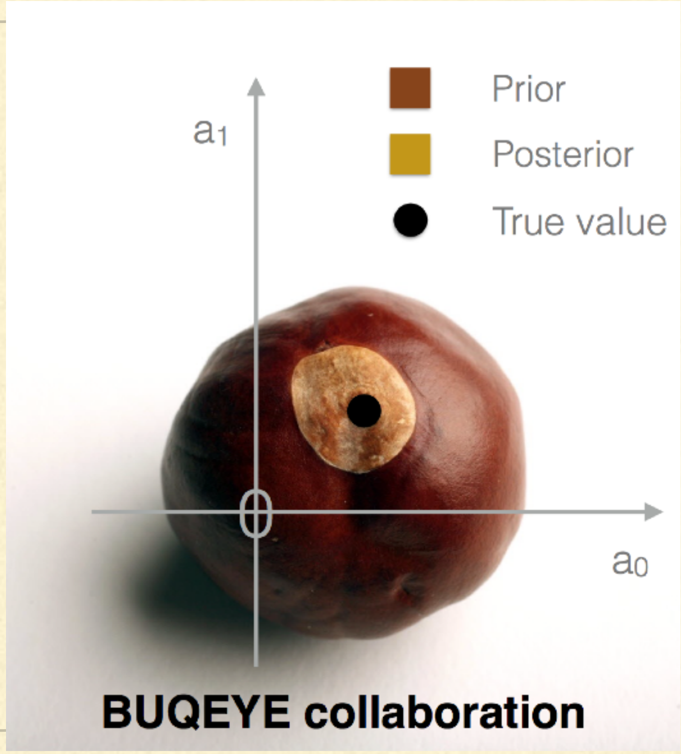
TALENT Course 11
Learning from Data: Bayesian methods and machine learning



Lecture 23: Model checking II

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Ohio University
TU Darmstadt
ExtreMe Matter Institute

TALENT Course 11 is possible thanks to funding from the STFC

An EFT expansion in pictures

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

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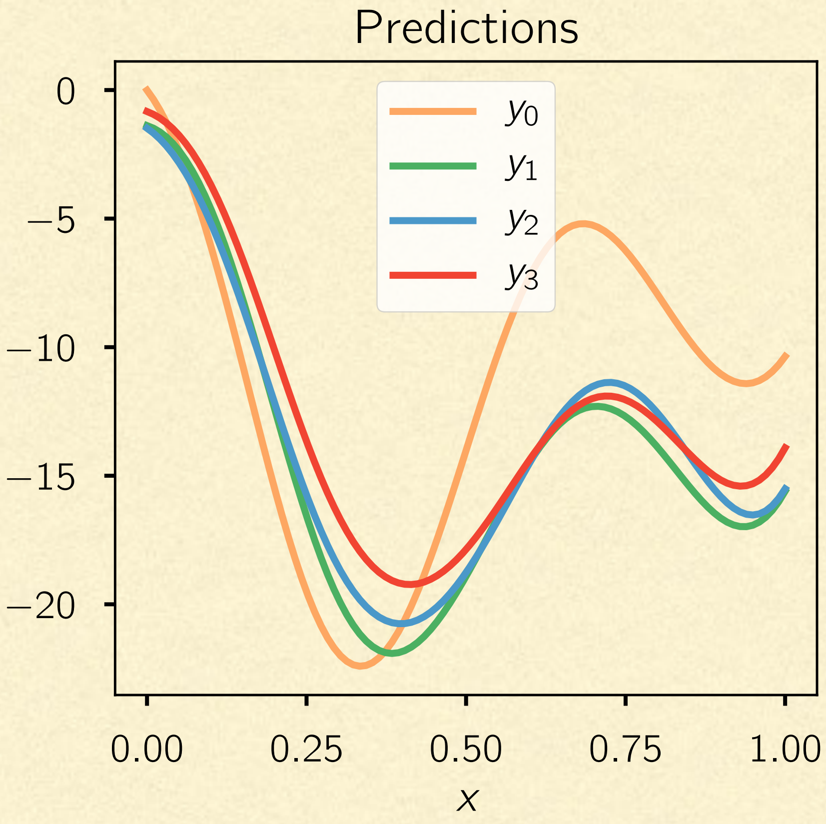

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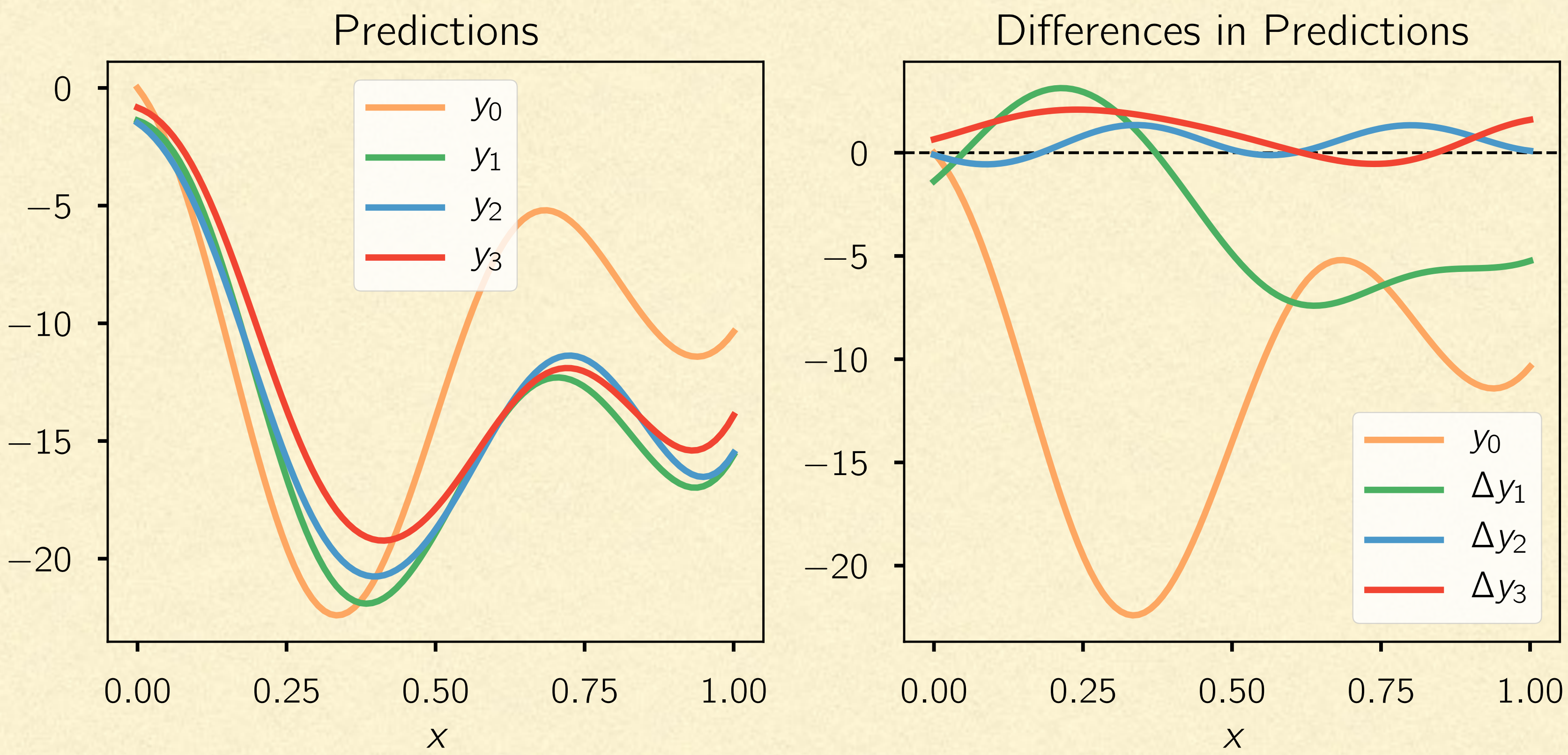

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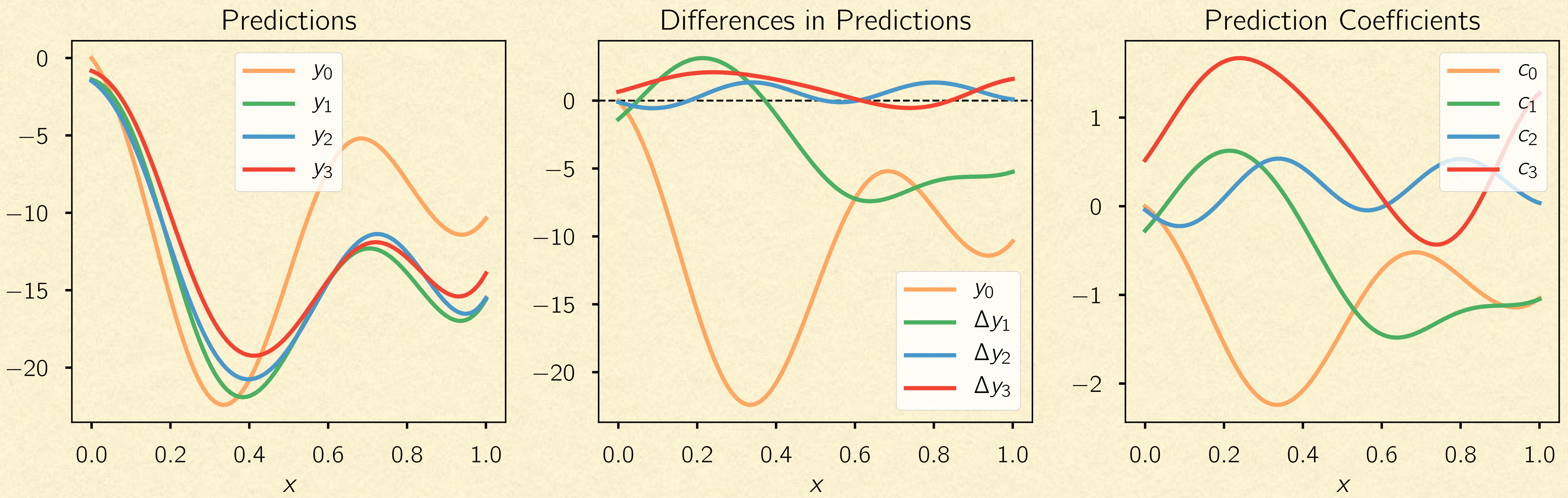

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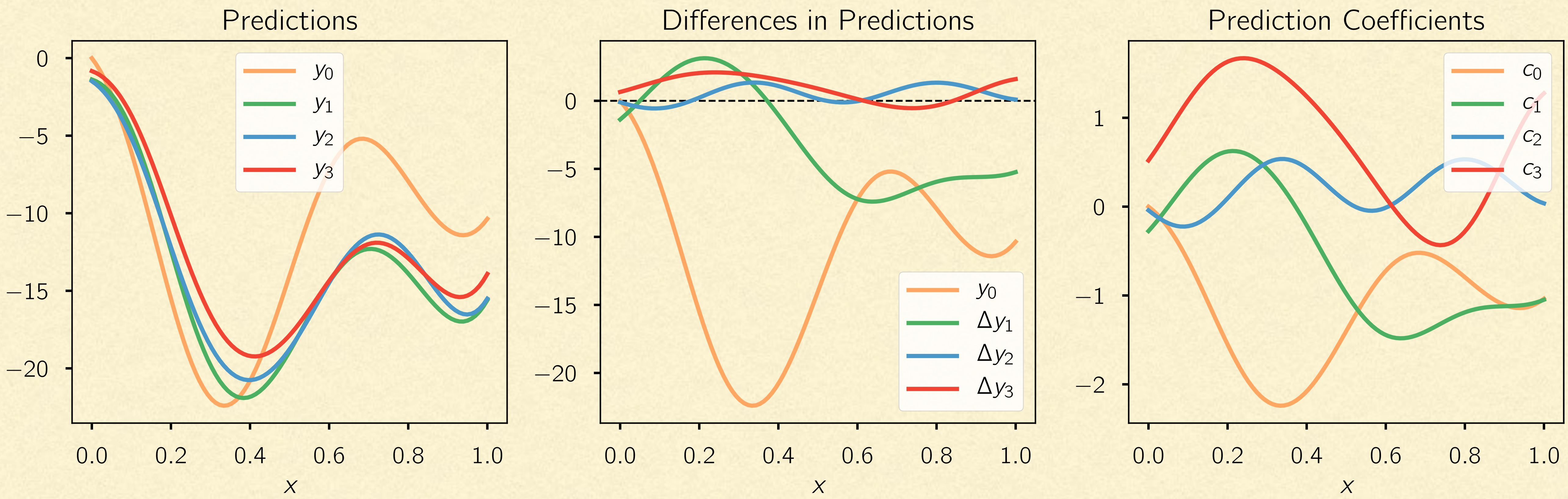

This is what a healthy observable expansion looks like: bounded coefficients, that do not grow or shrink with order.

Bayesian EFT Parameter Estimation

$$X(p) = X_0(p) \sum_{i=0}^{k} c_i(\{a_j\}) x^i$$

Bayesian EFT Parameter Estimation

- General EFT series for observable to order k: $X(p) = X_0(p) \sum_{i=0}^{k} c_i(\{a_j\}) x^i$
- Truncation error=$X_0(p)\ c_{k+1}\ x^{k+1}$ + ...
- Posterior for parameters **a**={a_0,...,a_k} by marginalizing:

$$\mathrm{pr}(\mathbf{a}|D,k,k_{\mathrm{max}}) = \int dc_{k+1} \ldots dc_{k_{\mathrm{max}}} \mathrm{pr}(\mathbf{a}, c_{k+1}, \ldots, c_{k_{\mathrm{max}}}|D,k,k_{\mathrm{max}})$$

and Bayesing $= \int dc_{k+1} \ldots dc_{k_{\mathrm{max}}} \dfrac{\mathrm{pr}(D|\mathbf{a}, c_{k+1}, \ldots, c_{k_{\mathrm{max}}}, k, k_{\mathrm{max}})\mathrm{pr}(\mathbf{a}|\bar{a}_{\mathrm{fix}}) \prod_{j=k+1}^{k_{\mathrm{max}}} \mathrm{pr}(c_j|\bar{c}_{\mathrm{fix}})}{\mathrm{pr}(D|k,k_{\mathrm{max}})}$

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- Marginalization over c's produces revised correlation matrix in standard likelihood, accounts for uncertainties (and correlation structure) induced by omitted terms

$$\mathrm{pr}(\mathbf{a}\,|\,D) \propto \exp\left(-\frac{1}{2}\mathbf{r}^T(\mathbf{\Sigma}_{\mathrm{exp}}+\mathbf{\Sigma}_{\mathrm{th}})^{-1}\mathbf{r}\right)\exp\left(-\frac{\mathbf{a}^2}{2\bar{a}^2}\right) \qquad \mathbf{r} \equiv \mathbf{y}_{\mathrm{exp}} - \mathbf{y}_{\mathrm{th}}$$

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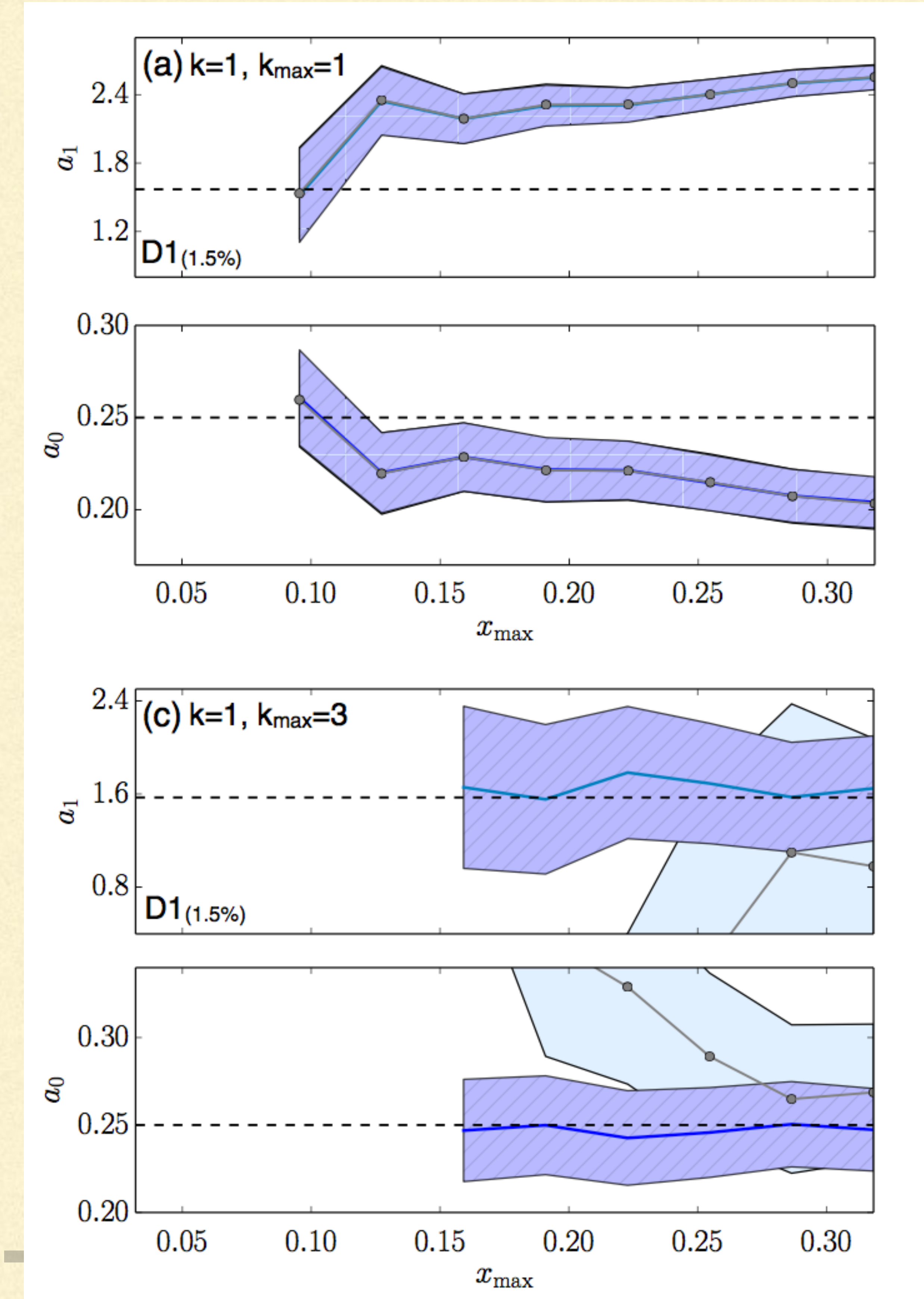
- Normal distribution for LECs. Here we take a fixed $\bar{a}$, could also marginalize over it.

Truncation Errors Help



Wesolowski et al., JPG (2016)

$$(\boldsymbol{\Sigma}_{\text{th,corr}})_{ij} = (\mathbf{y}_{\text{ref}})_i(\mathbf{y}_{\text{ref}})_j\bar{c}^2 \sum_{n=k+1}^{k_{\text{max}}} x_i^n x_j^n$$

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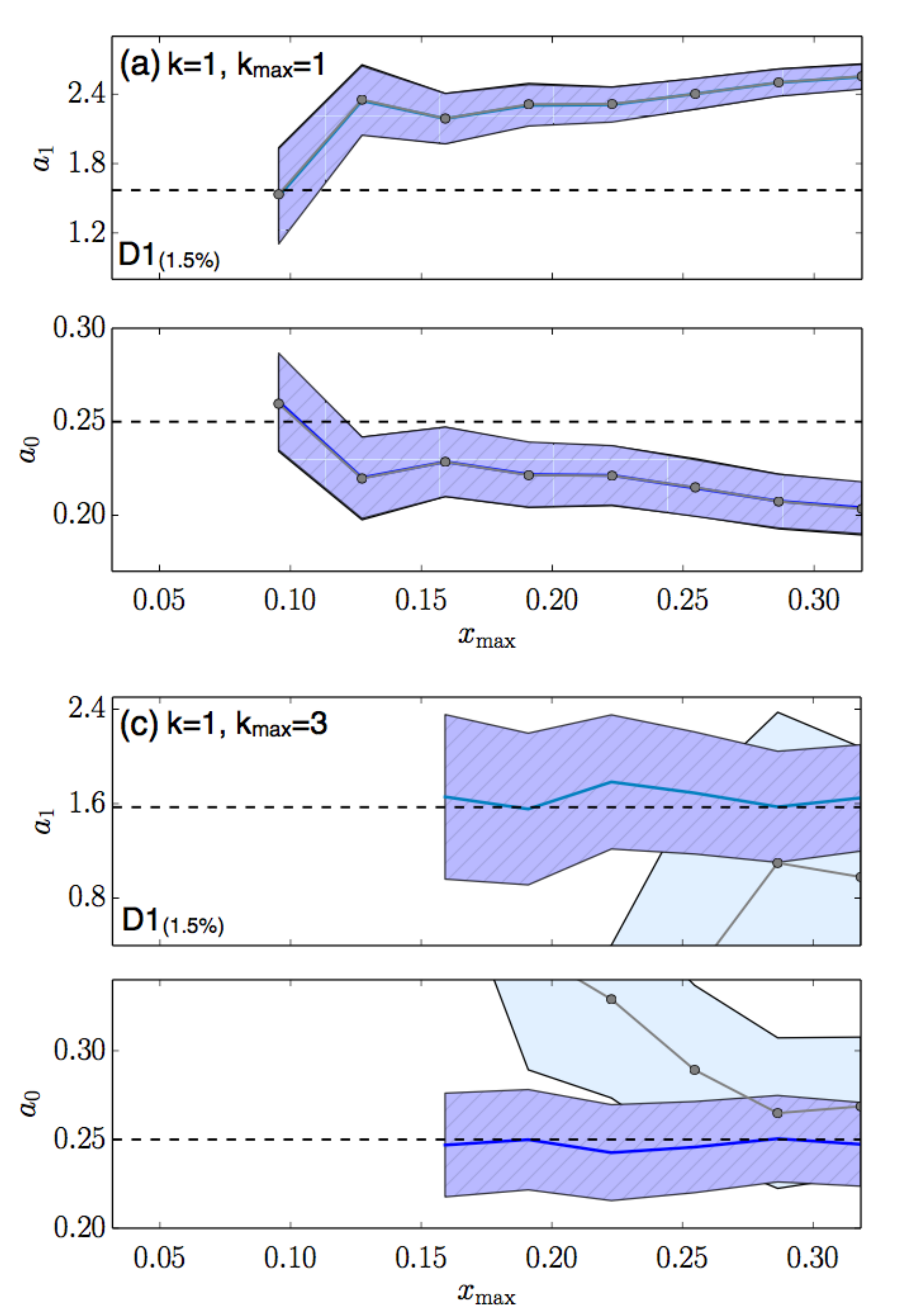

