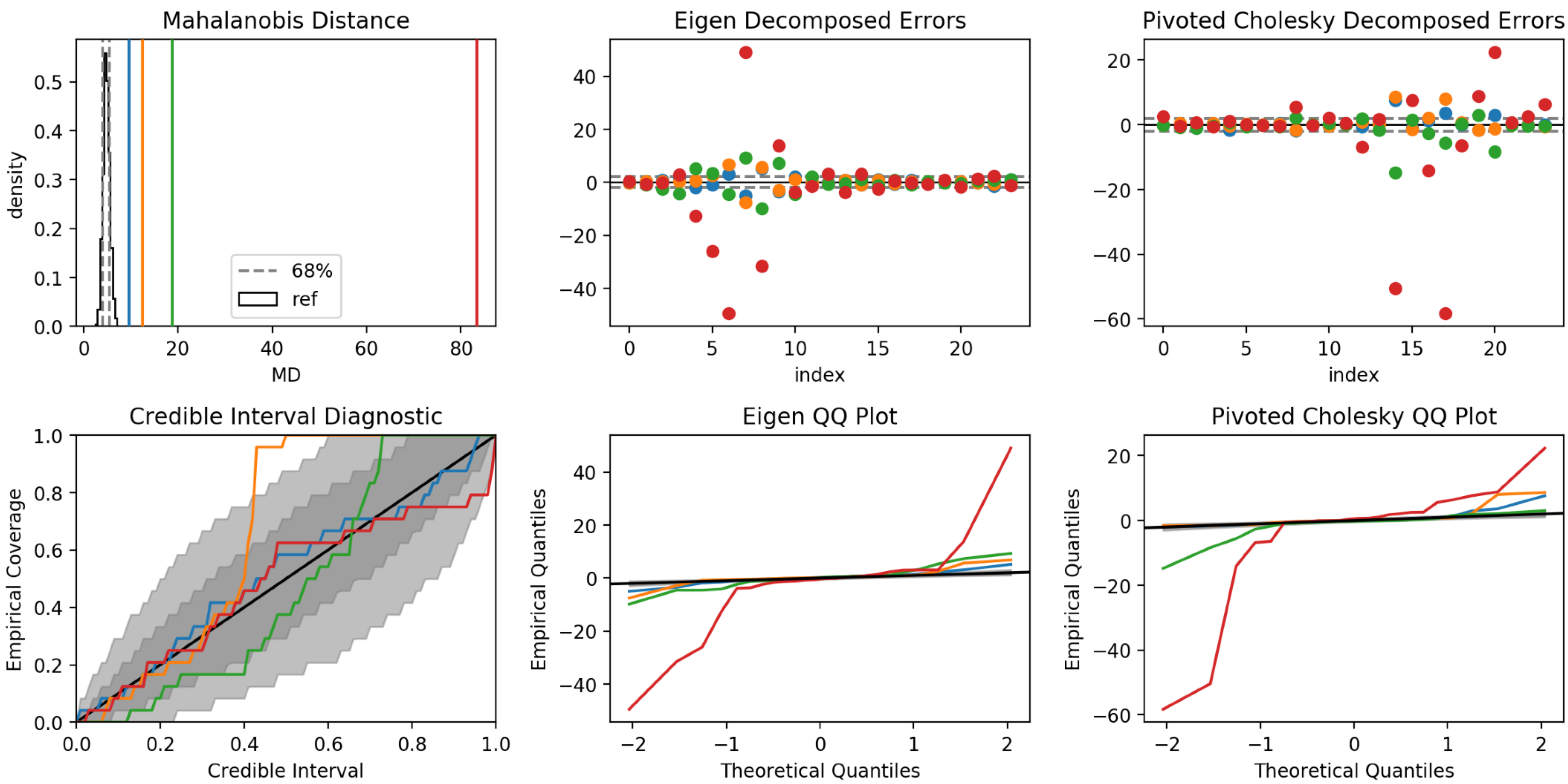
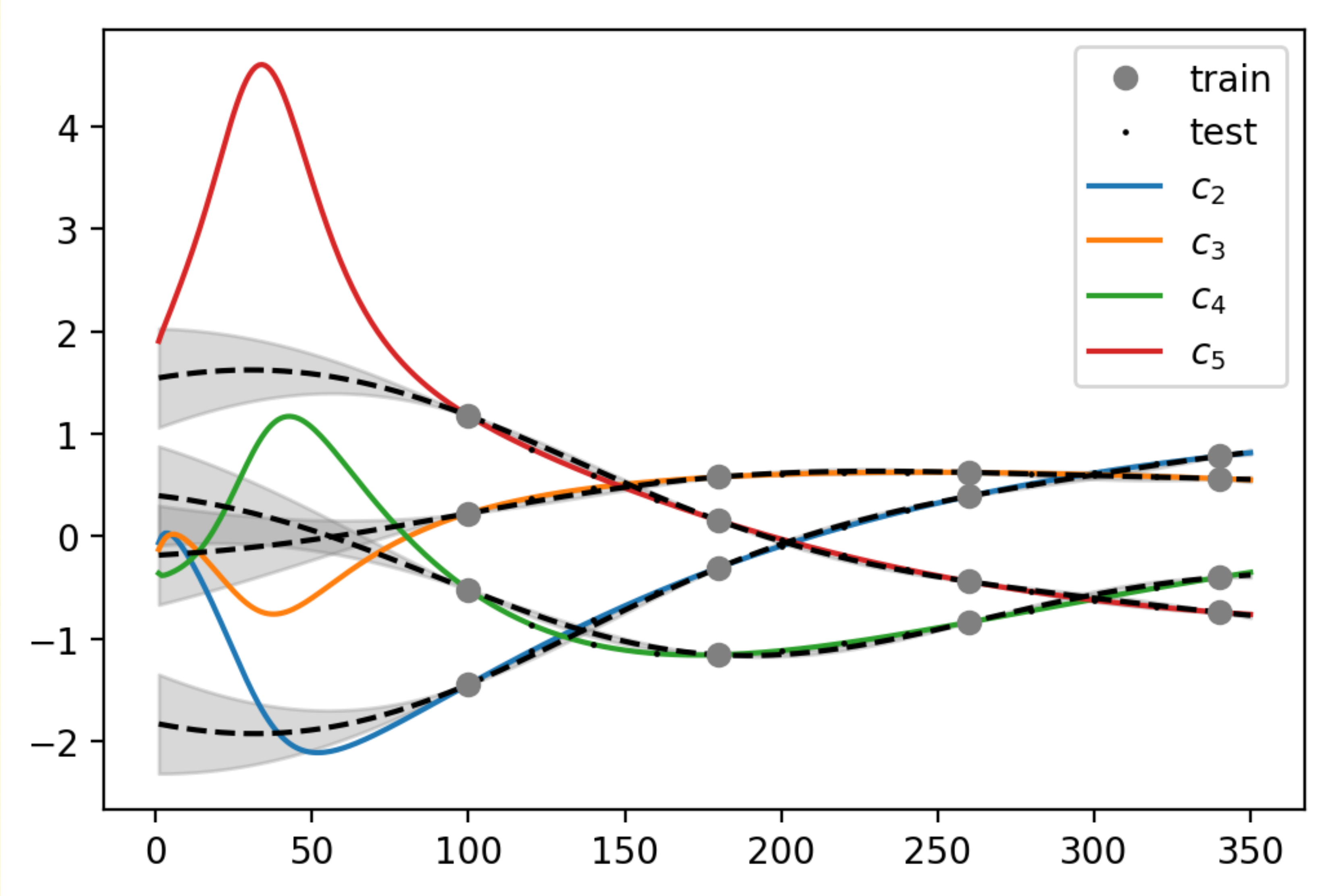


- Even with change of expansion parameter built in, change of length scale messes up GP estimation: "non-stationarity"

One way to deal with low energies



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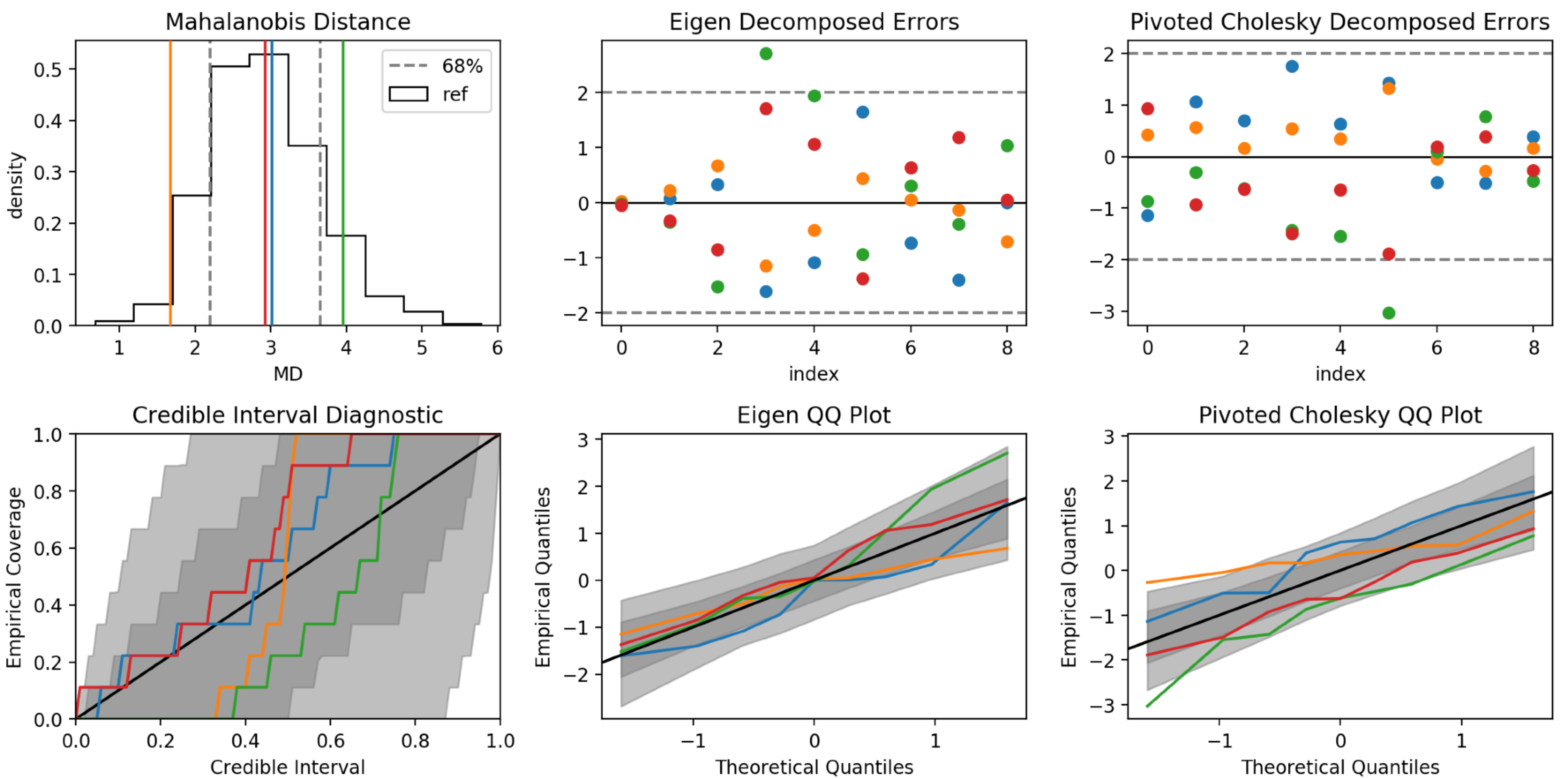