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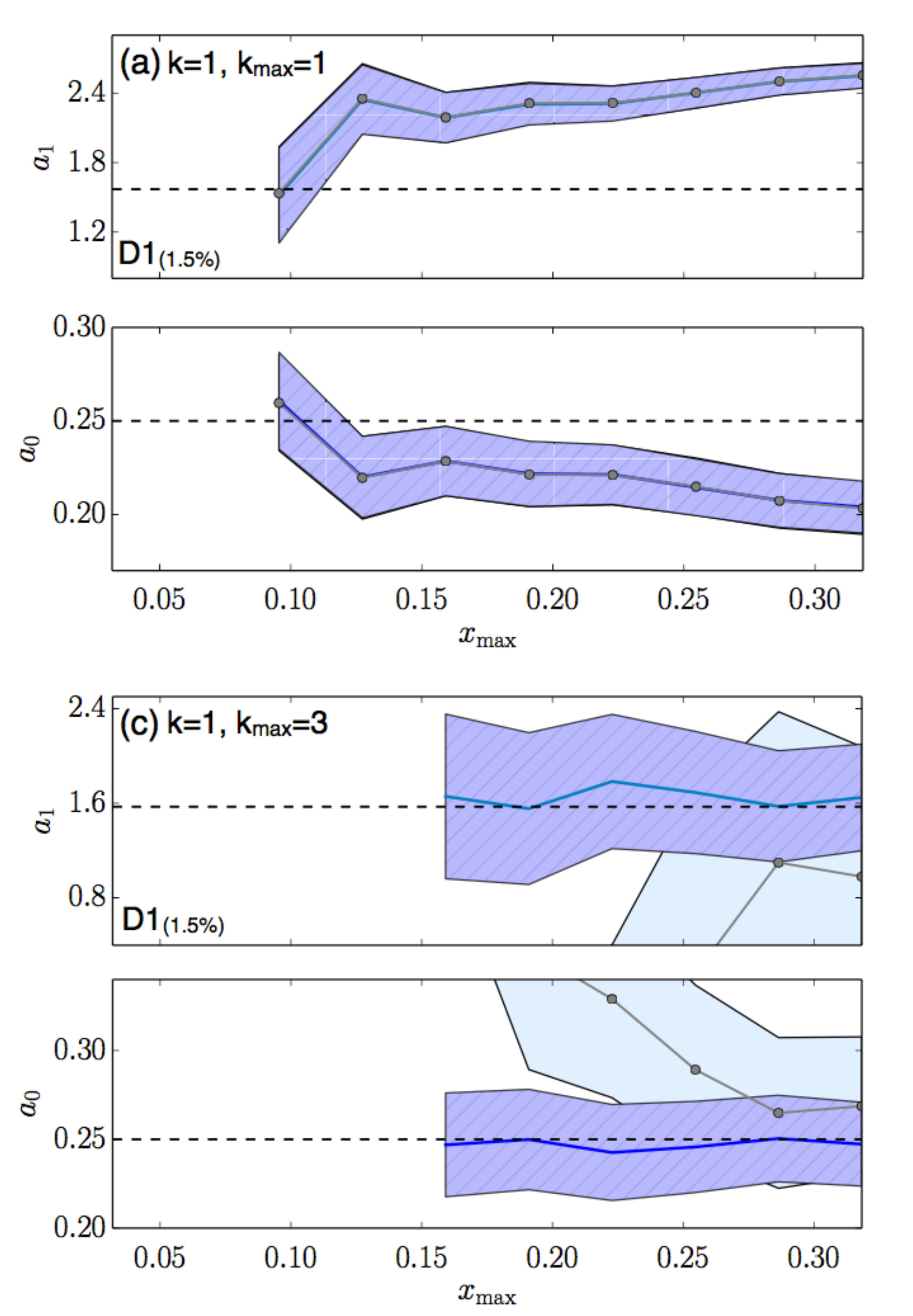

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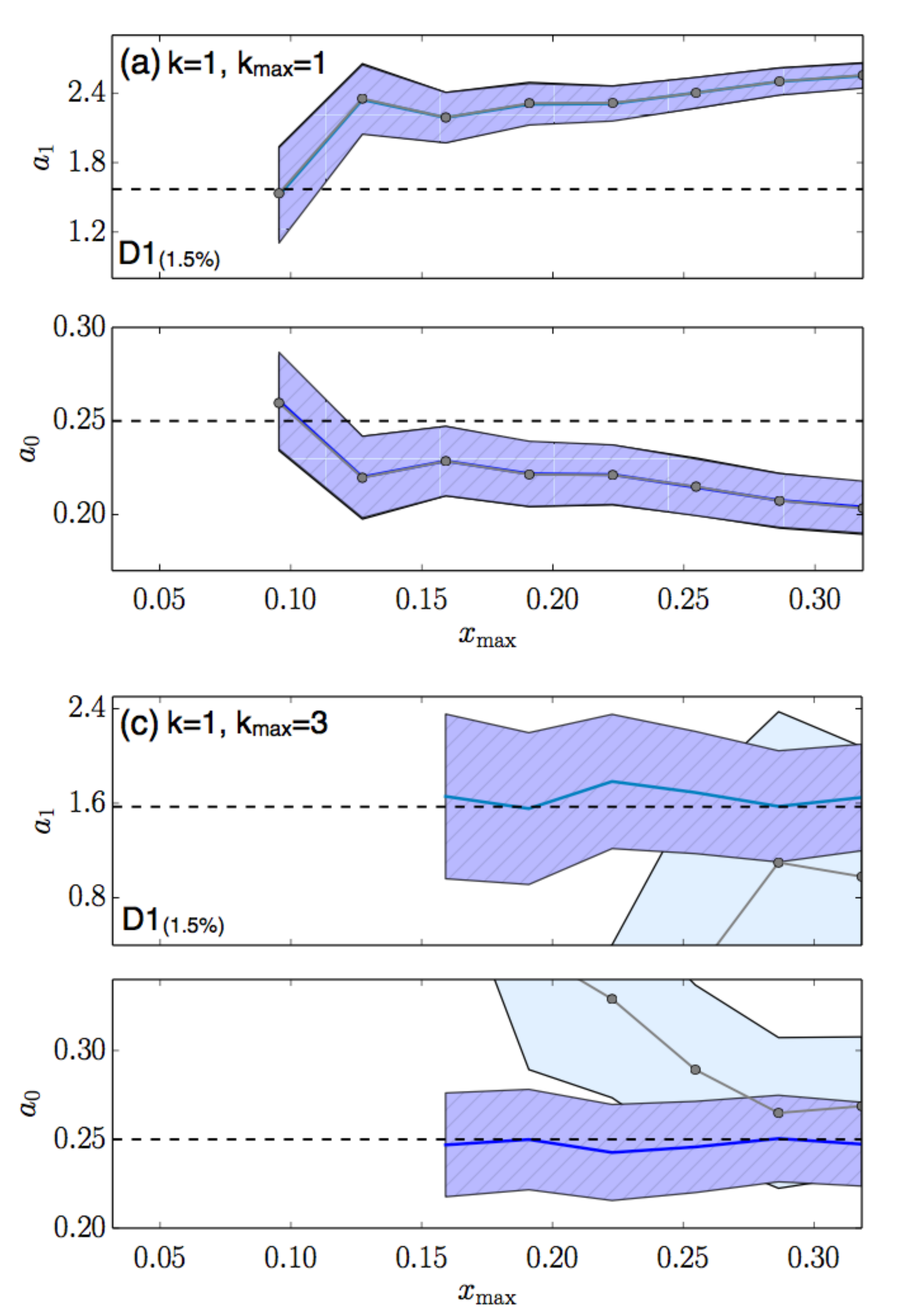

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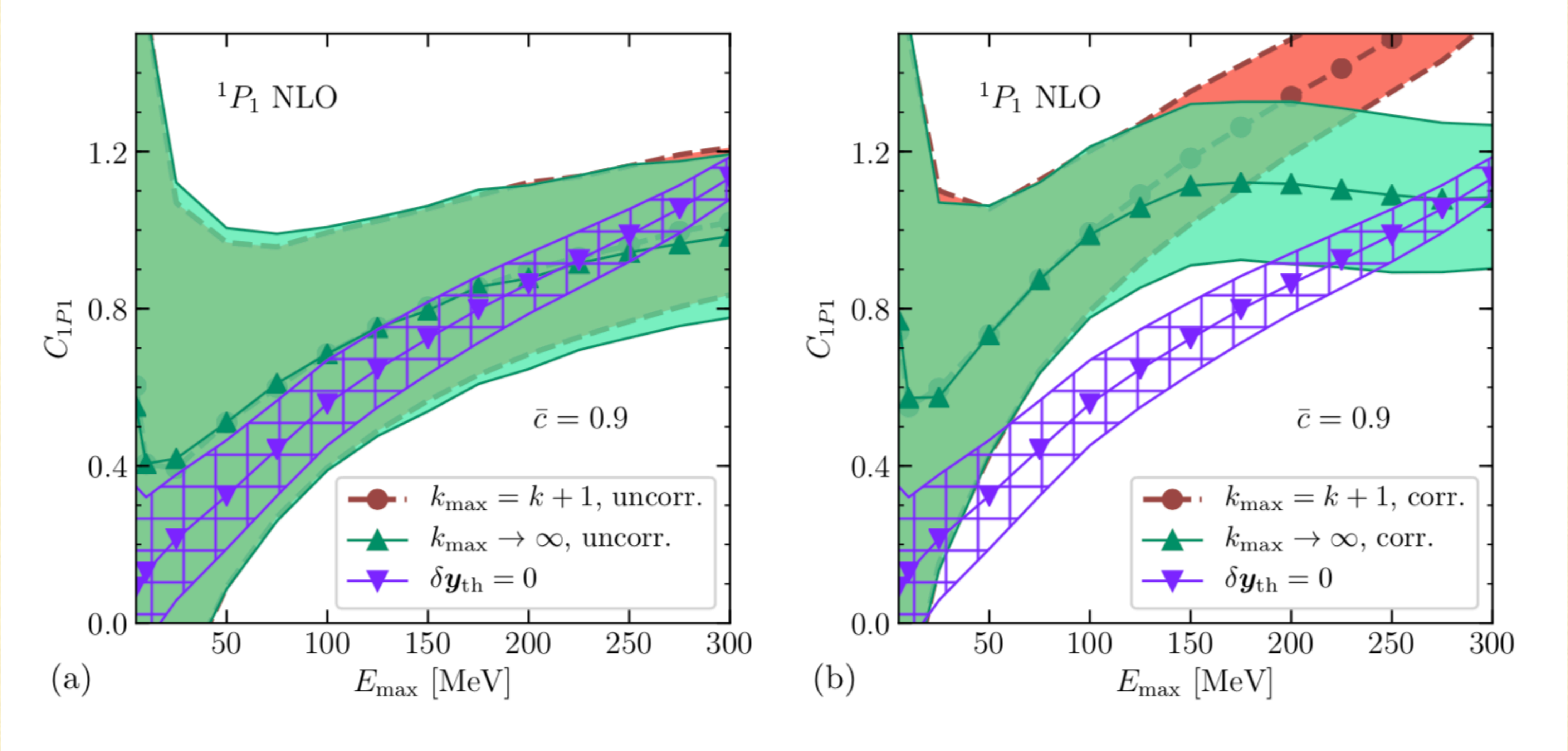
- Lack of stability for $k=k_{max}=1$. Underfitting.
- $k=1$, $k_{max}=3$: once truncation errors are incorporated correct result is achieved earlier, and with smaller error bars, than for uniform-prior (least-squares) result

E_{max} plots for NN

Wesolowski, Furnstahl, Melendez, DP, JPG (2019)

Epelbaum, Krebs, Meißner, EPJA 51, 53 (2015)

- EKM semi-local potential with R=0.9 fm



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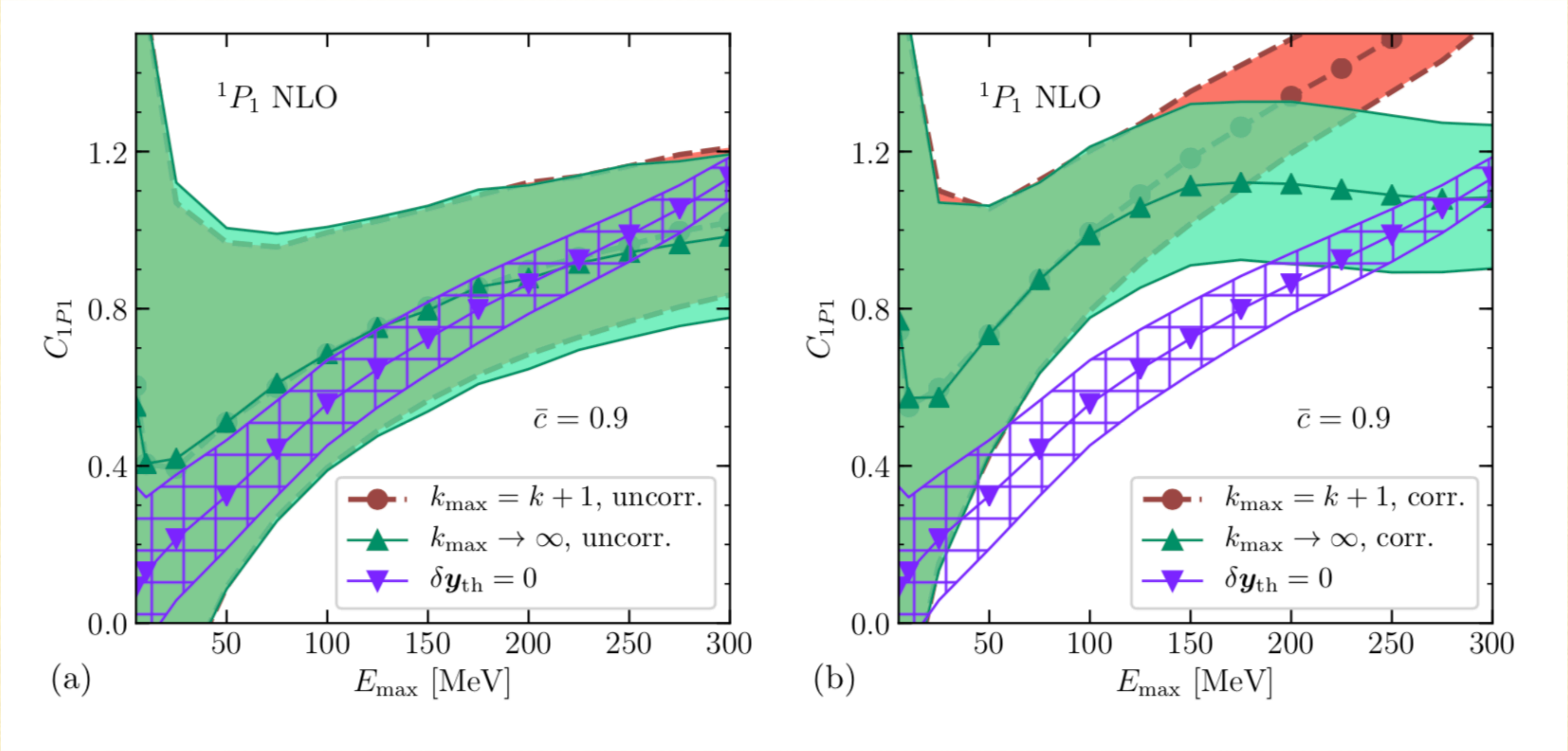

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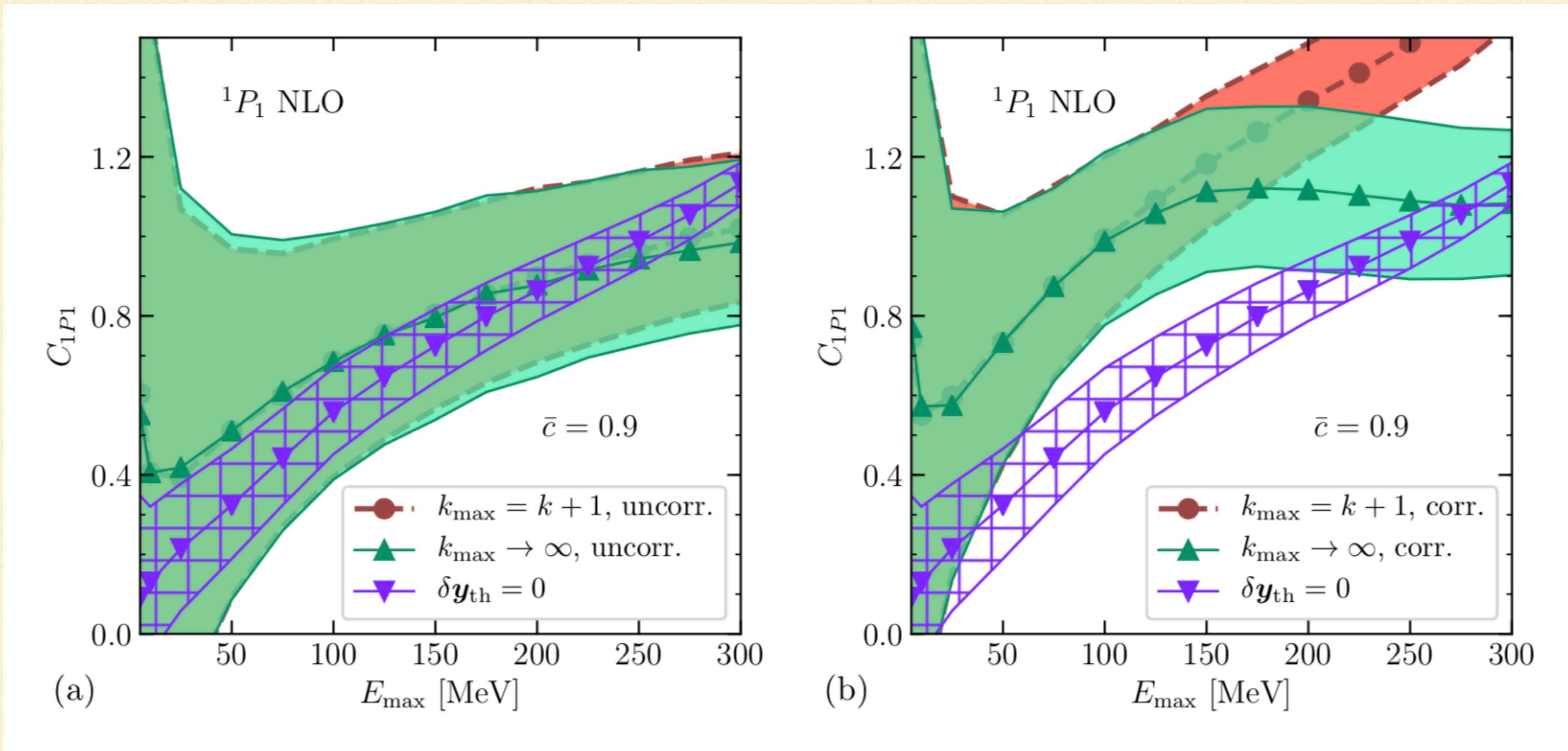

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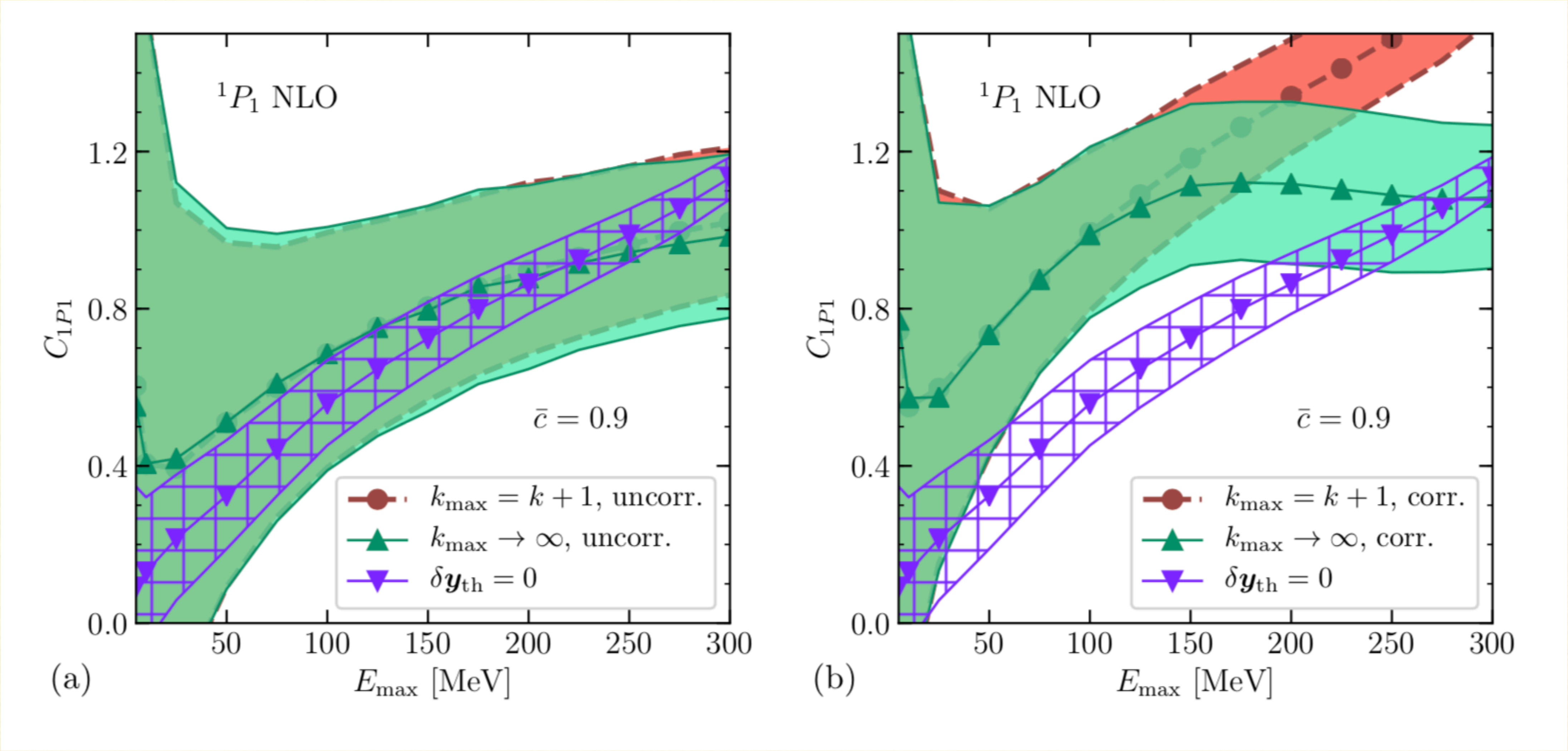

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- Can resum truncation error to all orders (under assumptions about its correlation across orders): tests validity of FOTA

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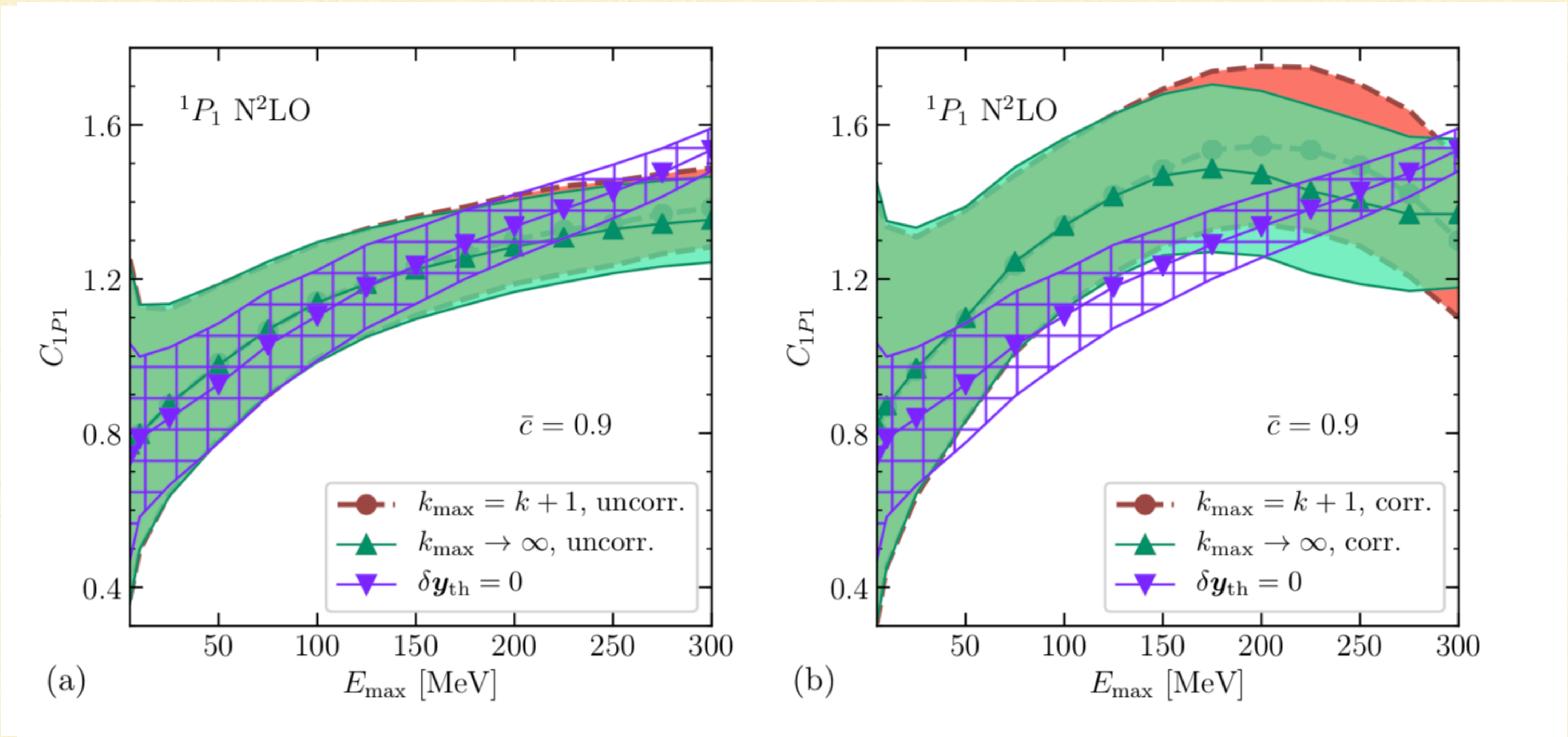

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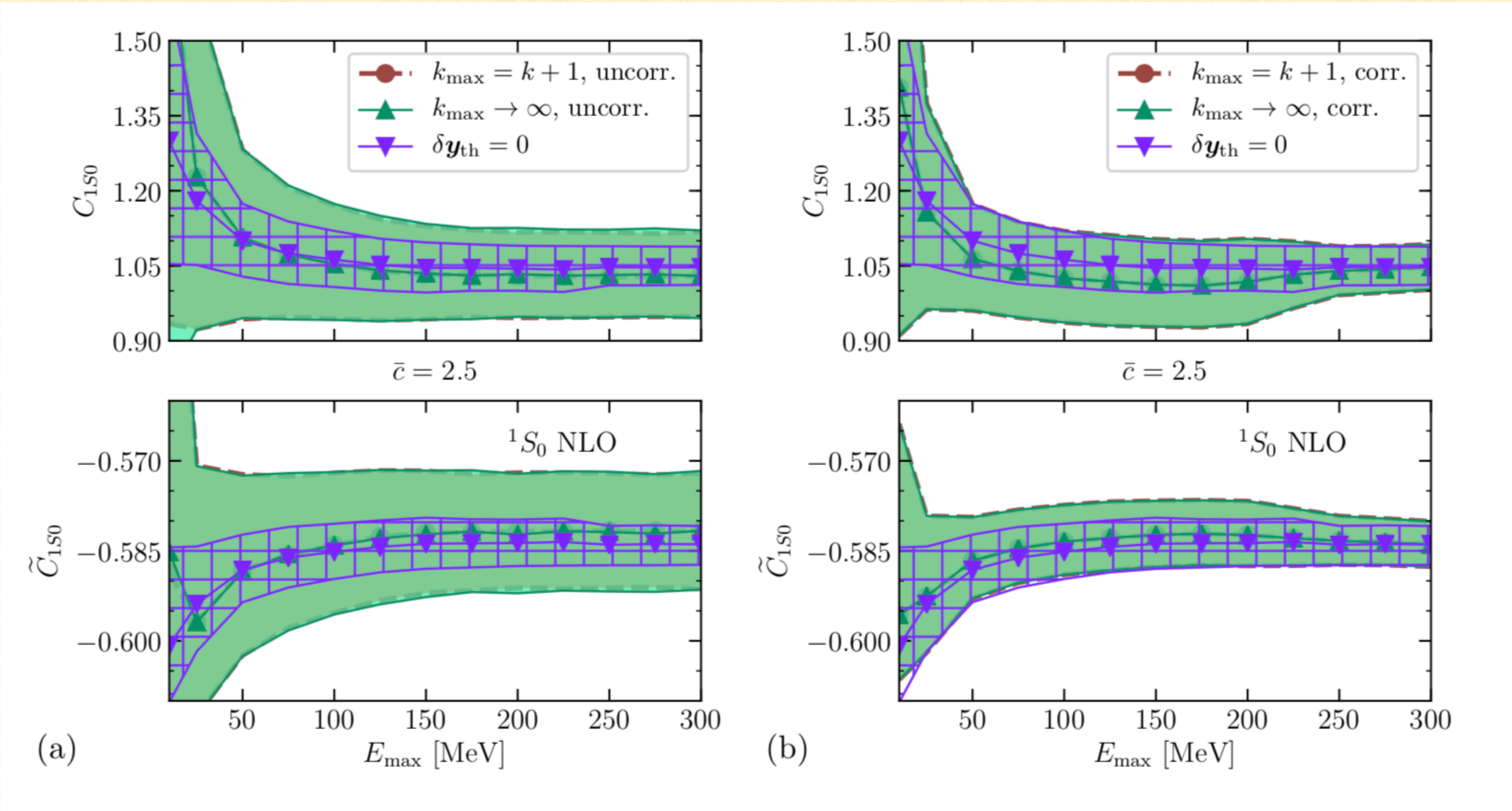
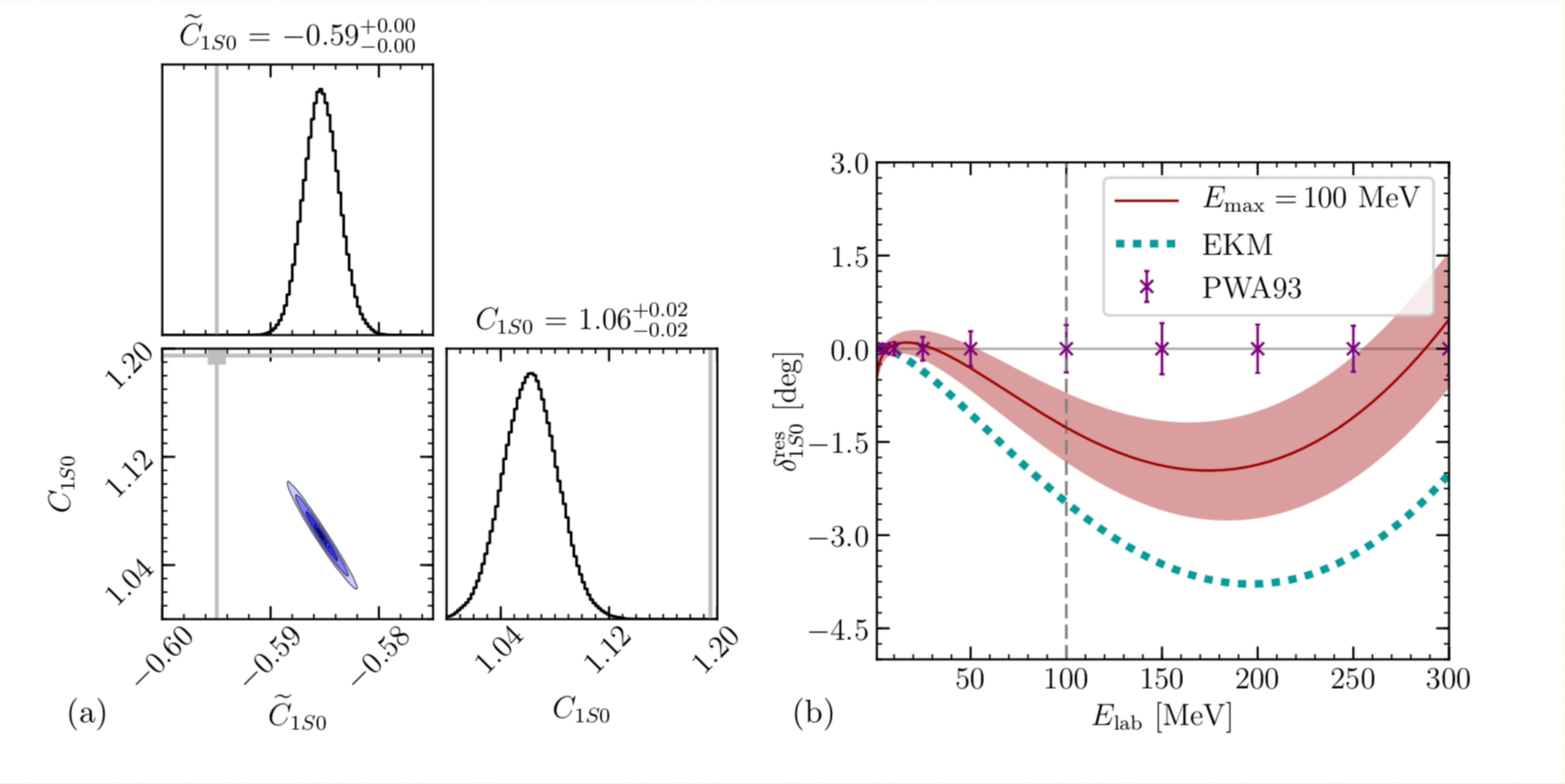
E_{max} plot in the $^1S_0$ at NLO

NLO potential in $^1S_0$ channel $V^{(2)}_{1S0}(p',p) = \frac{4\pi}{f_\pi^2}\left(\tilde{C}^{np}_{1S0} + C_{1S0}\frac{p^2+p'^2}{\Lambda_b^2}\right)$



Changes in Parameter Estimates



Including truncation errors changes central values and (esp.) errors

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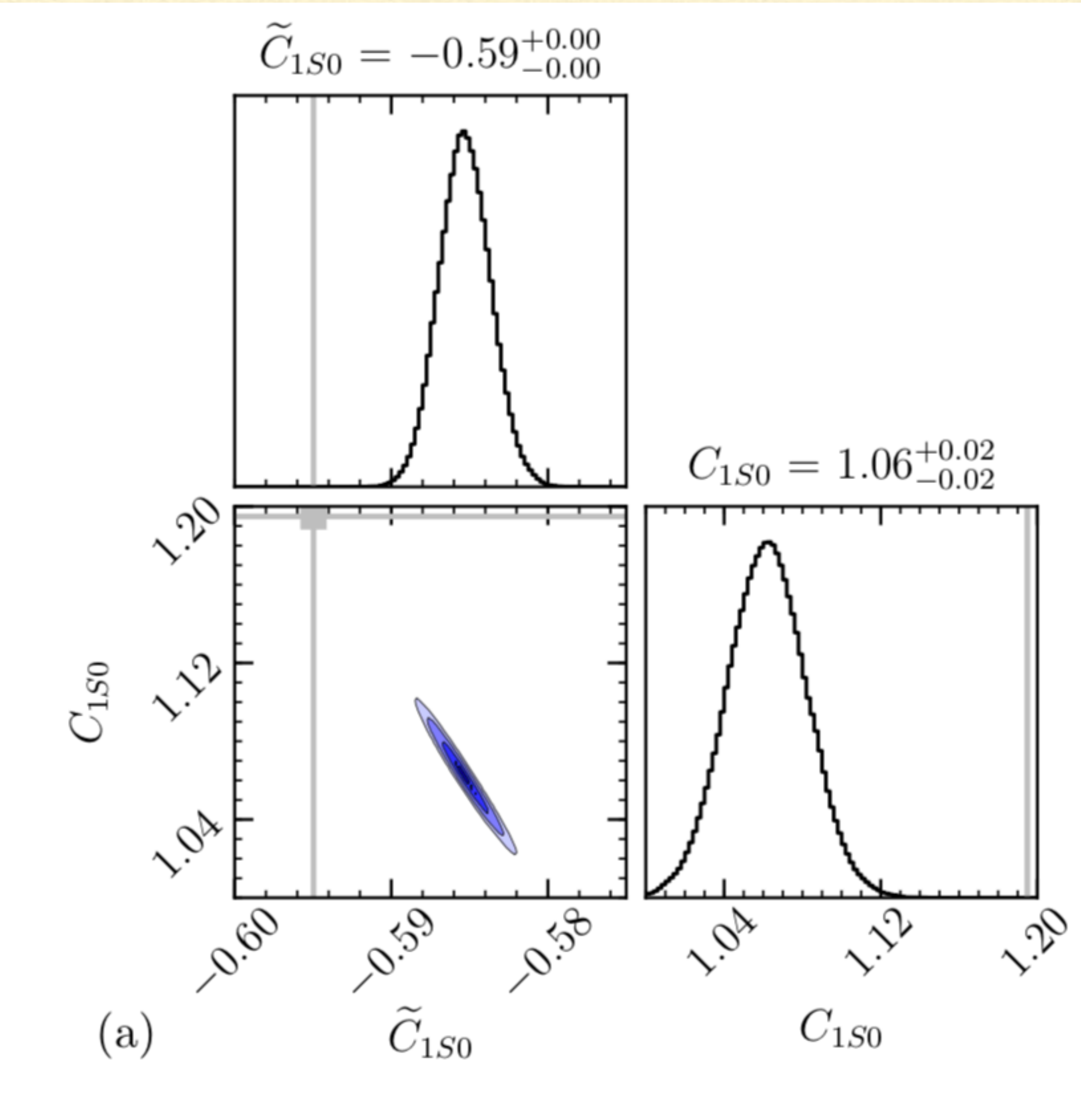

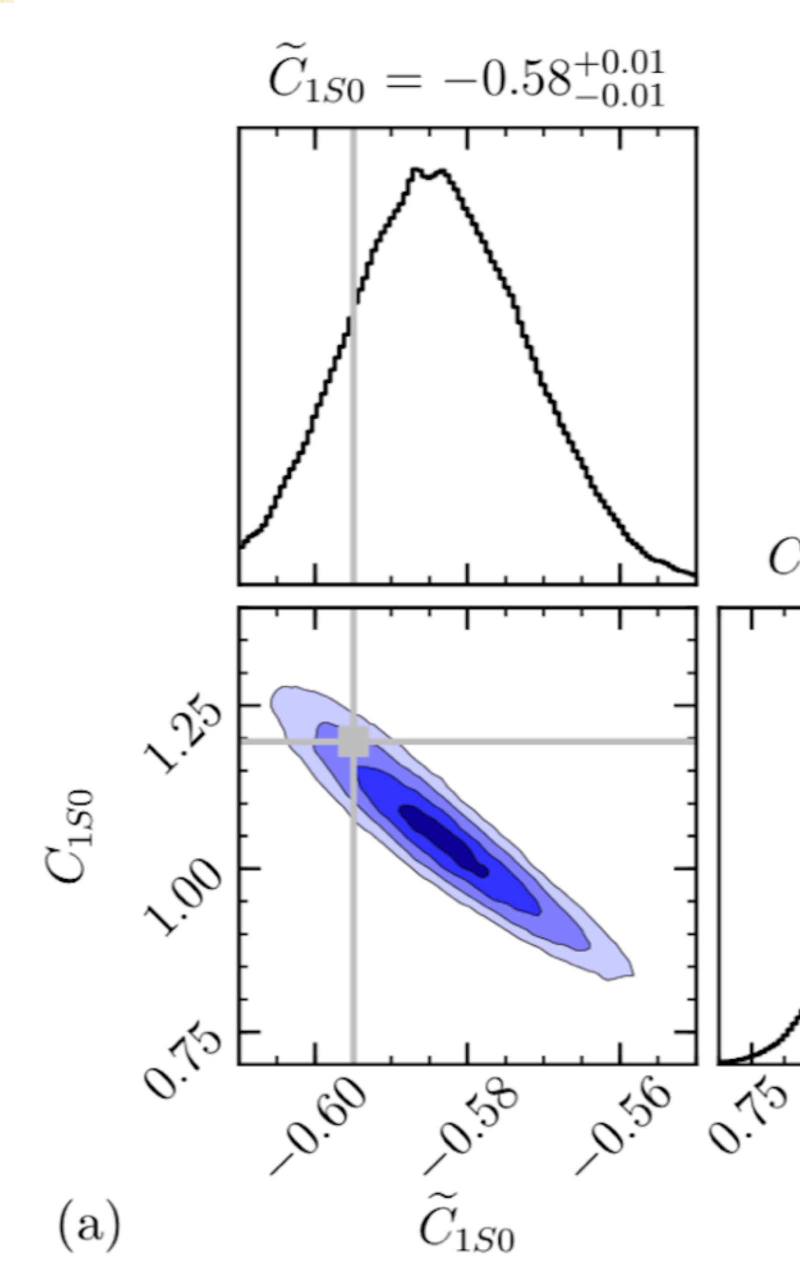

Uncorrelated

Λ_b=600 MeV

Including truncation errors changes central values and (esp.) errors

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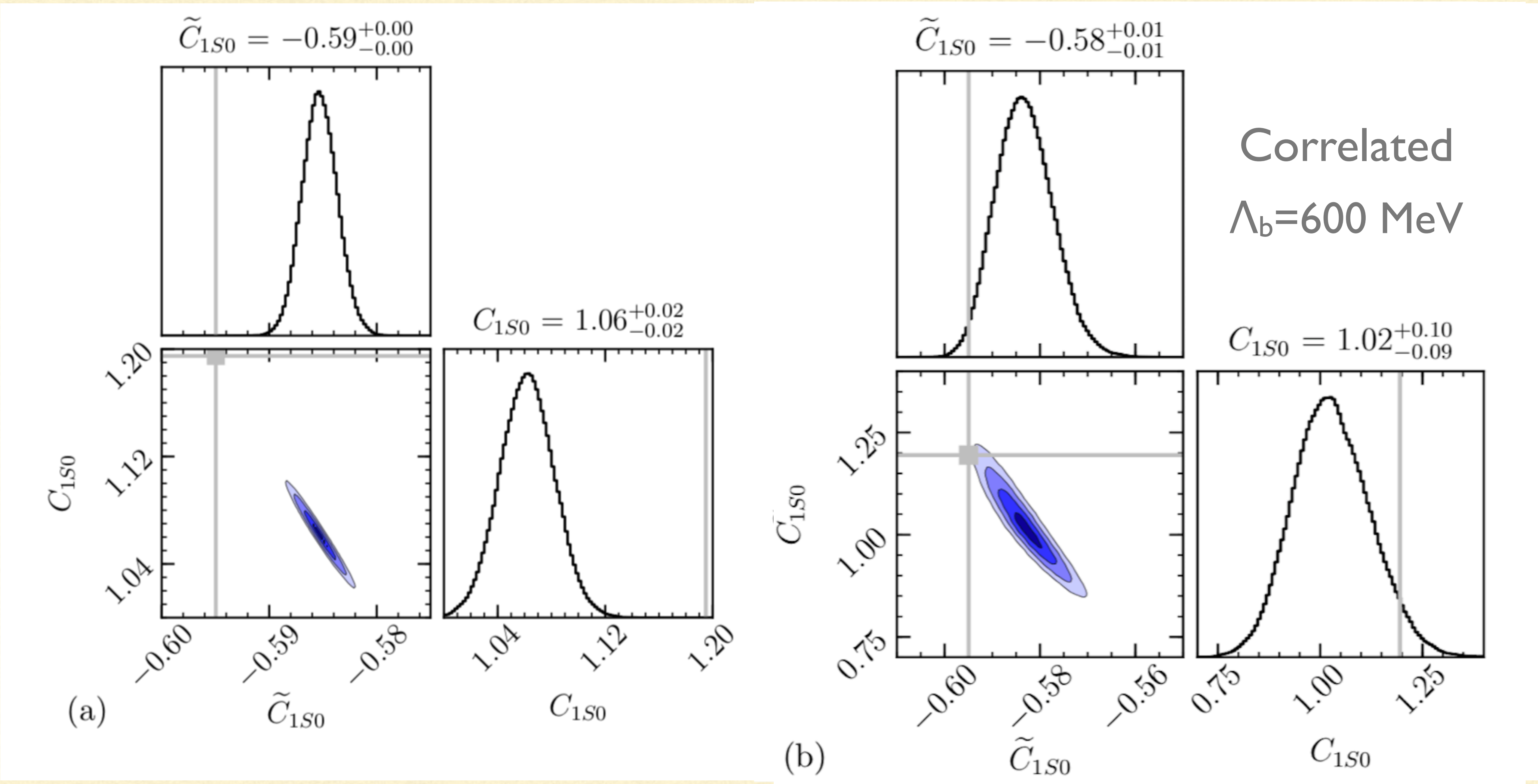