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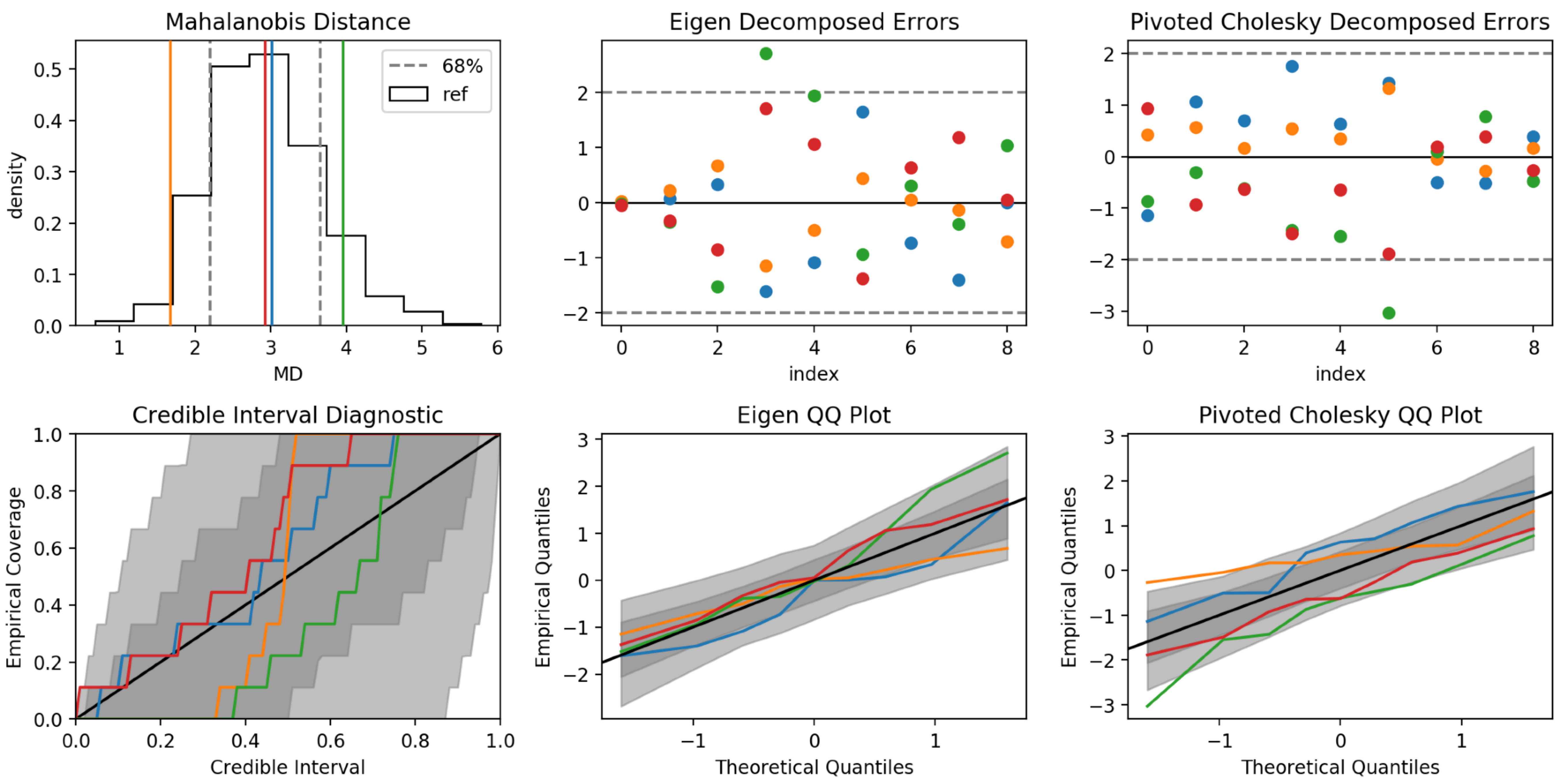
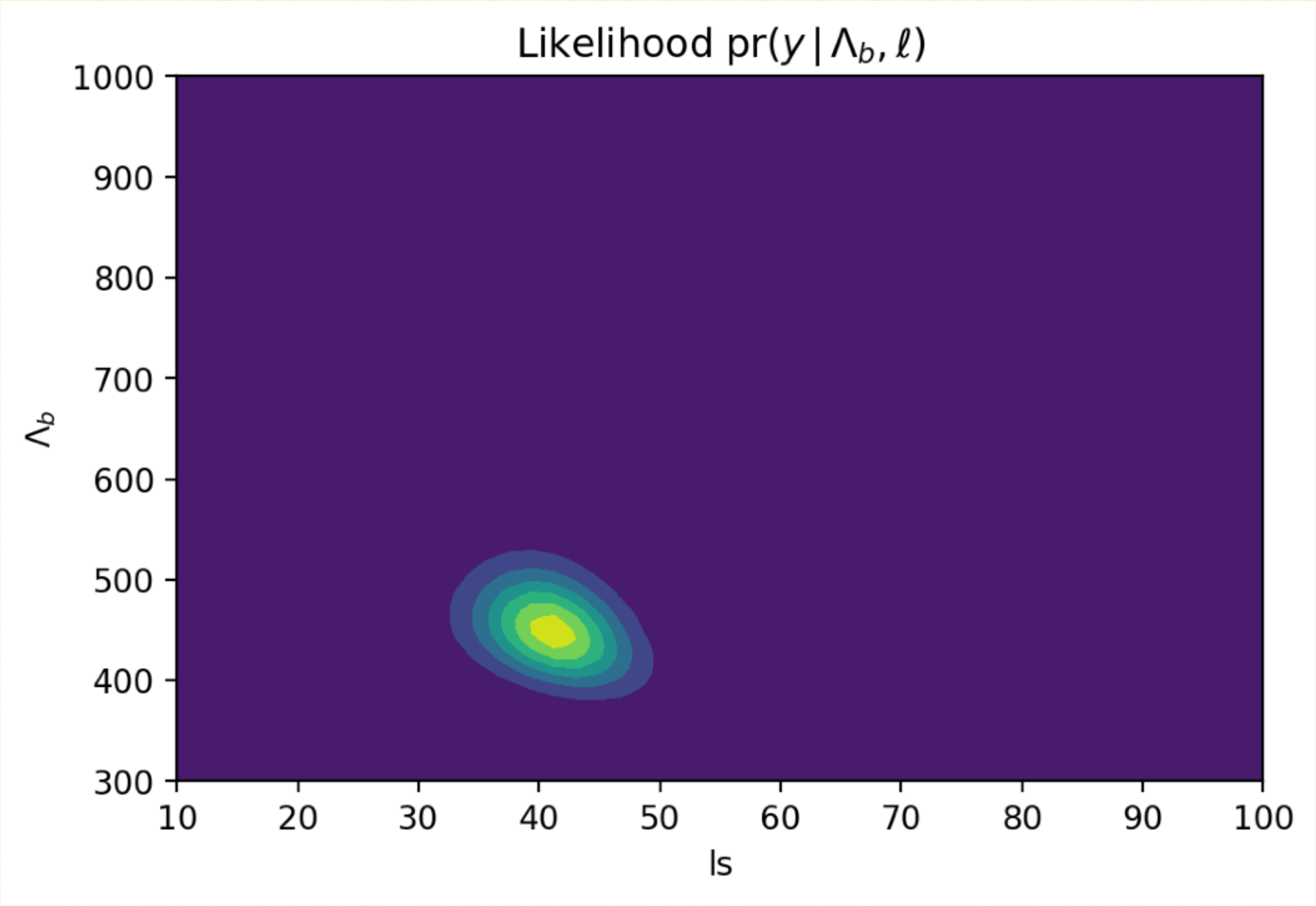