Including truncation errors changes central values and (esp.) errors

NN scattering

Epelbaum, Krebs, Meißner, PRC, 2015

Employ "semi-local" potentials of Epelbaum, Krebs, and Meißner

χEFT: $\mathscr{L}(N,\pi) \to V^{(k)} \to \delta \to \sigma_{np}$

$$\sigma_{np}(E_{\mathrm{lab}}) = \sigma_{\mathrm{LO}} \sum_{n=0}^{k} c_n(p_{\mathrm{rel}}) \left(\frac{p_{\mathrm{rel}}}{\Lambda_b}\right)^n$$

$$x = \frac{p_{\mathrm{rel}}}{\Lambda_b}$$

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χEFT: $\mathscr{L}(N,\pi) \to V^{(k)} \to \delta \to \sigma_{np}$

- NN cross section at T_{lab}=50, 96, 143, 200 MeV
- Potential regulated by local function, parameterized by R
- EKM identify Λ_b=600 MeV for smaller R values
- Here: R=0.9 fm data
- Results at LO, NLO, N²LO, N³LO, N⁴LO (k=0, 2, 3, 4, 5)

$$\sigma_{np}(E_{\rm lab}) = \sigma_{\rm LO} \sum_{n=0}^{k} c_n(p_{\rm rel}) \left(\frac{p_{\rm rel}}{\Lambda_b}\right)^n$$

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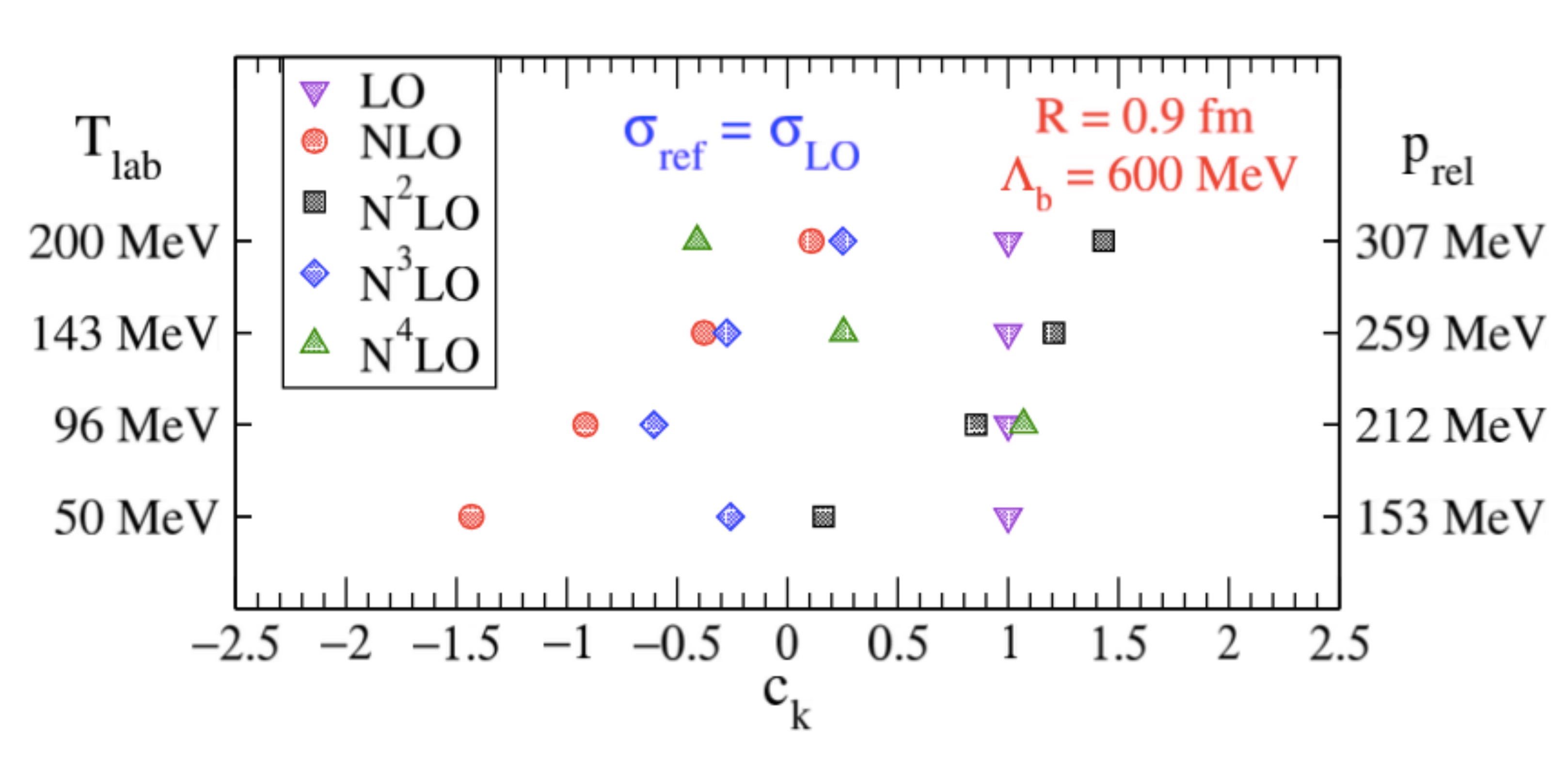

EFT truncation error model checking

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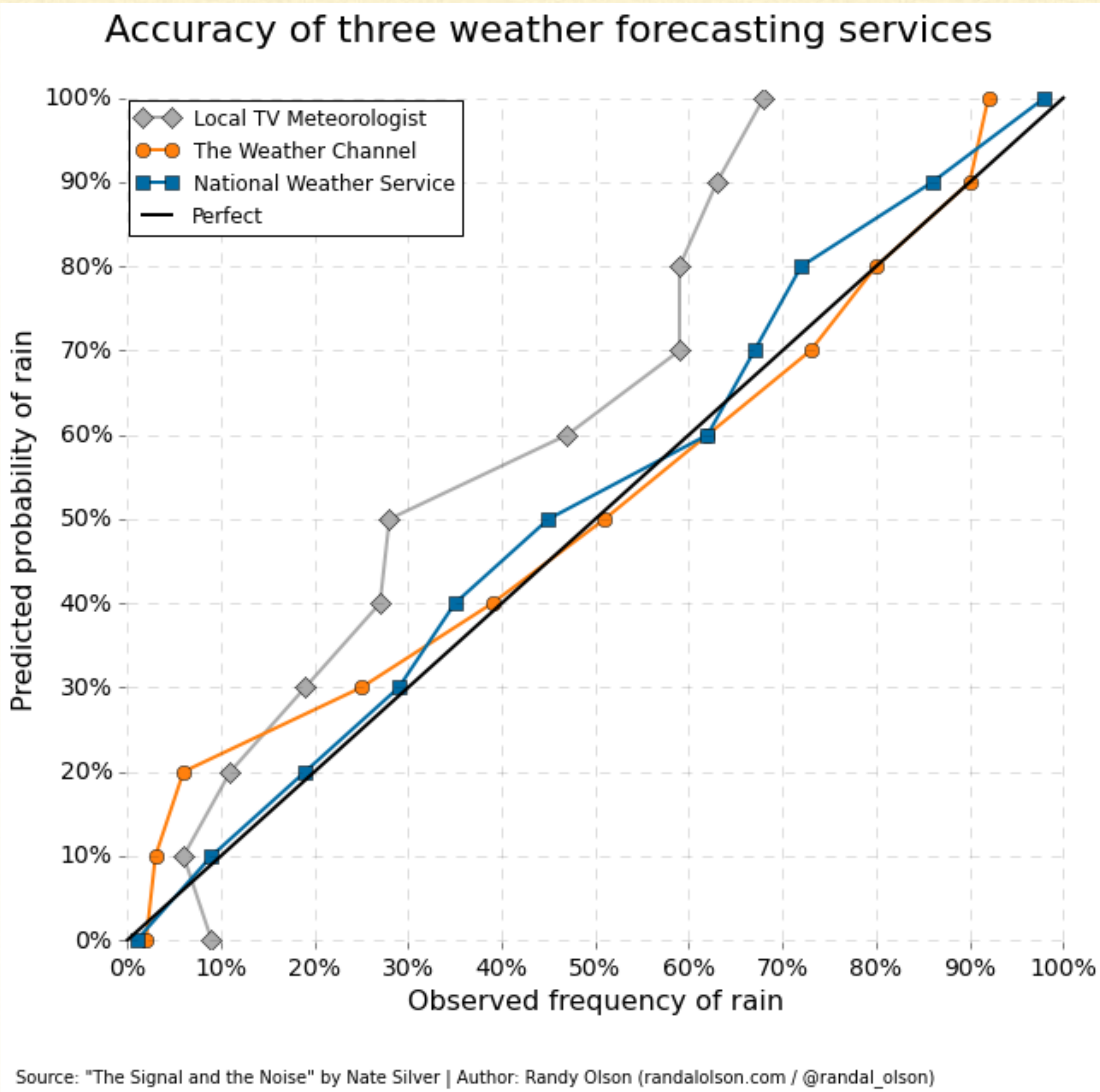

Melendez, Furnstahl, Wesolowski, PRC, 2017
after Furnstahl, Klco, DP, Wesolowski, PRC, 2015
after Bagnaschi, Cacciari, Guffanti, Jenniches, 2015

- 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

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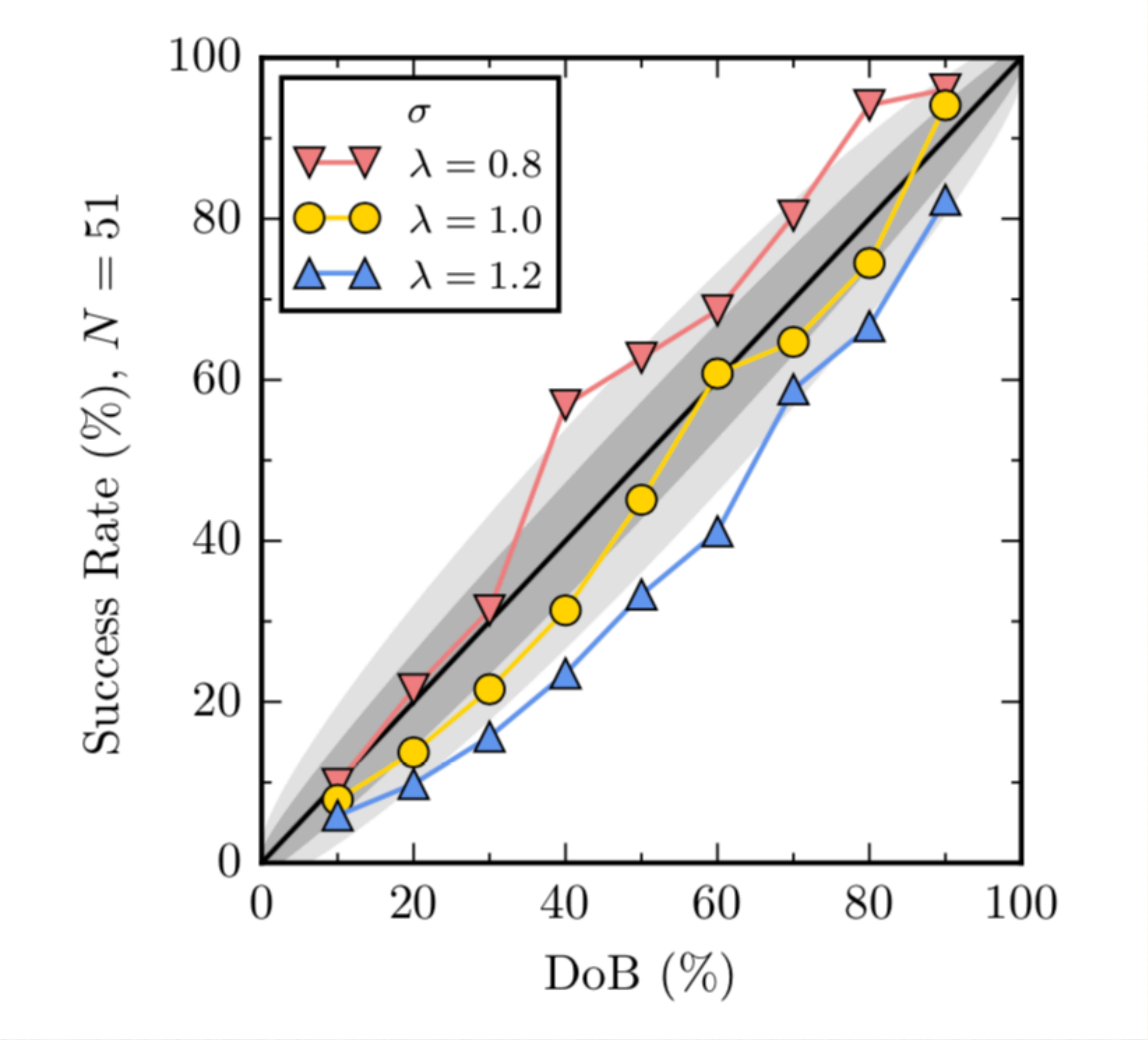

- Consider predictions at each order, with their error bars, as data and test them to see if the procedure is consistent
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- Look at this for EKM predictions at three different orders and 17 different energies
- Interpret in terms of rescaling of Λ_b by a factor λ

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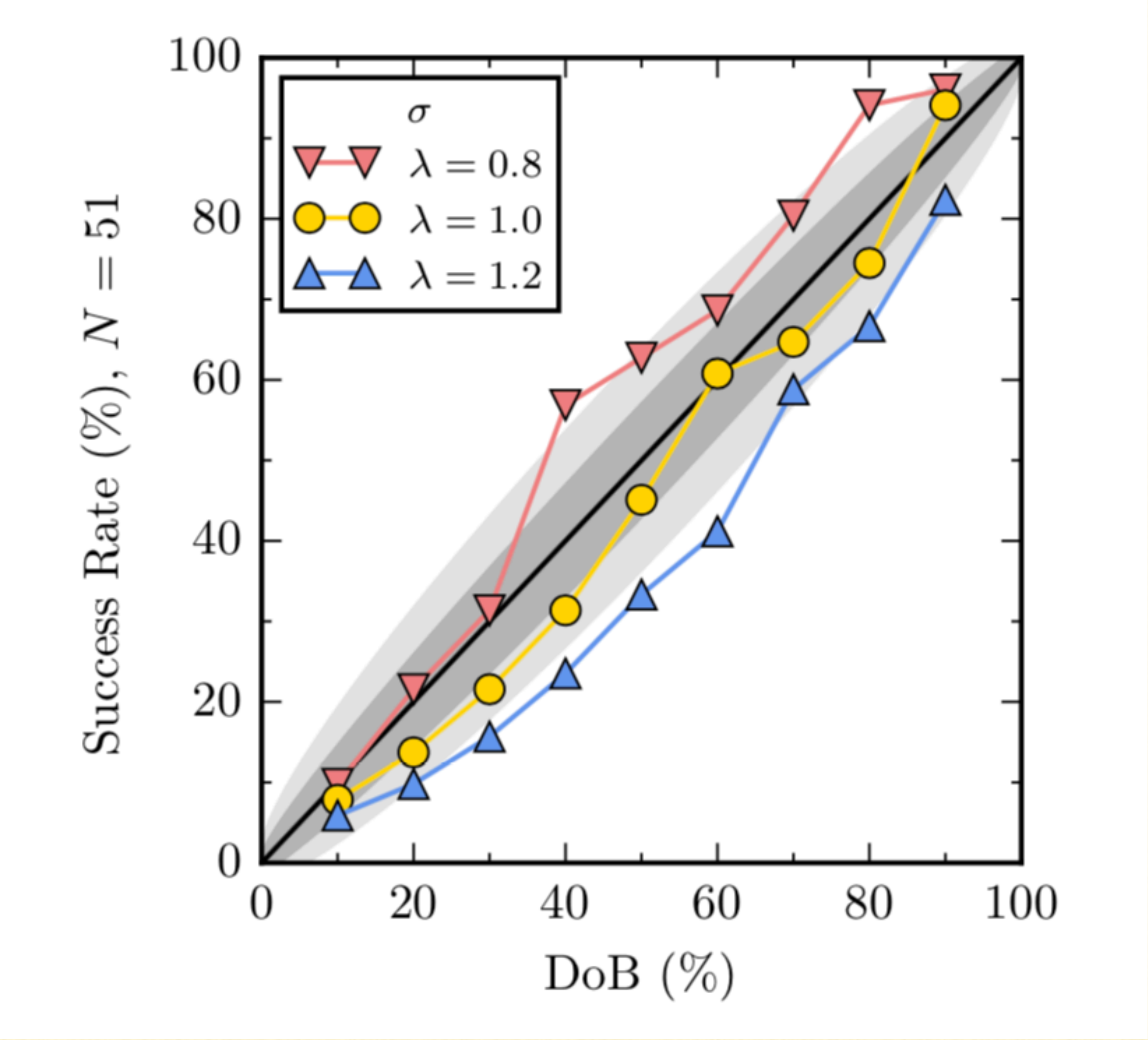

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No evidence for significant rescaling of Λ_b

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 $\mathrm{pr}(c_n|c_0, c_1, \ldots, c_k)$: 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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At one energy:

$$\mathrm{pr}(\Lambda_b|b_2,\ldots,b_k) \propto \frac{1}{\Lambda_b}\left(\frac{\Lambda_b^{k+2}}{(k+1)\langle b^2\rangle}\right)^{\frac{k-1}{2}}$$

(NLO: k=2, NNLO: k=3, N^3LO: k=4, etc.)

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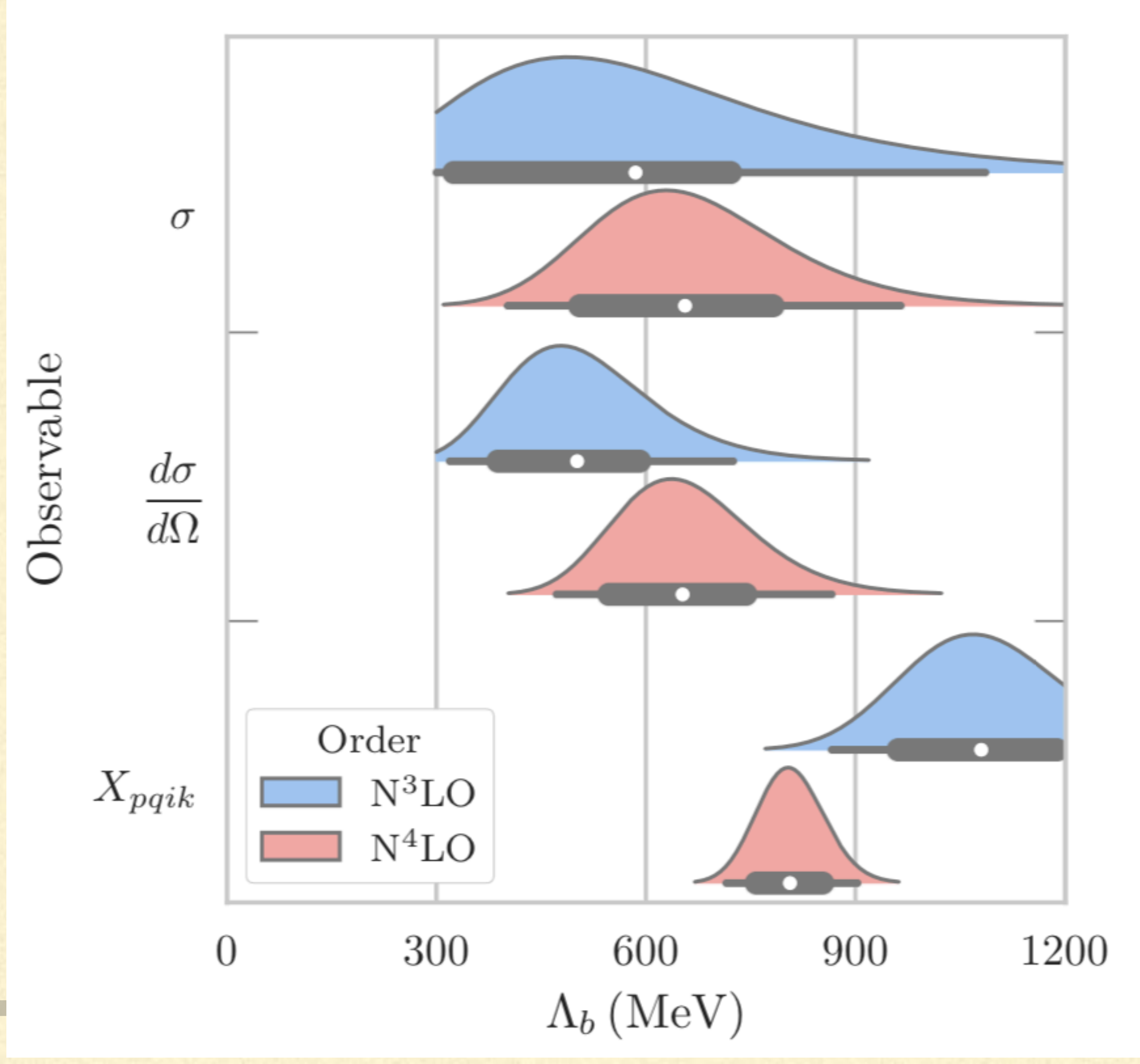
Using 5 energies (and 2 angles):



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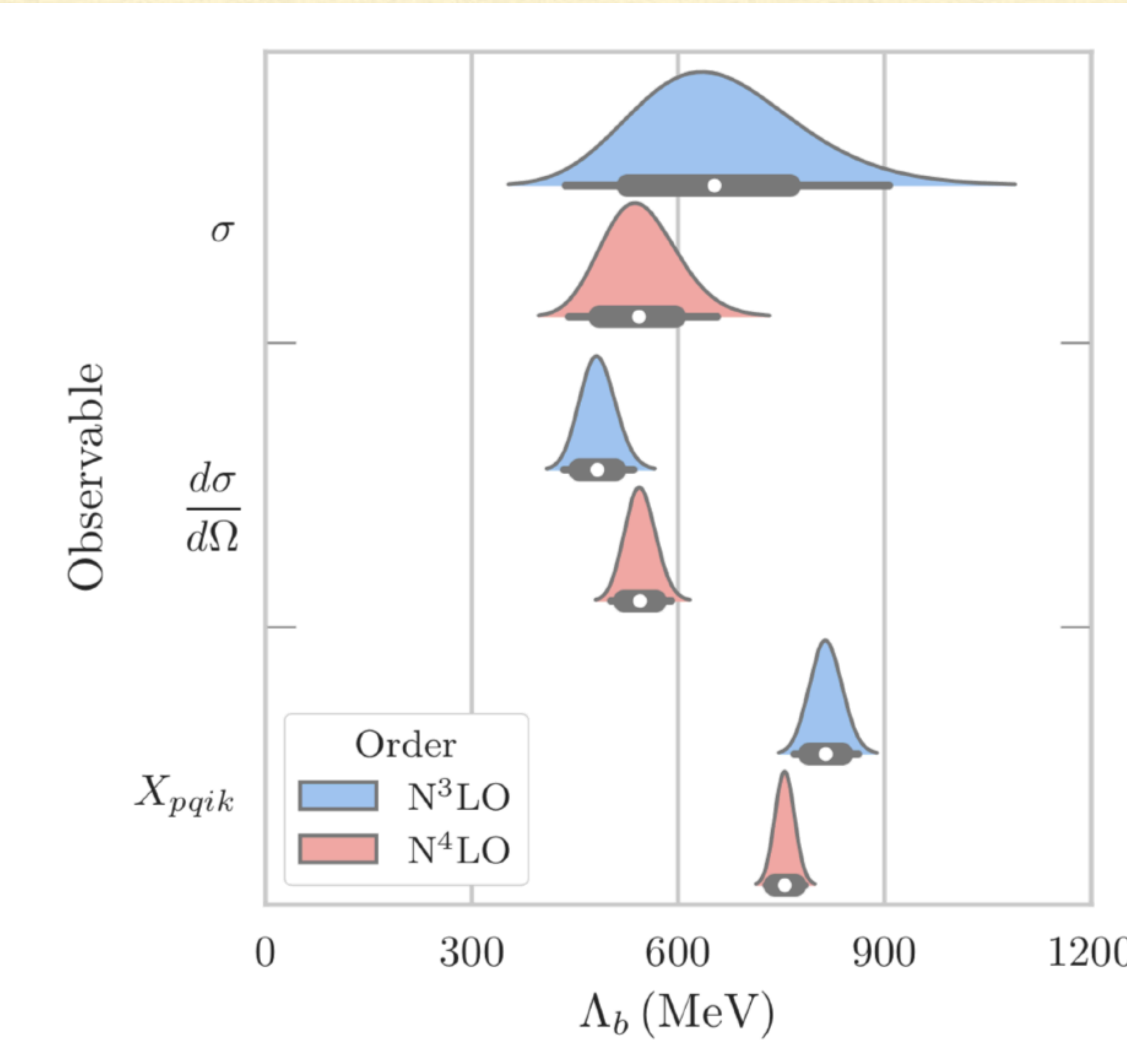
Using 17 energies (and 7 angles):



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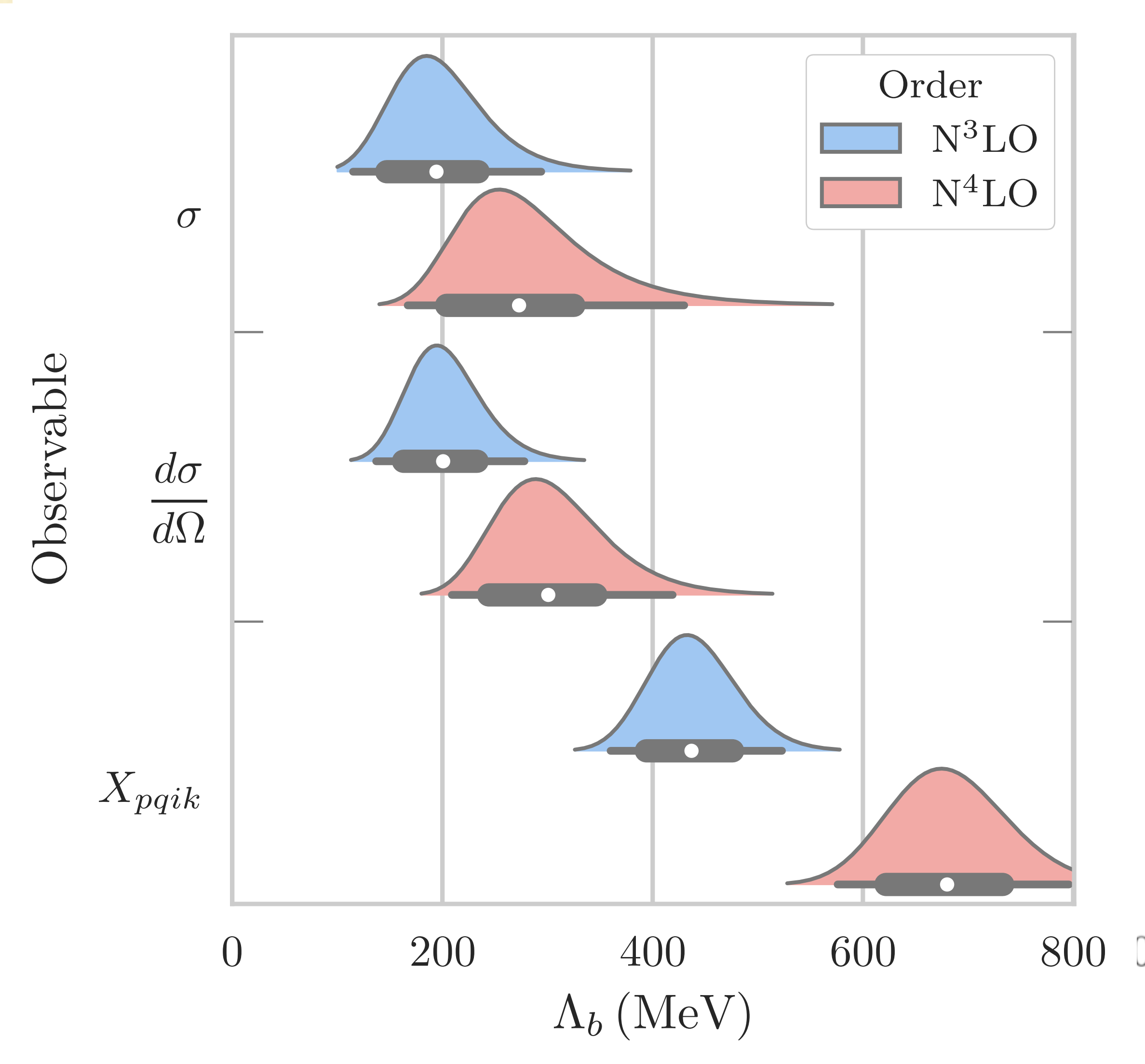
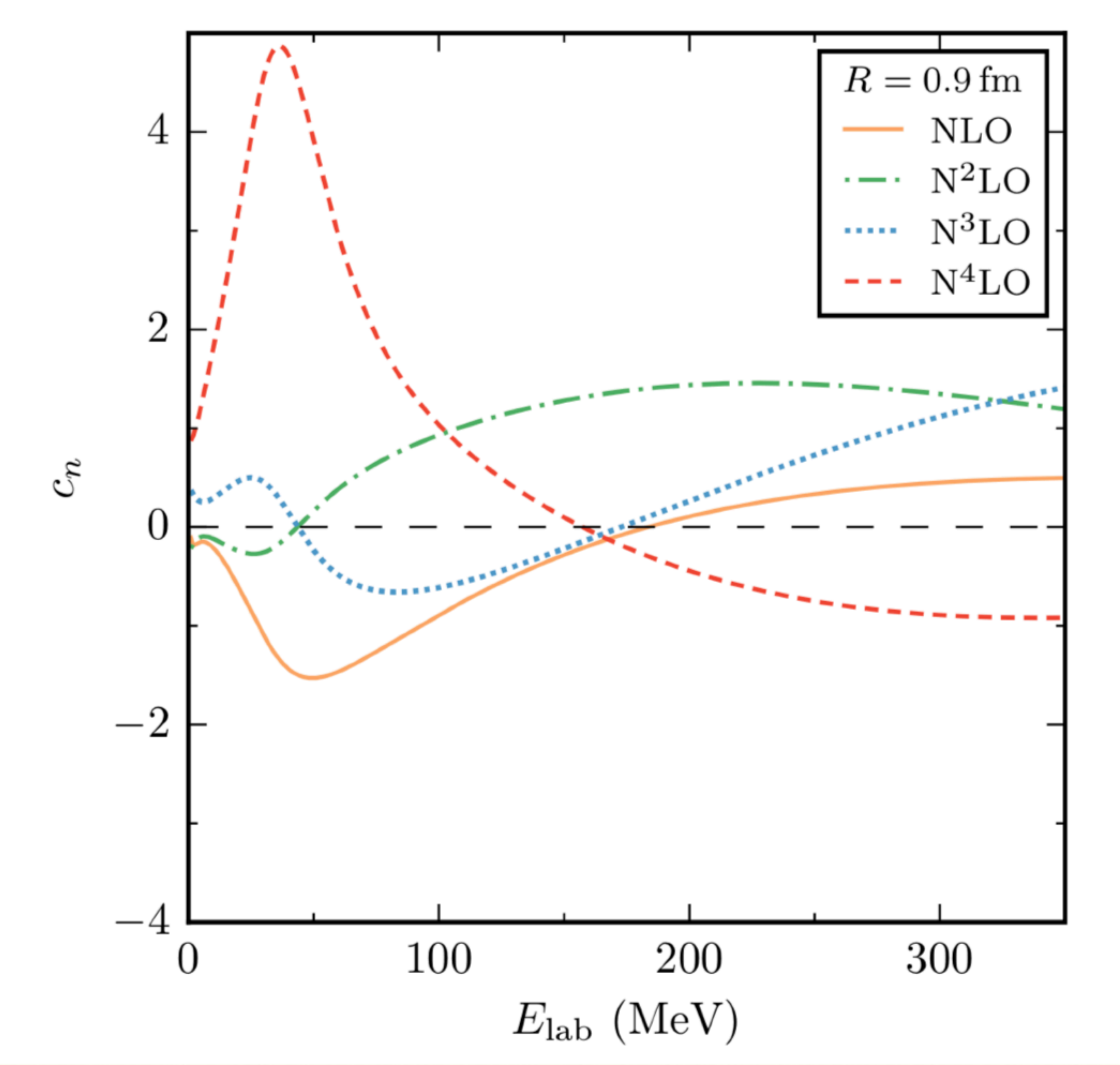
Using 17 energies (and 7 angles):

R=1.2 fm



Functional Data

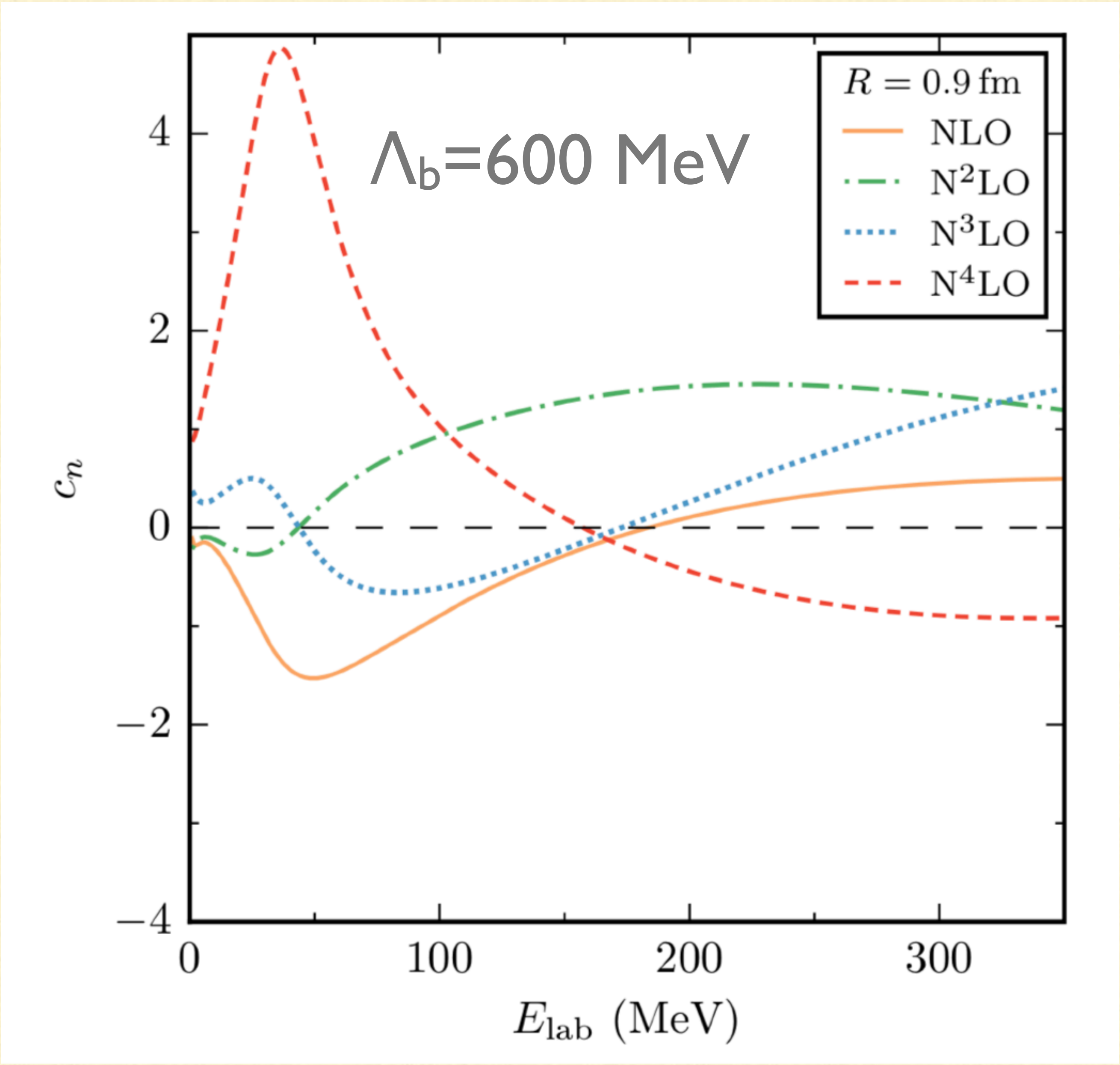
- Truncation-error analysis assumed we have 119 independent data points
- But we don't
- We have a function for each observable at each order
- Can we understand the properties of these functions, and so do Λ_b inference and compute success ratios rigorously?



$$\sigma(E) = \sigma_0(E)\left[1 + c_2(E)x^2 + c_3(E)x^3 + c_4(E)x^4 + c_5(E)x^5\right]$$

Observations and Questions

- c_n's do not grow or shrink with n: good Λ_b choice
- Bounded functions, mostly between -2 and 2
- Each "takes a turn" at being largest
- Not oscillating quickly in this energy range



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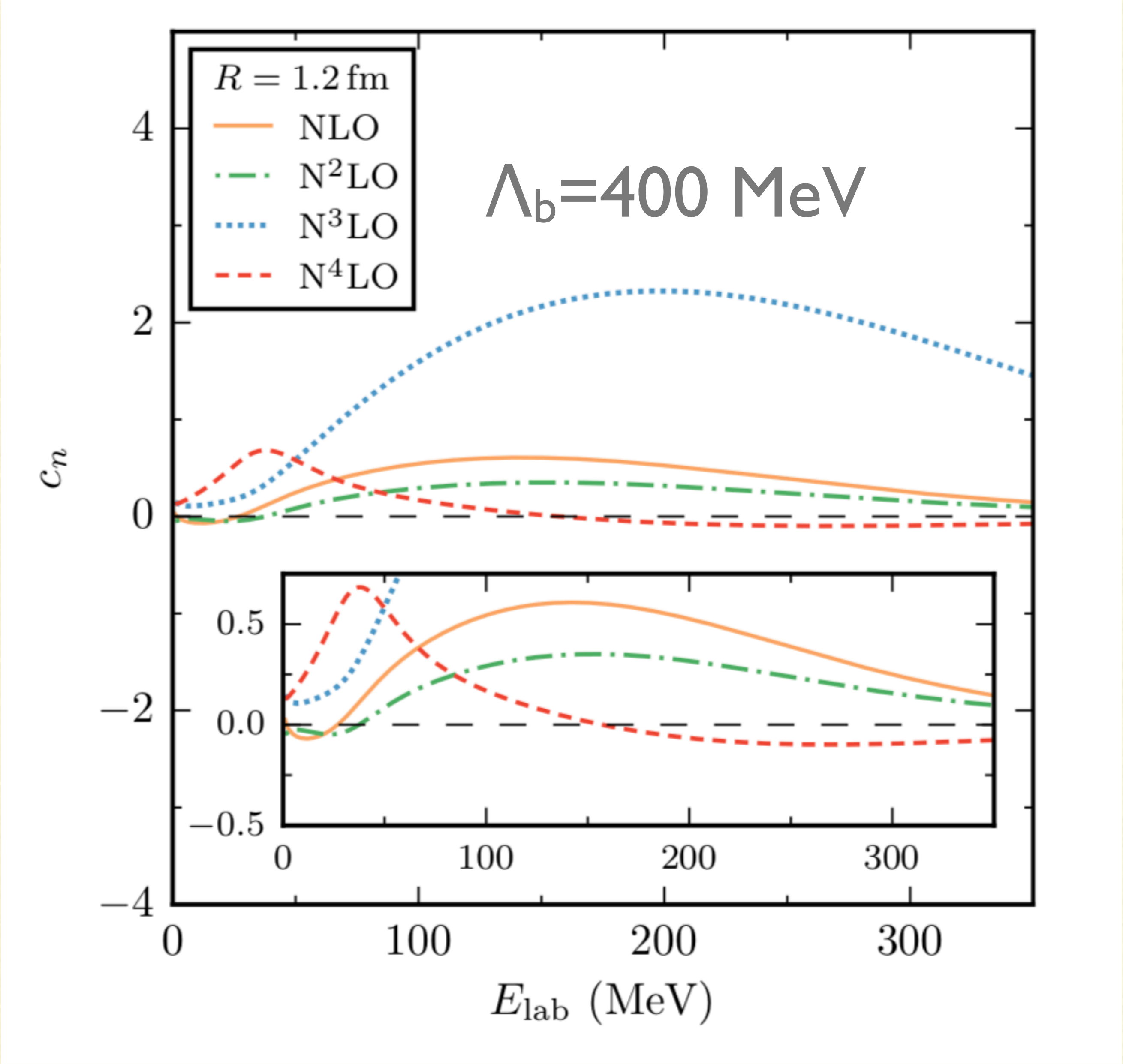

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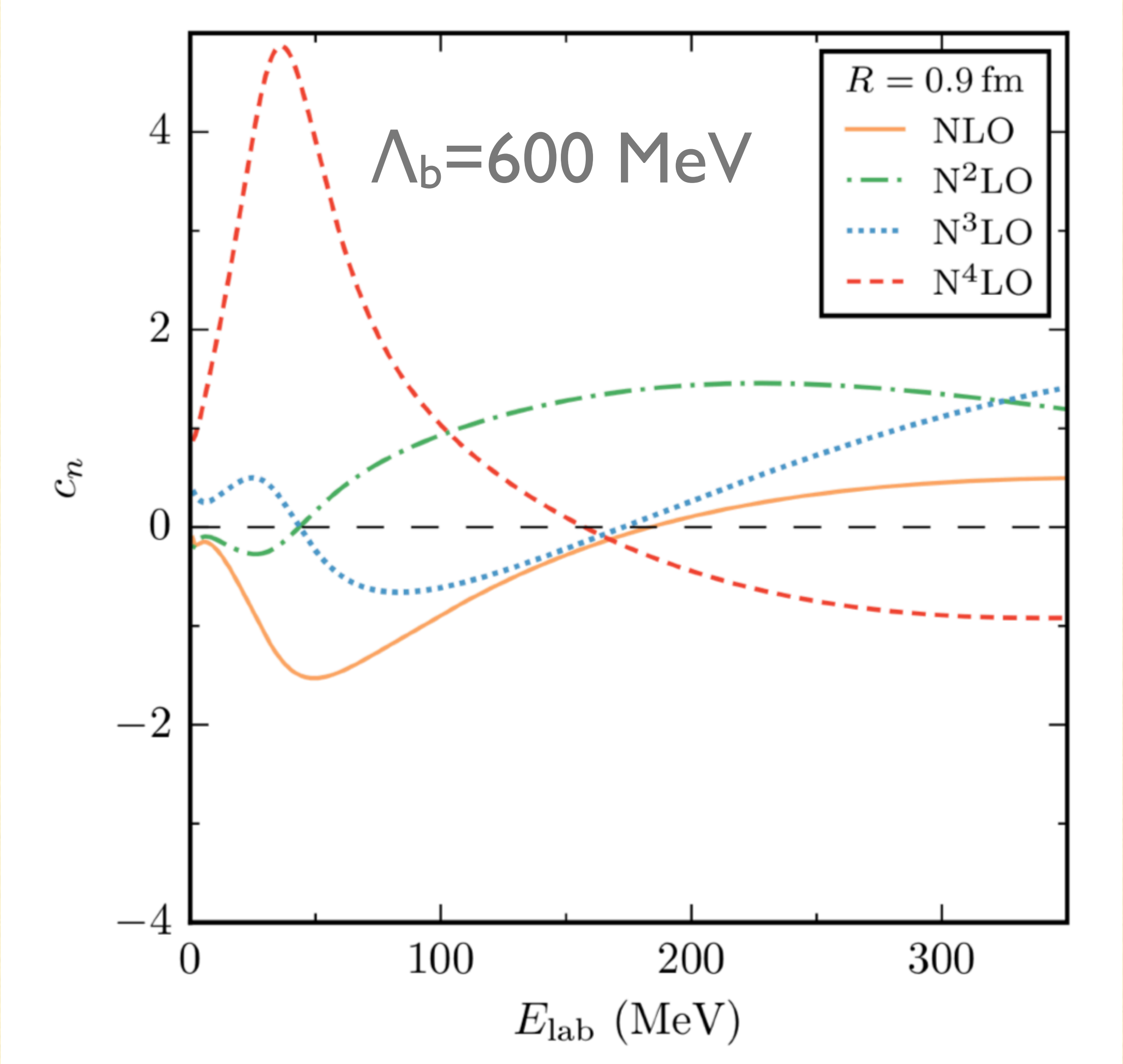