- Hypothesis of EFT coefficients as draws from a GP looks very healthy for cross section at E_{lab}>100 MeV: next we need to model change of behavior

Λ_b and ℓ inference

PRELIMINARY



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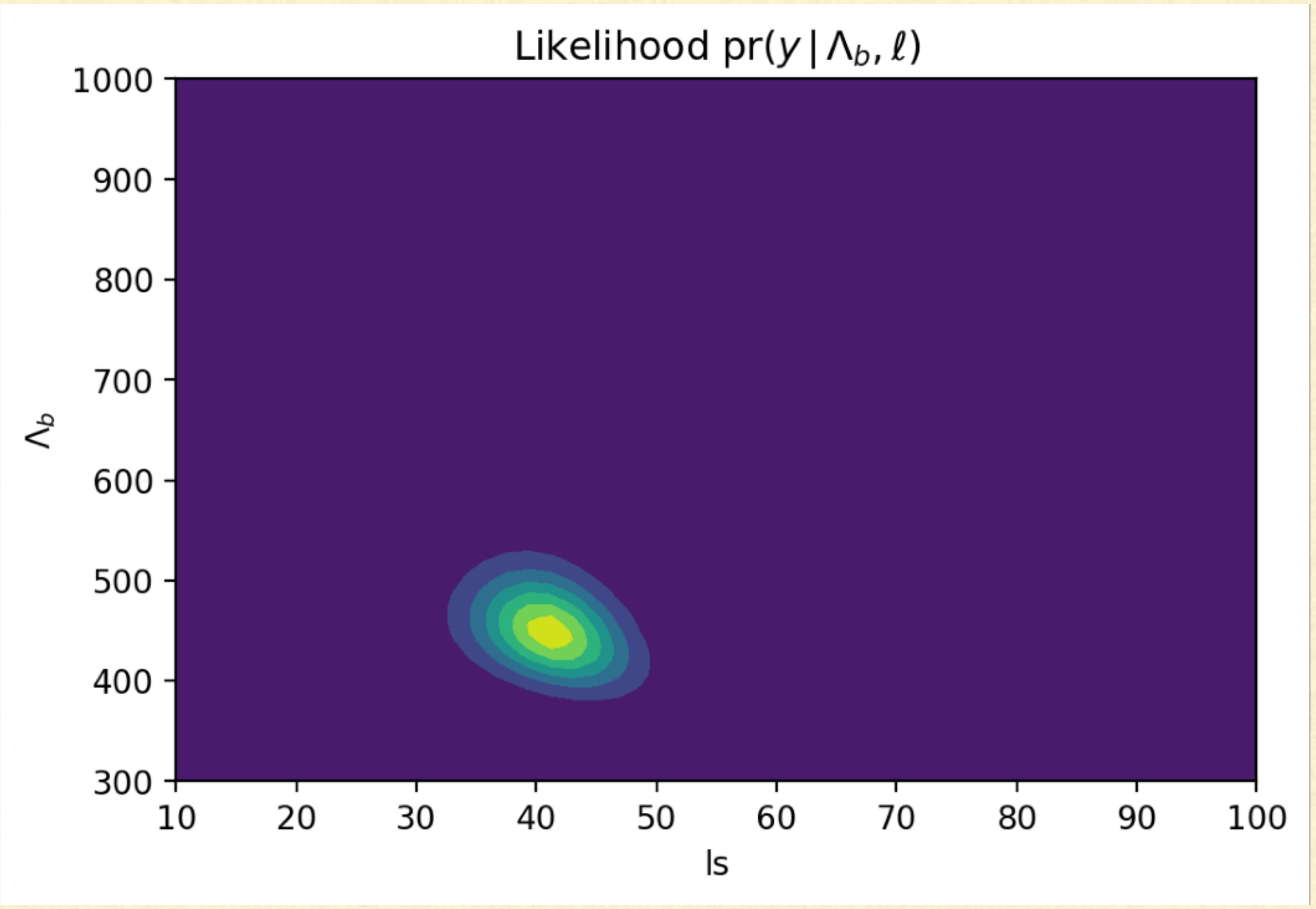

RKE potential; Λ=500 MeV;
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$\ell \approx 40$ MeV

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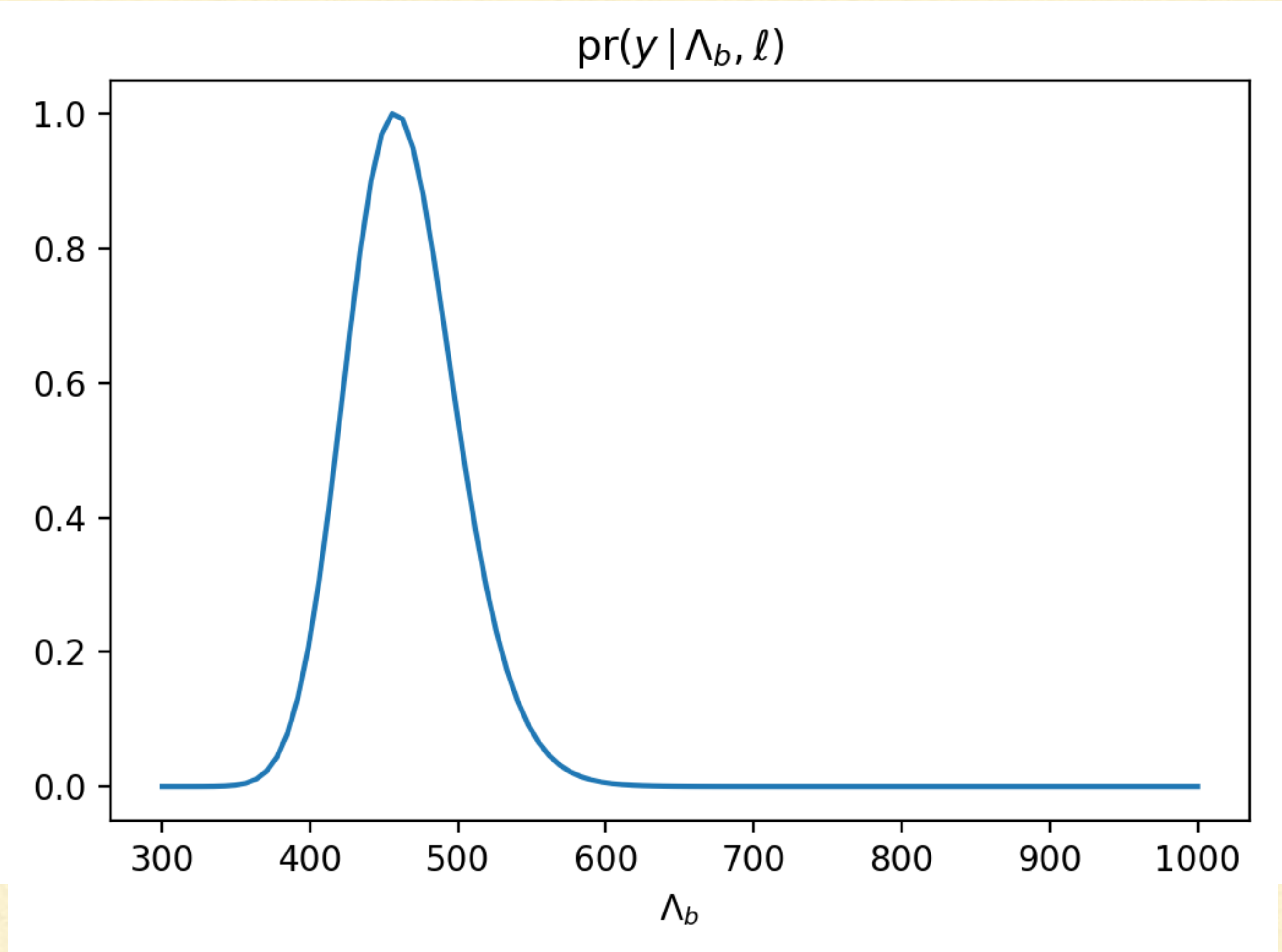