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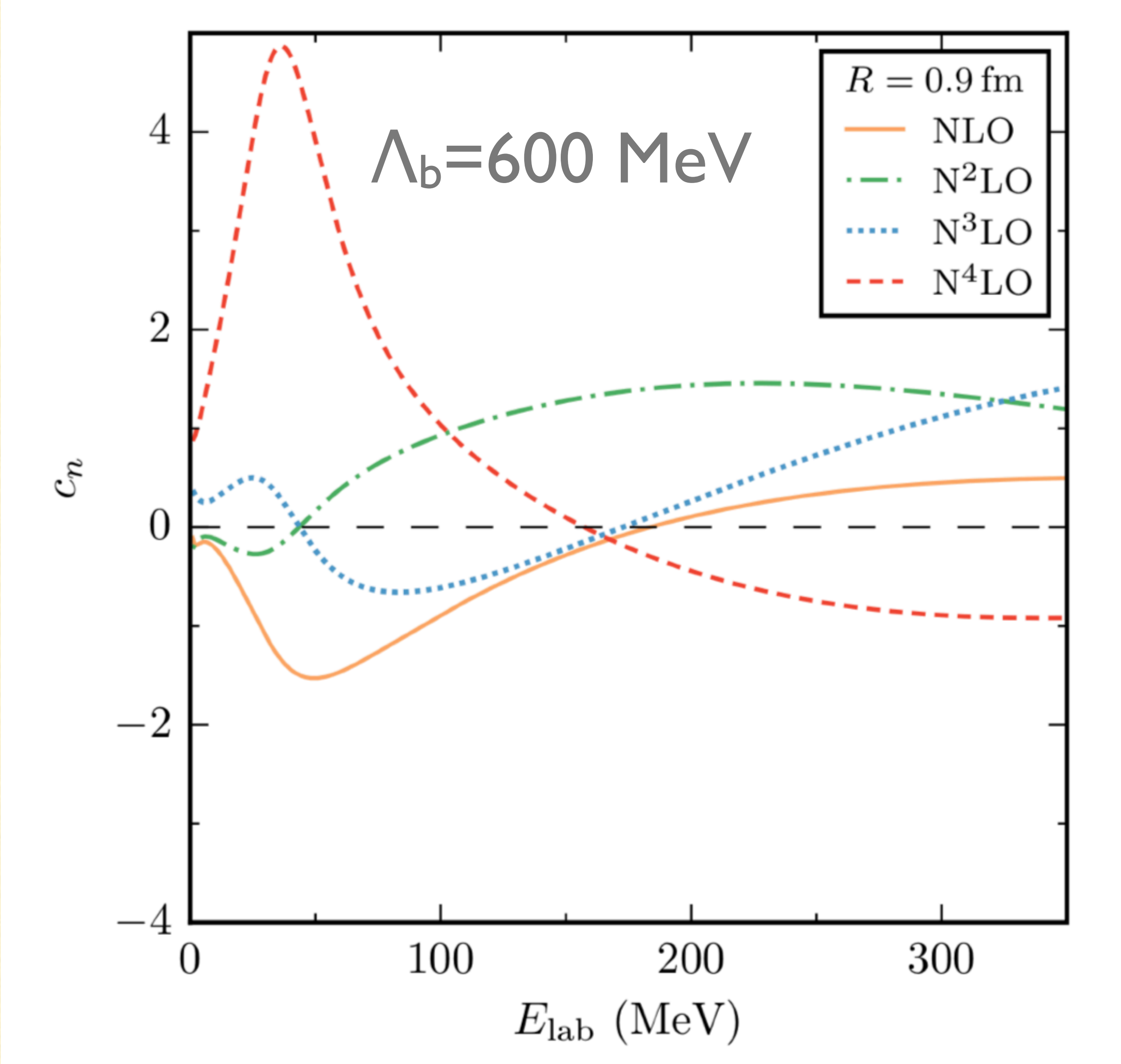
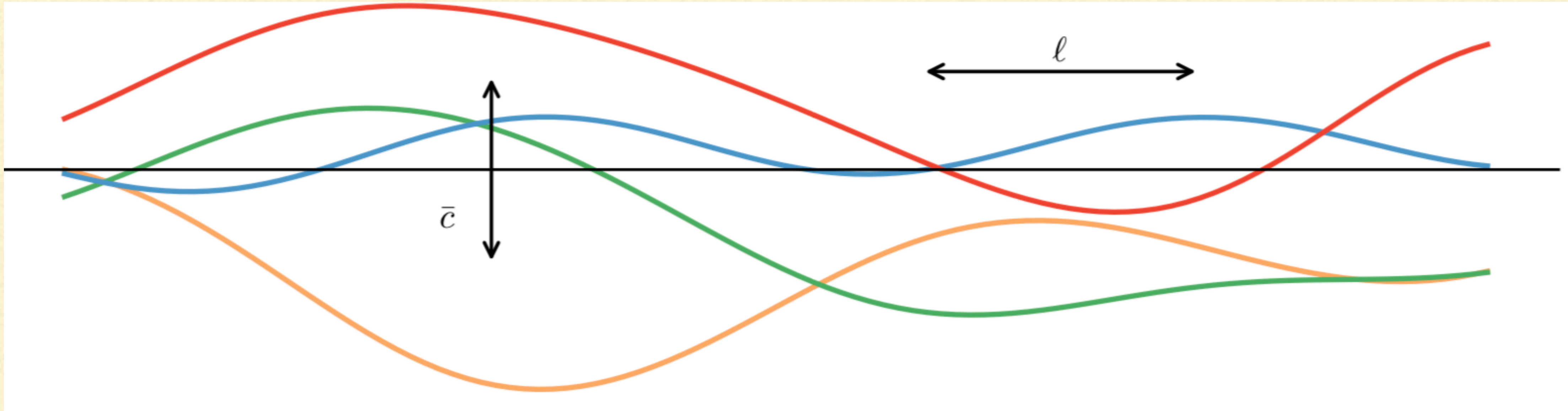


Physics questions:

- Do curves all fluctuate around zero with some common variance?
- What is the correlation length? Is it different at each order?

Hypothesis: the c_n's are a GP

Melendez, Furnstahl, DP, Pratola, Wesolowski (2019)



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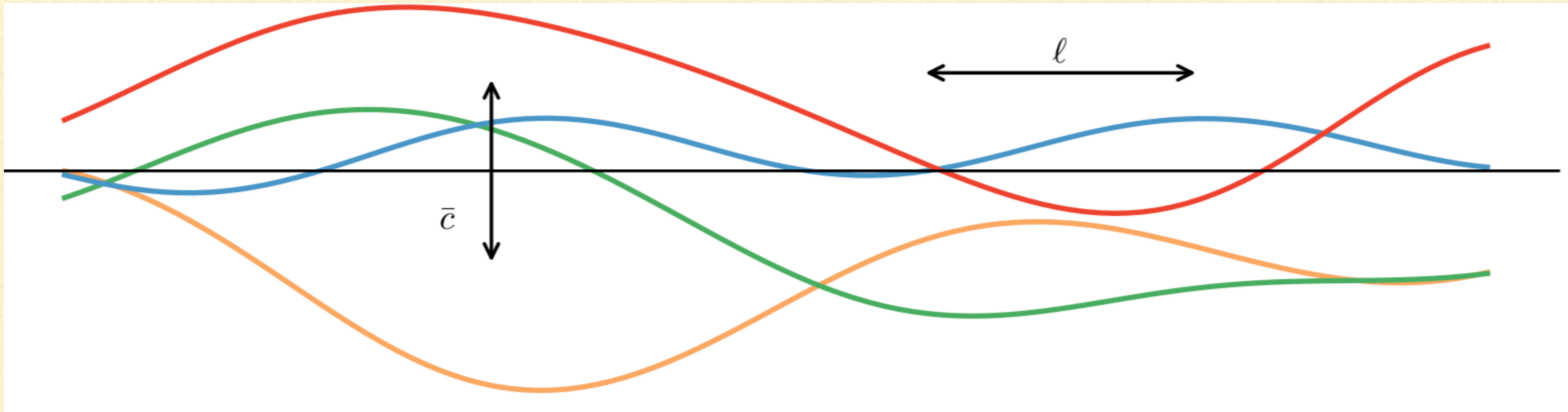

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Our hypothesis:

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

Gaussian Process model

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

Gaussian Process model

- Specify correlation matrix of c_n at x and y, e.g.:

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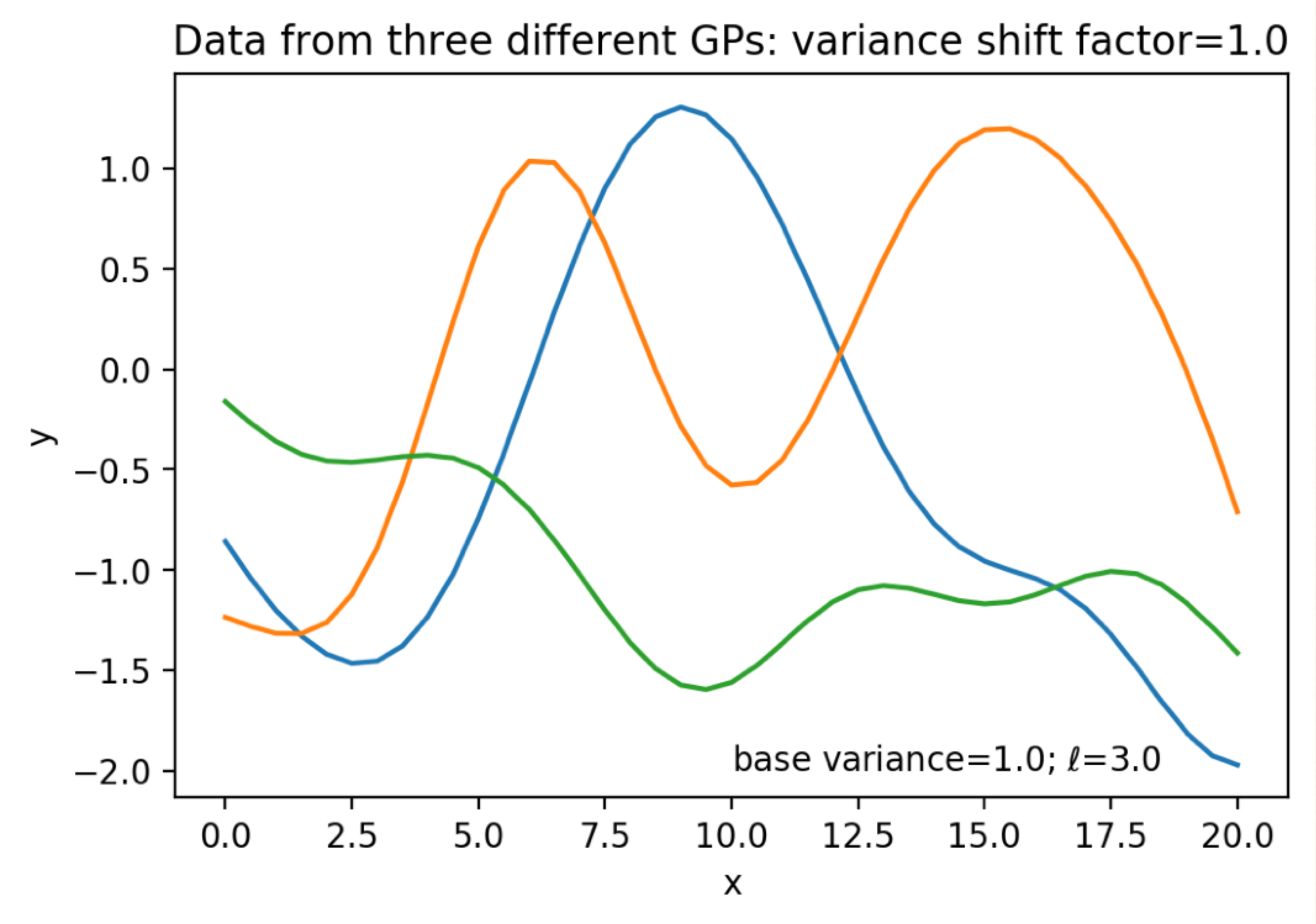
- Need to estimate two parameters: cbar (variance) and ℓ (correlation length)

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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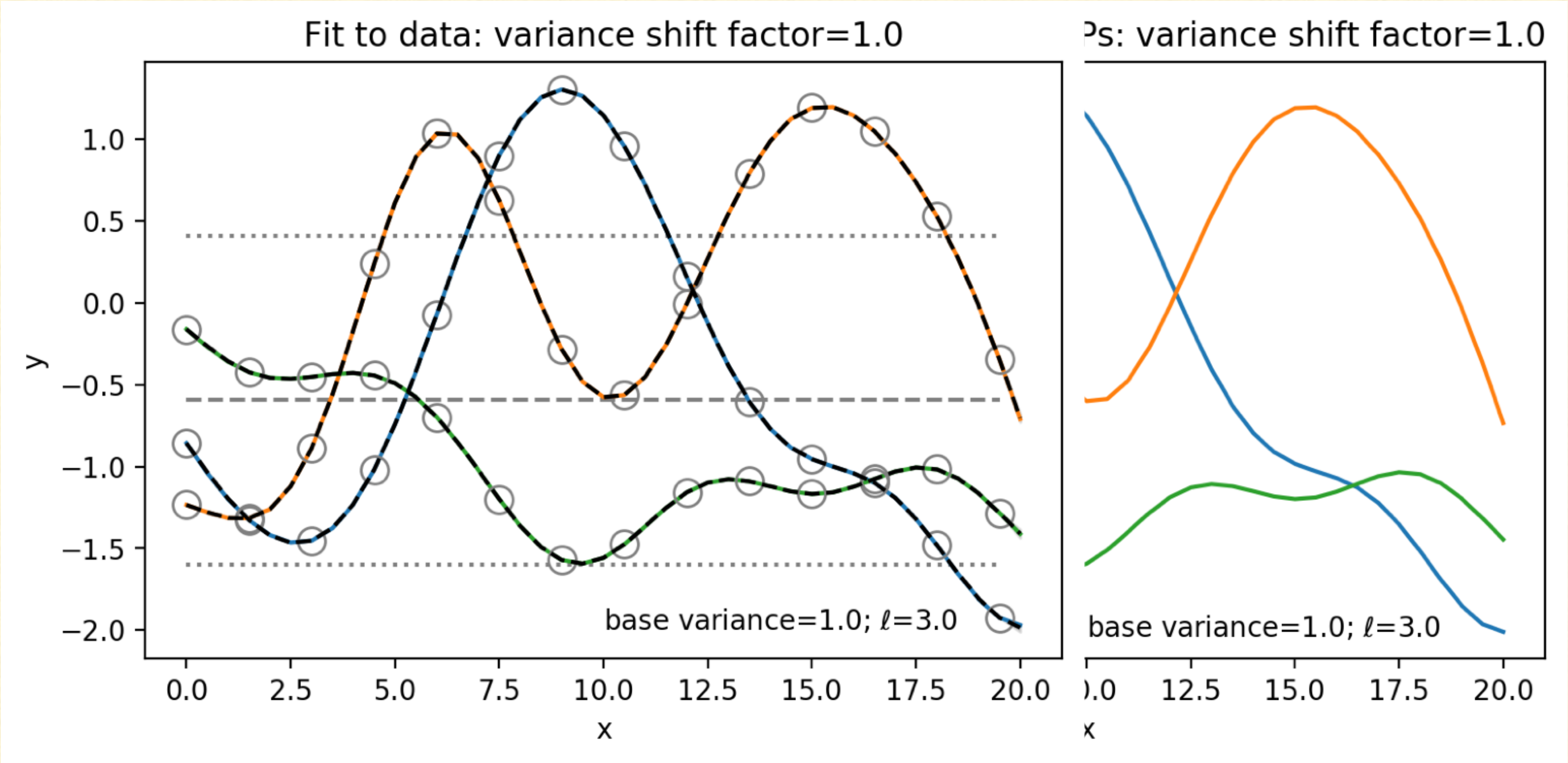

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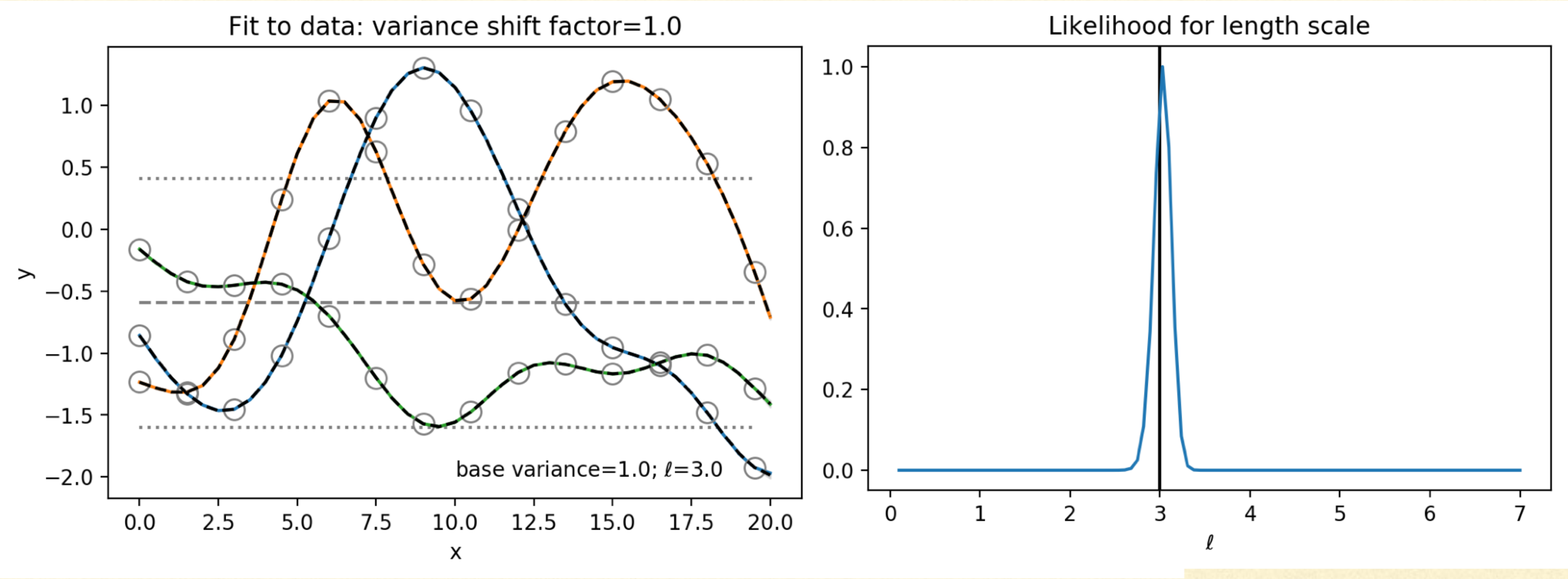

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GP diagnostics sumnmary

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Melendez, Furnstahl, DP, Pratola, Wesolowski (2019)

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GP c

2009

(2019)

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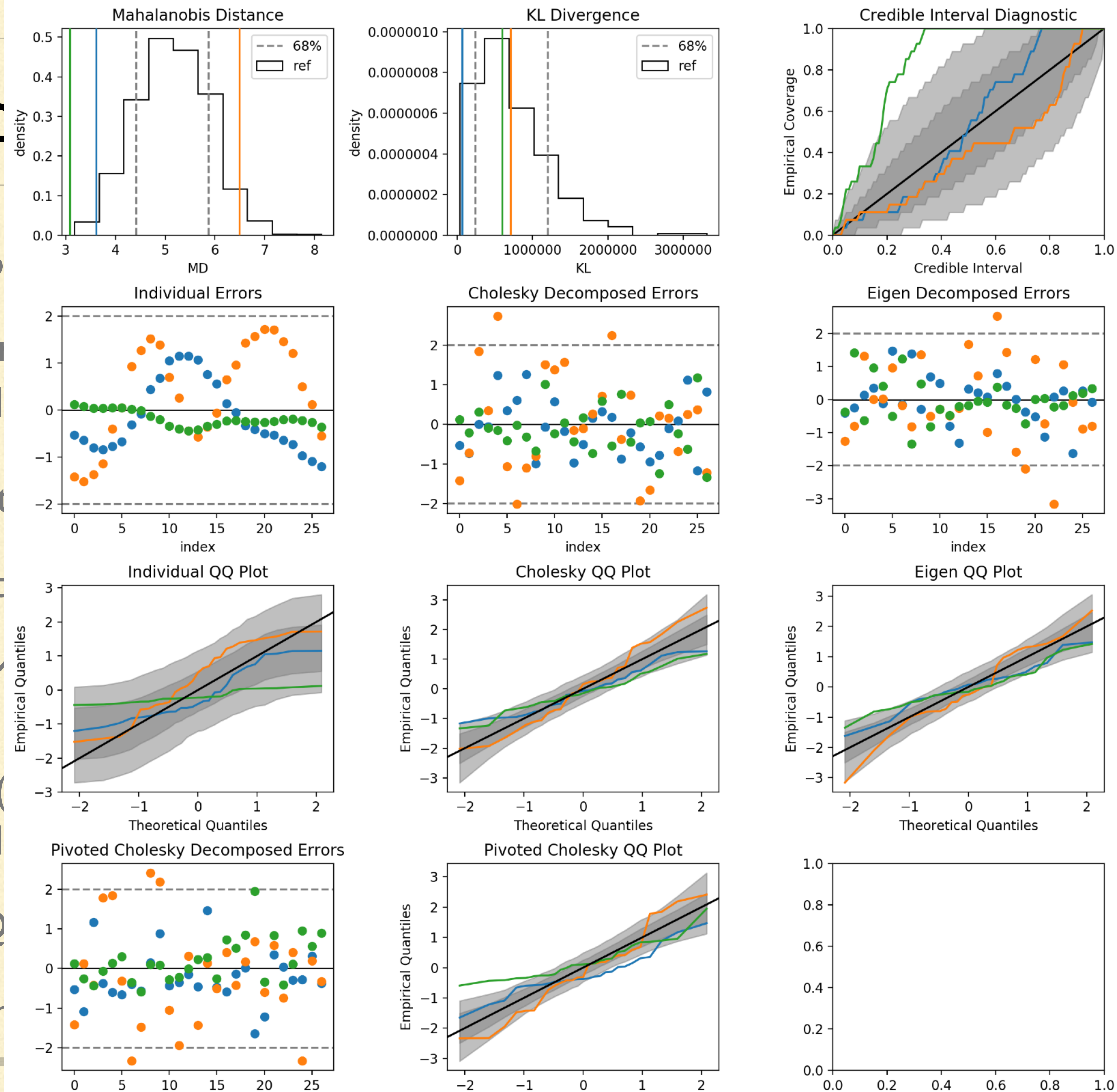