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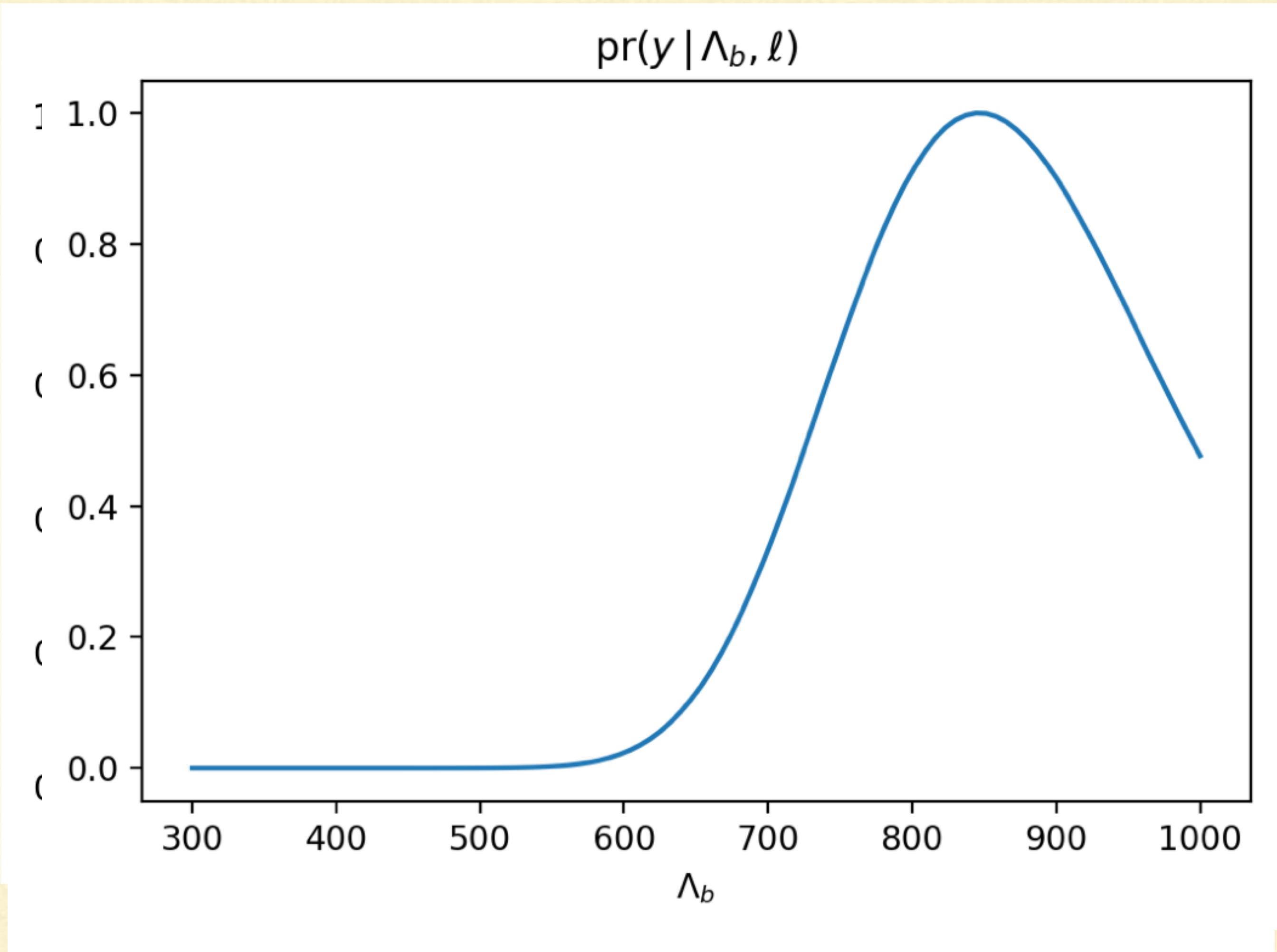

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Restricted domain

$\ell \approx 116$ MeV

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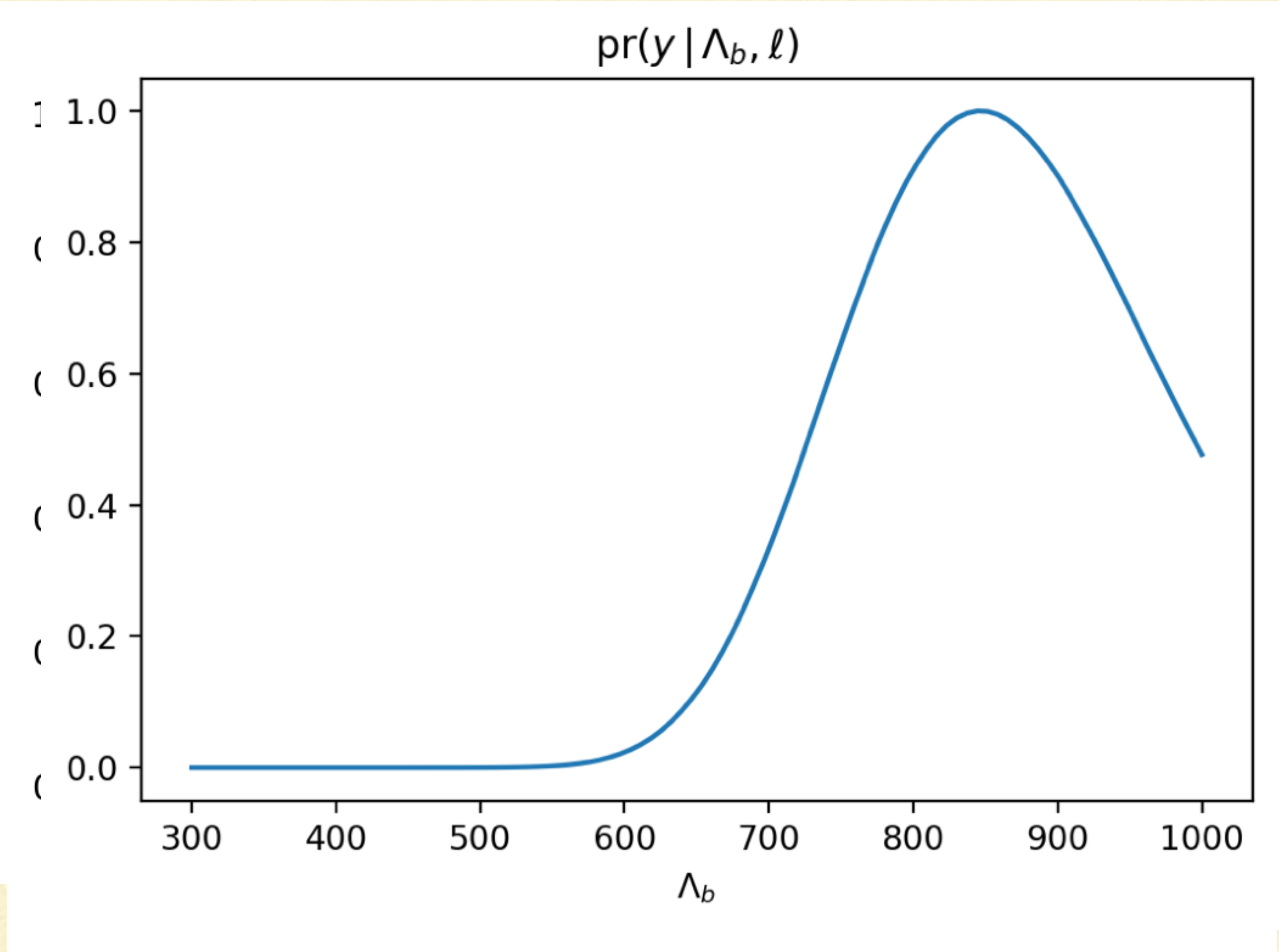

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To do:

- Model non-stationarity
- Play with "switch over" of expansion parameter at $p \approx m_\pi$
- Include other observables in analysis

Applications/future work

- Analyze different ChiEFT NN potentials for breakdown-scale, order-by-order calibration, etc.
- Gaussian Process models for ChiEFT expansion of E/N in nuclear and neutron matter