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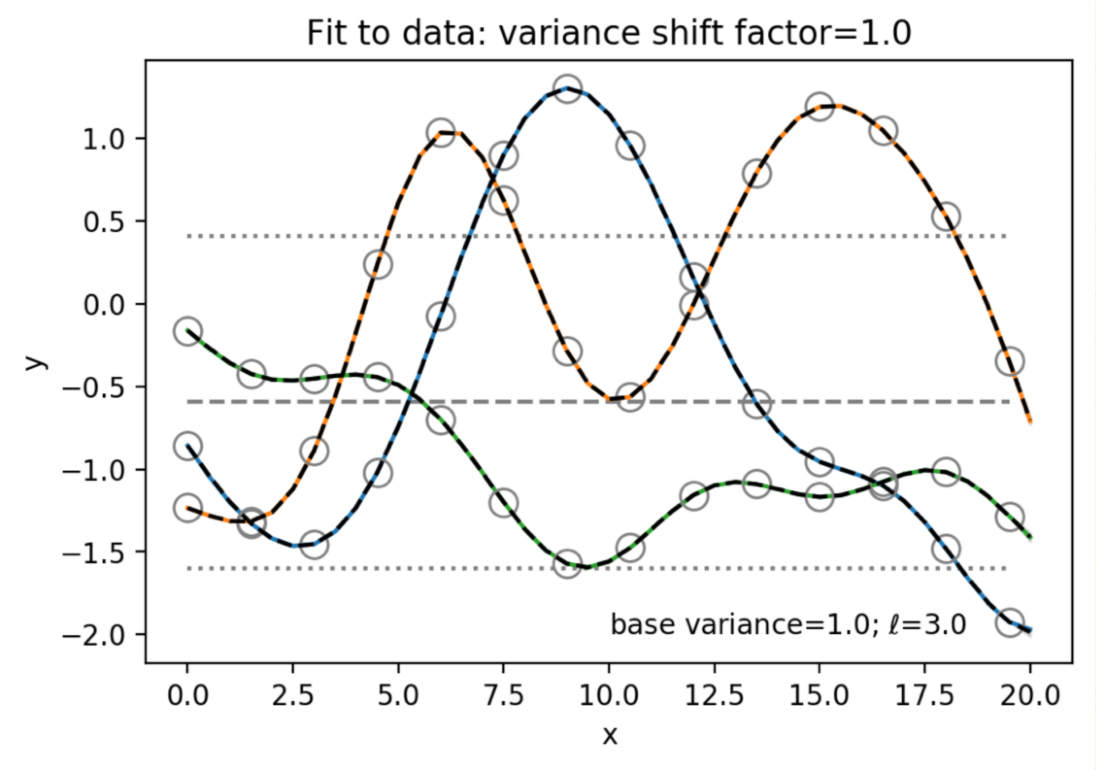

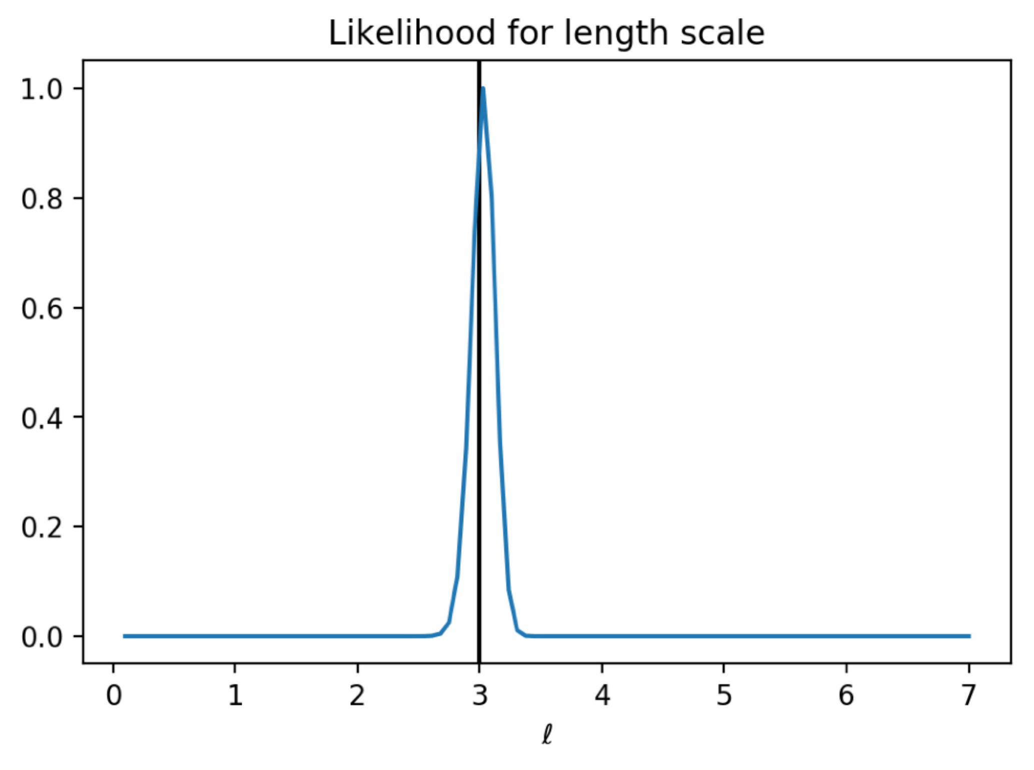

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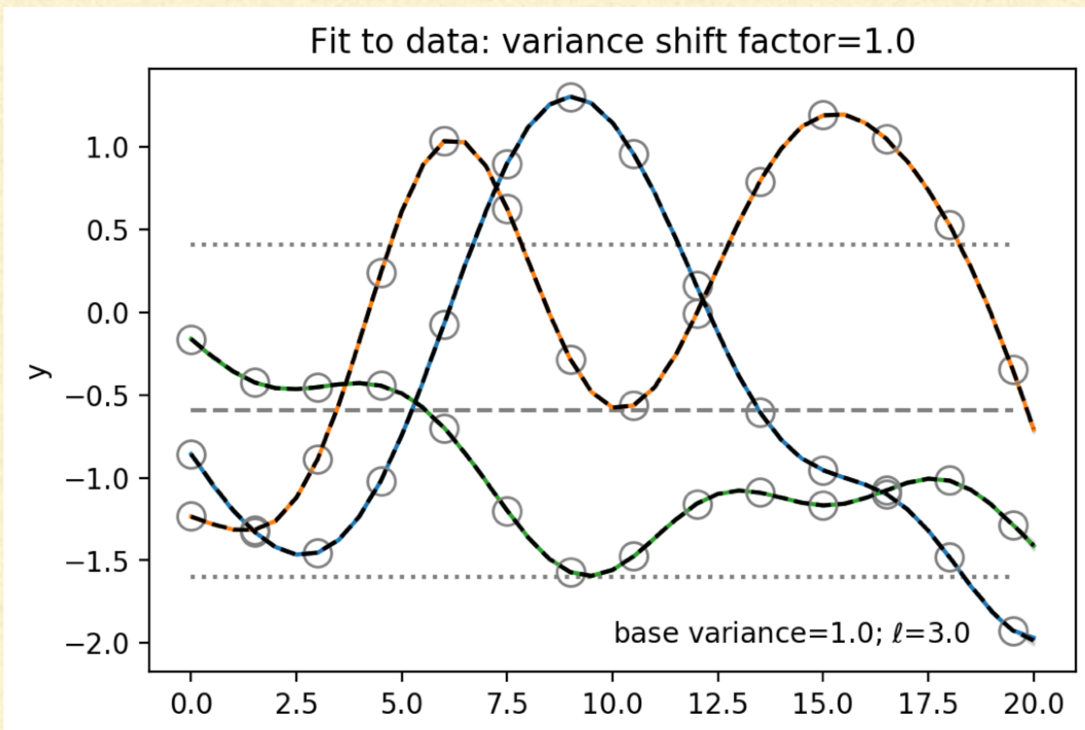

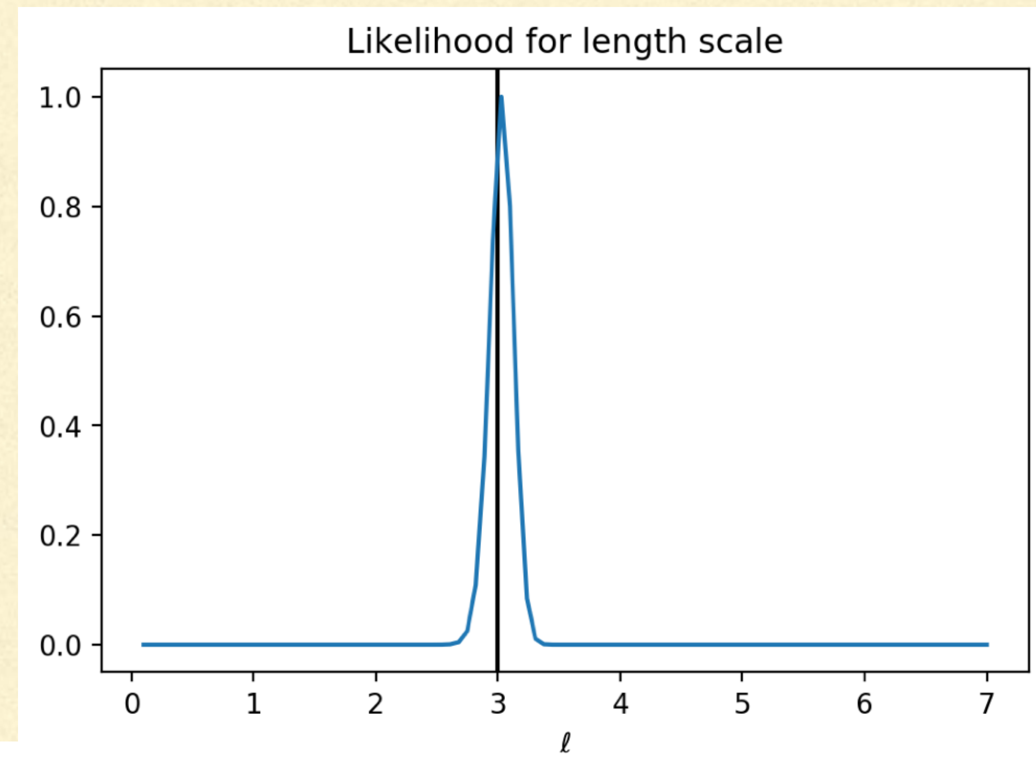

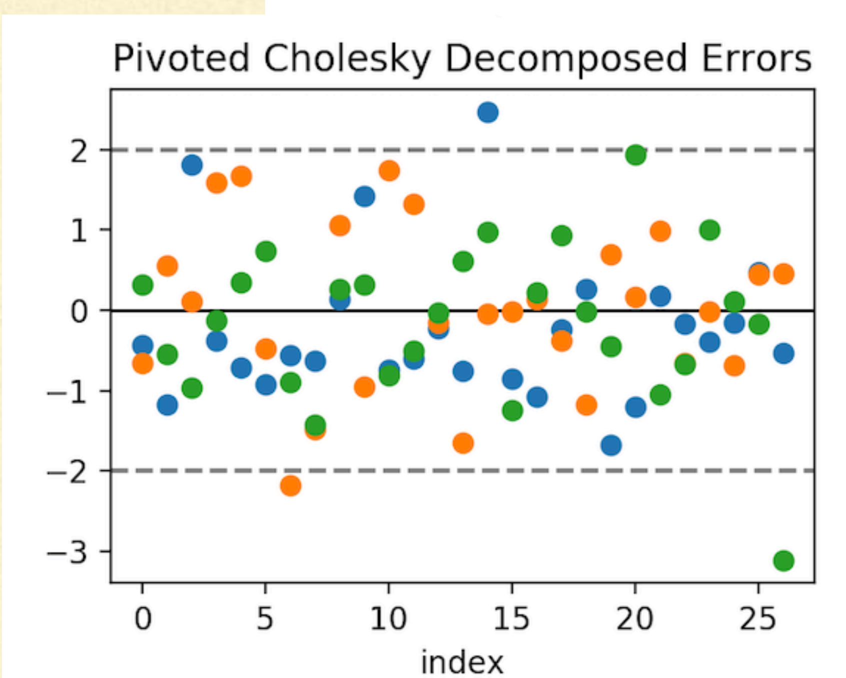

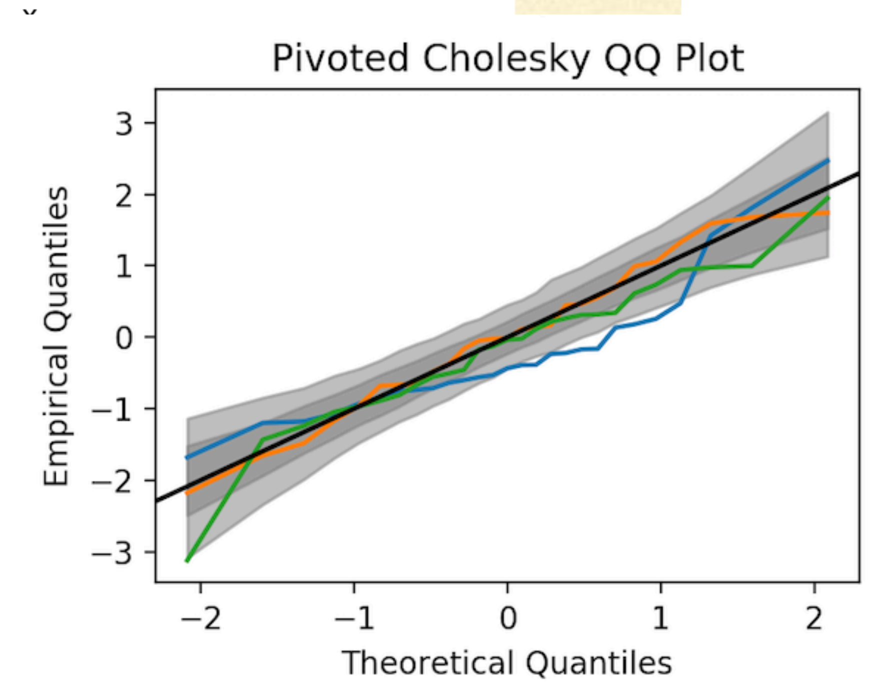

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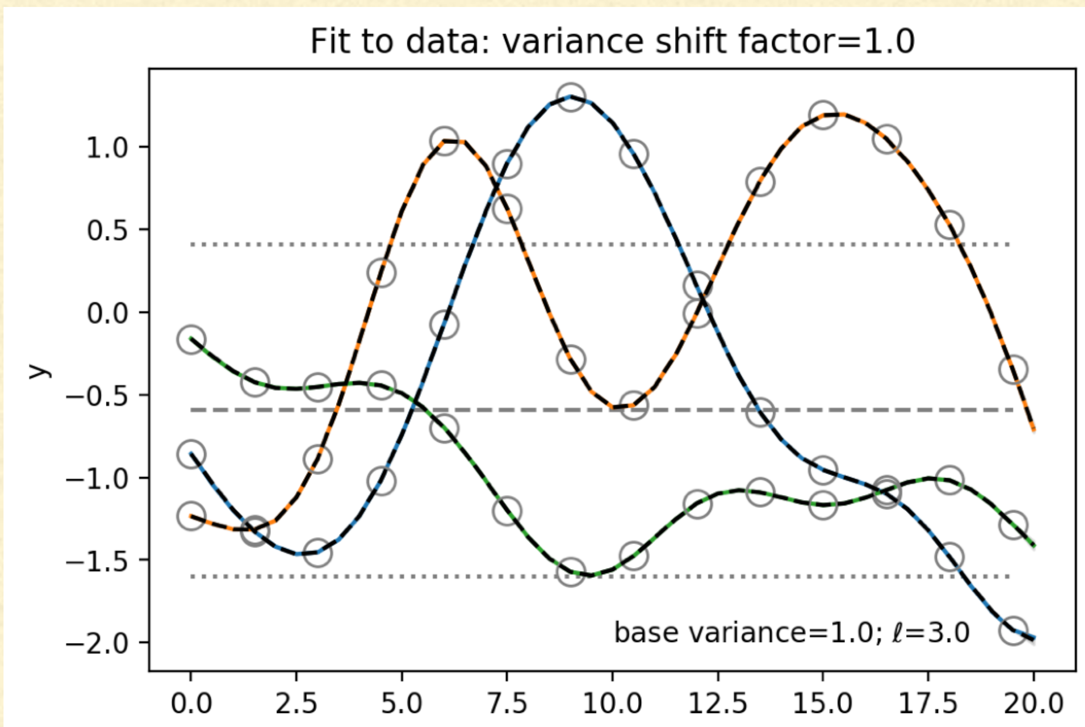