  With C. Drischler
- Gaussian Process models of Compton scattering observables

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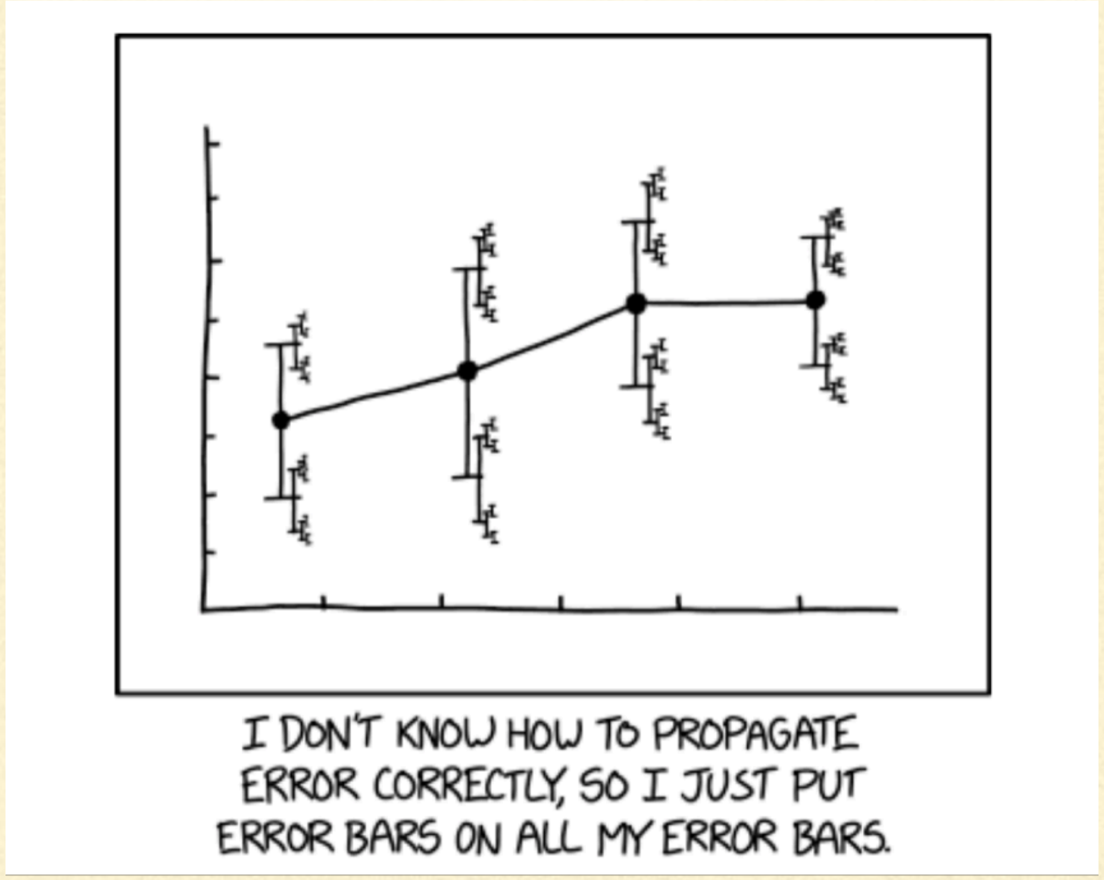
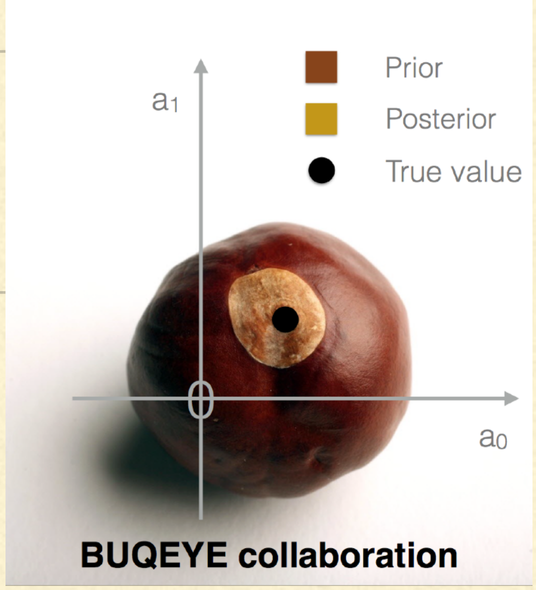


http://xkcd.com

Summary



- Bayesian analysis makes explicit what the assumptions about the EFT convergence pattern are
- A rigorous treatment of truncation errors can validate (or falsify) claims that potentials respect the ChiEFT power counting
- And improve parameter estimation

Sarah's talk

- But to do this properly we need a good model for the way that truncation errors are correlated across different observables
- Gaussian Process models of EFT truncation errors provide understanding of those correlations

gsum package

- Also provide an inexpensive way to simulate expensive observables
- Honest parameter estimation, calibration plots, breakdown-scale inference…

A Generic EFT

$$g(x) = \sum_{i=0}^{k} \mathcal{A}_i(x) x^i \qquad x = \frac{p}{\Lambda_b}$$

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- Suppose we are interested in a quantity as a function of a momentum, p, that is small compared to some high scale, Λ_b.
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$$\mathcal{A}_i(x) = c_i(\mu) + f_i(x, \mu) \qquad c_i, f_i = \mathcal{O}(1) \text{ for } \mu \sim \Lambda_b, x \sim 1$$

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- $f_i(x, \mu)$ is a calculable function, that encodes IR physics at order i
- c_i is a low-energy constant (LEC): encodes UV physics at order i. Must be fit to data
- Complications: multiple light scales, multiple functions at a given order, skipped orders, ….

Bayesian tools

Thomas Bayes (1701?-1761)

http://www.bayesian-inference.com

$$\mathrm{pr}(A|B,I) = \frac{\mathrm{pr}(B|A,I)\mathrm{pr}(A|I)}{\mathrm{pr}(B|I)}$$

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Posterior

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Allows us to integrate out "nuisance" (e.g. higher-order) parameters