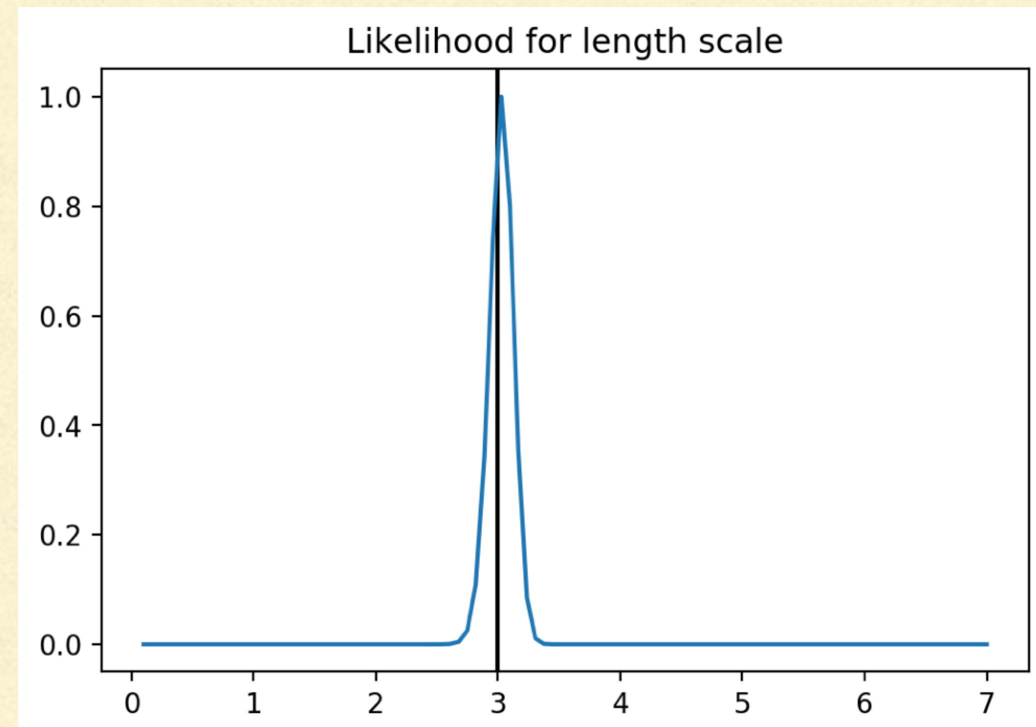

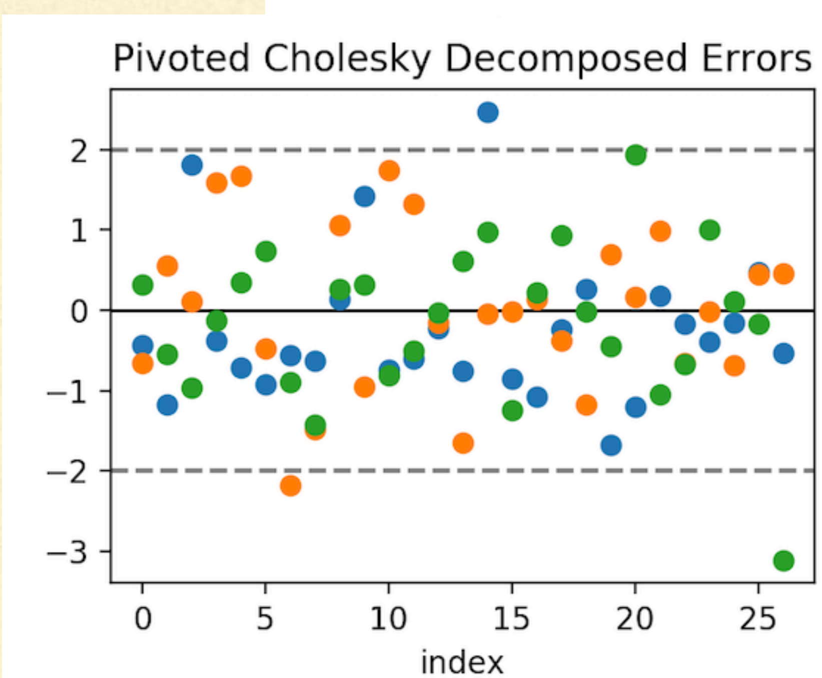

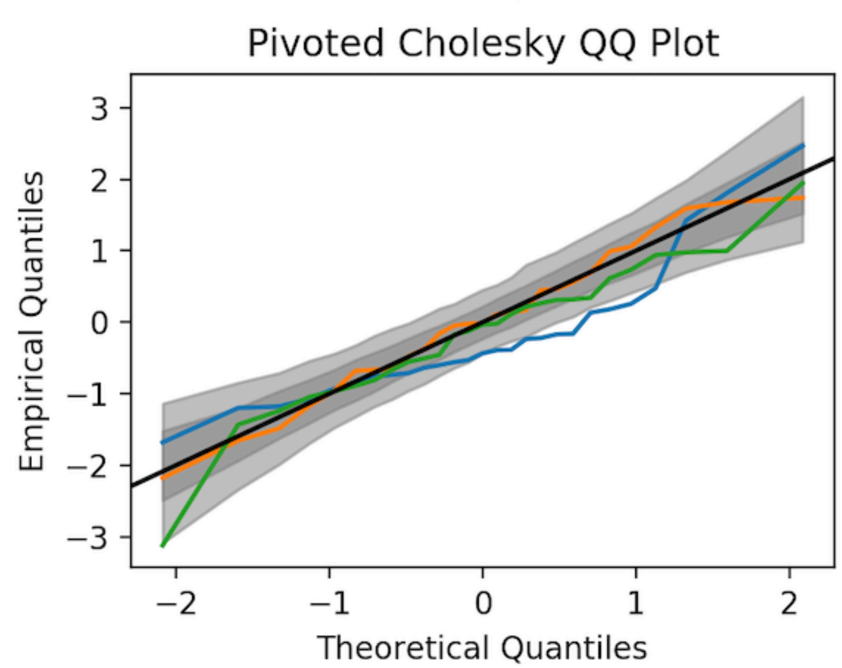

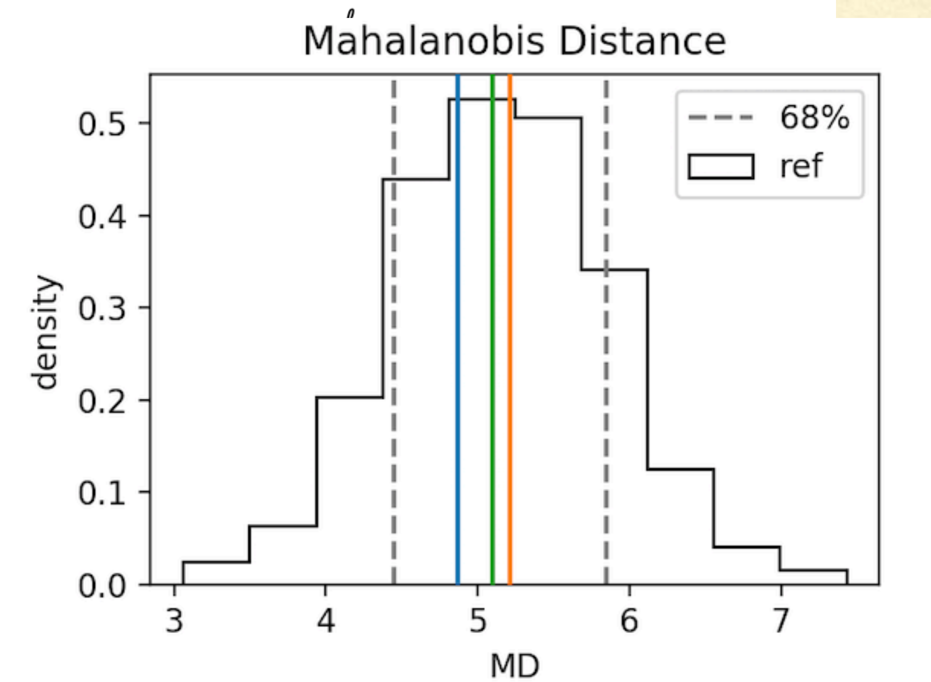

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- Try to fit a single GP to data generated using different variances

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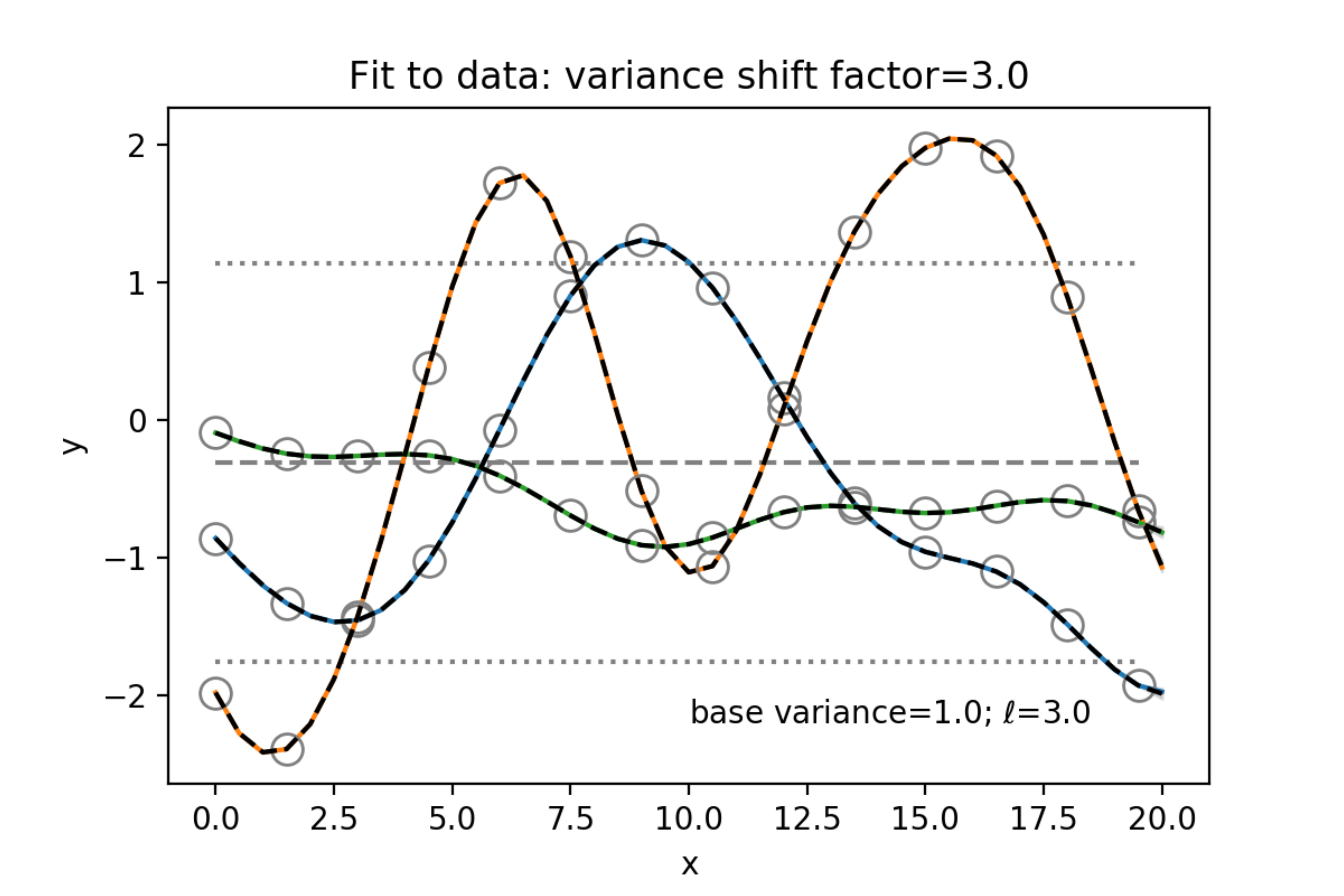

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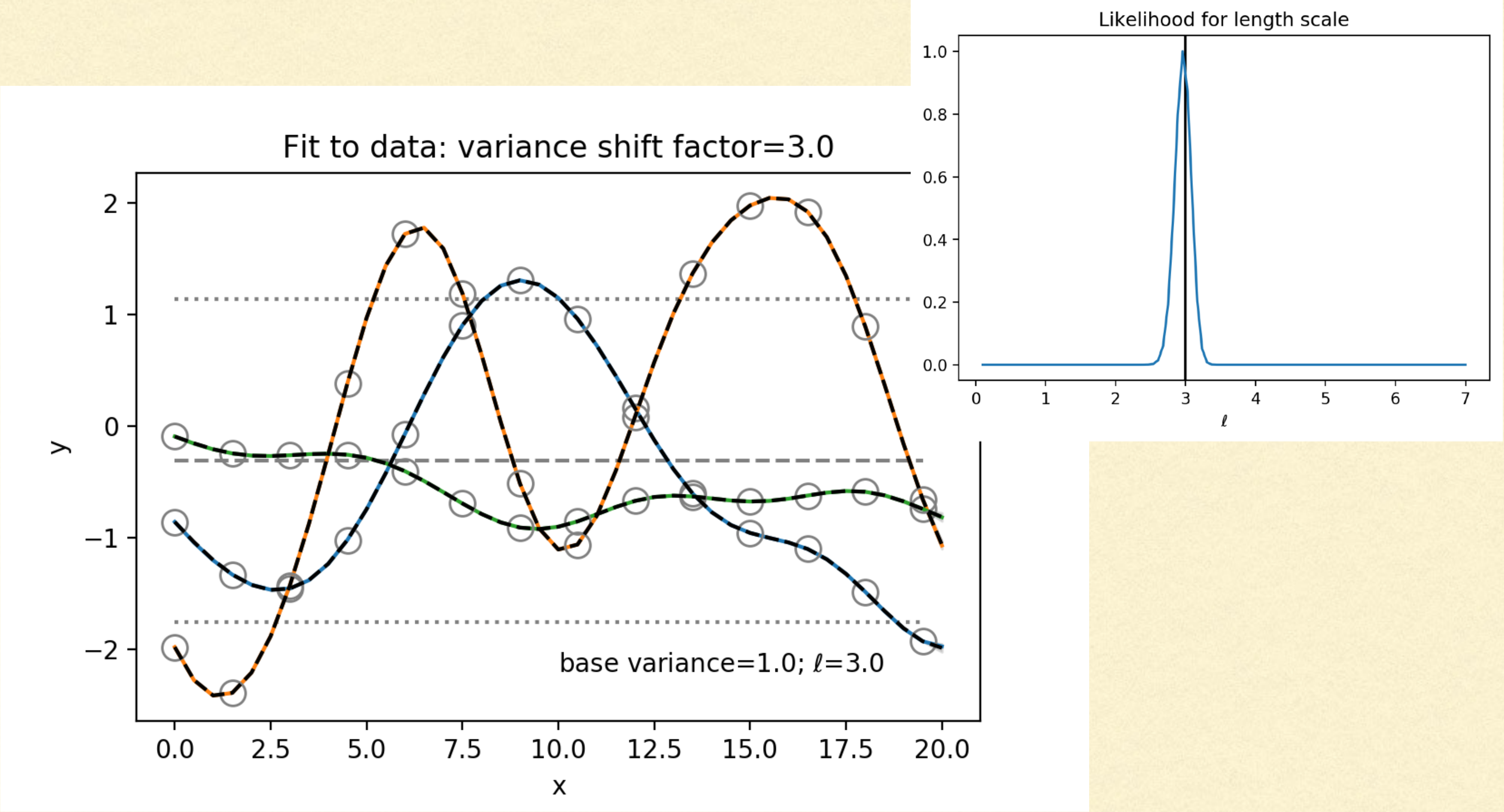

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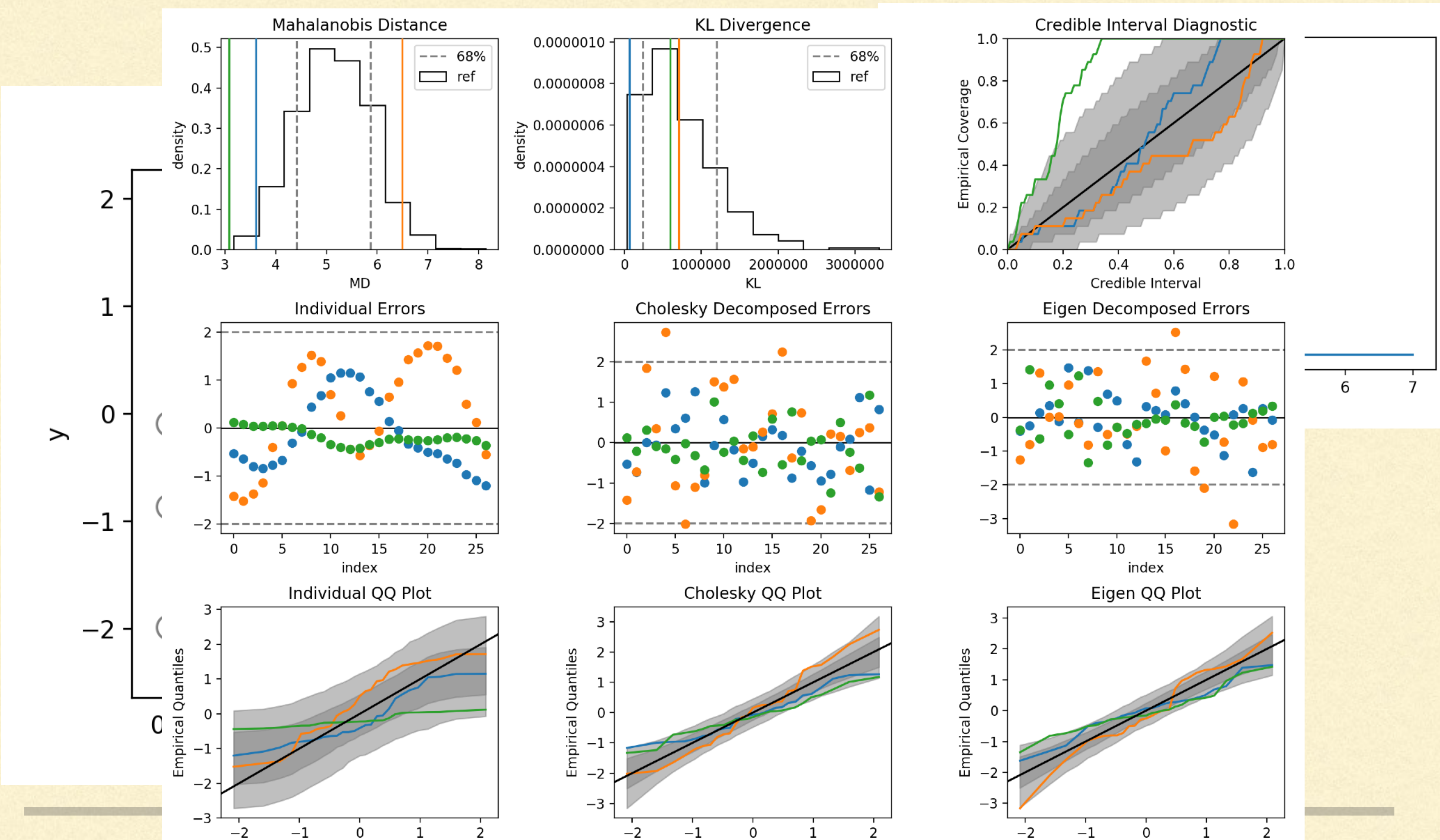

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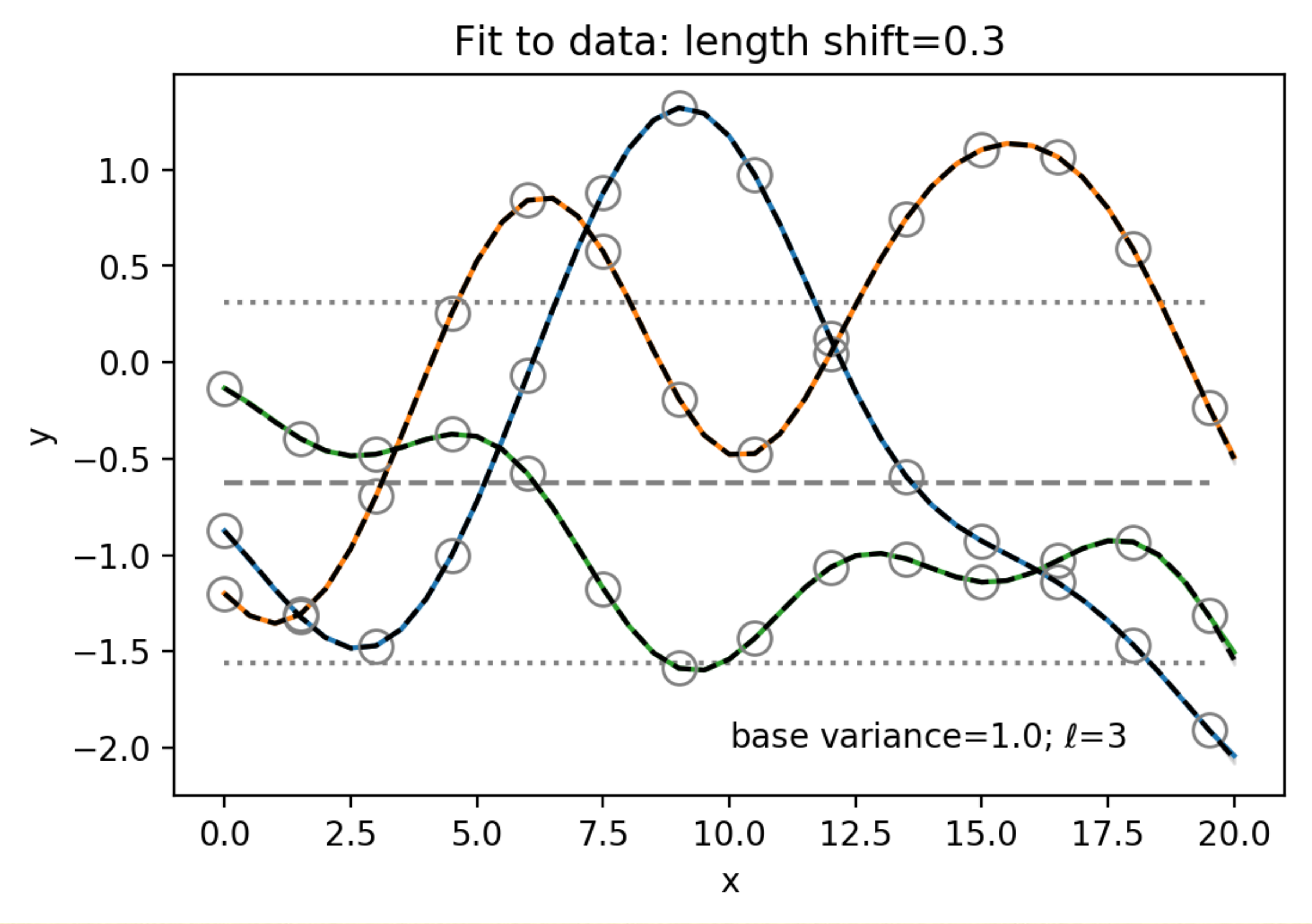

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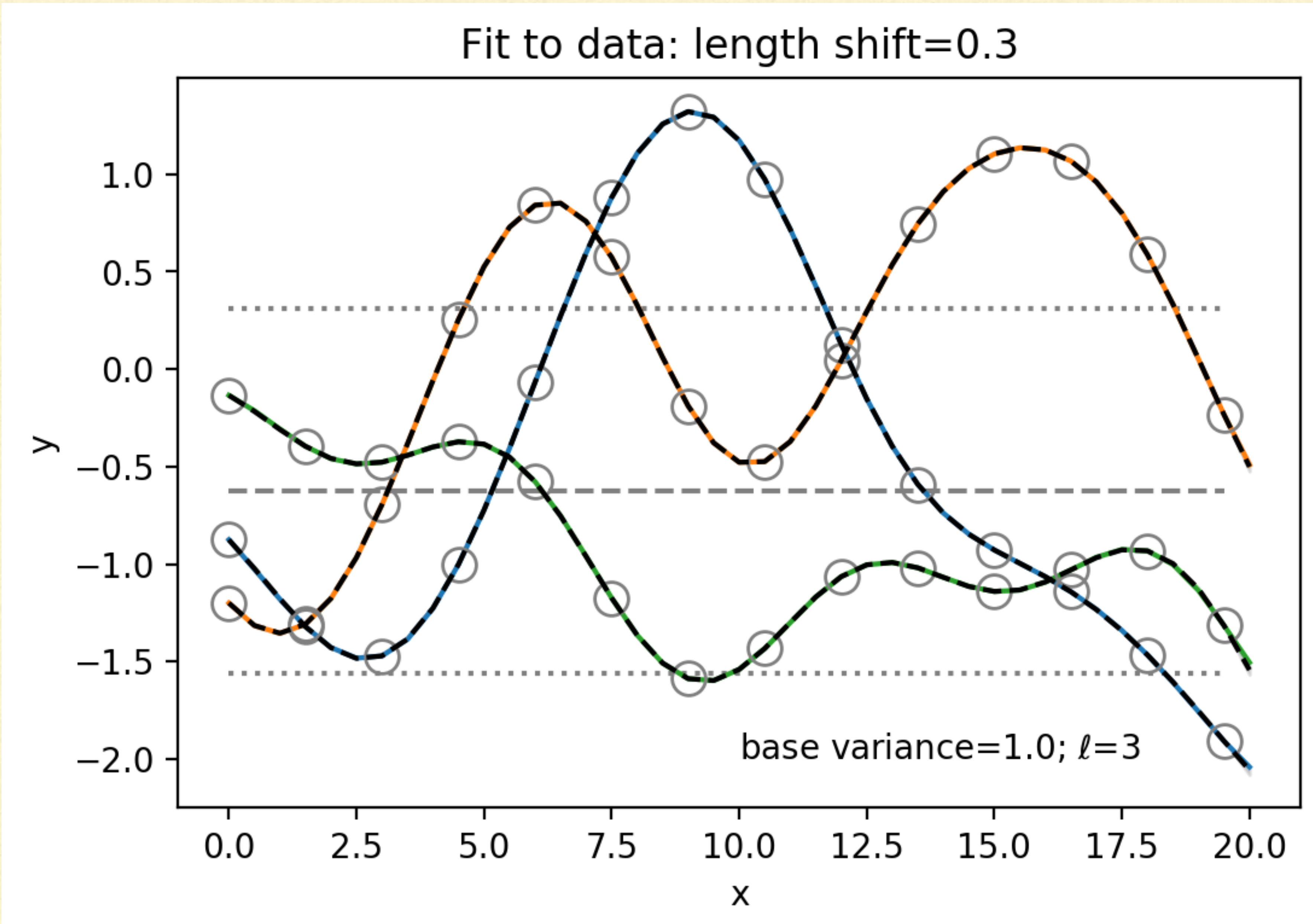

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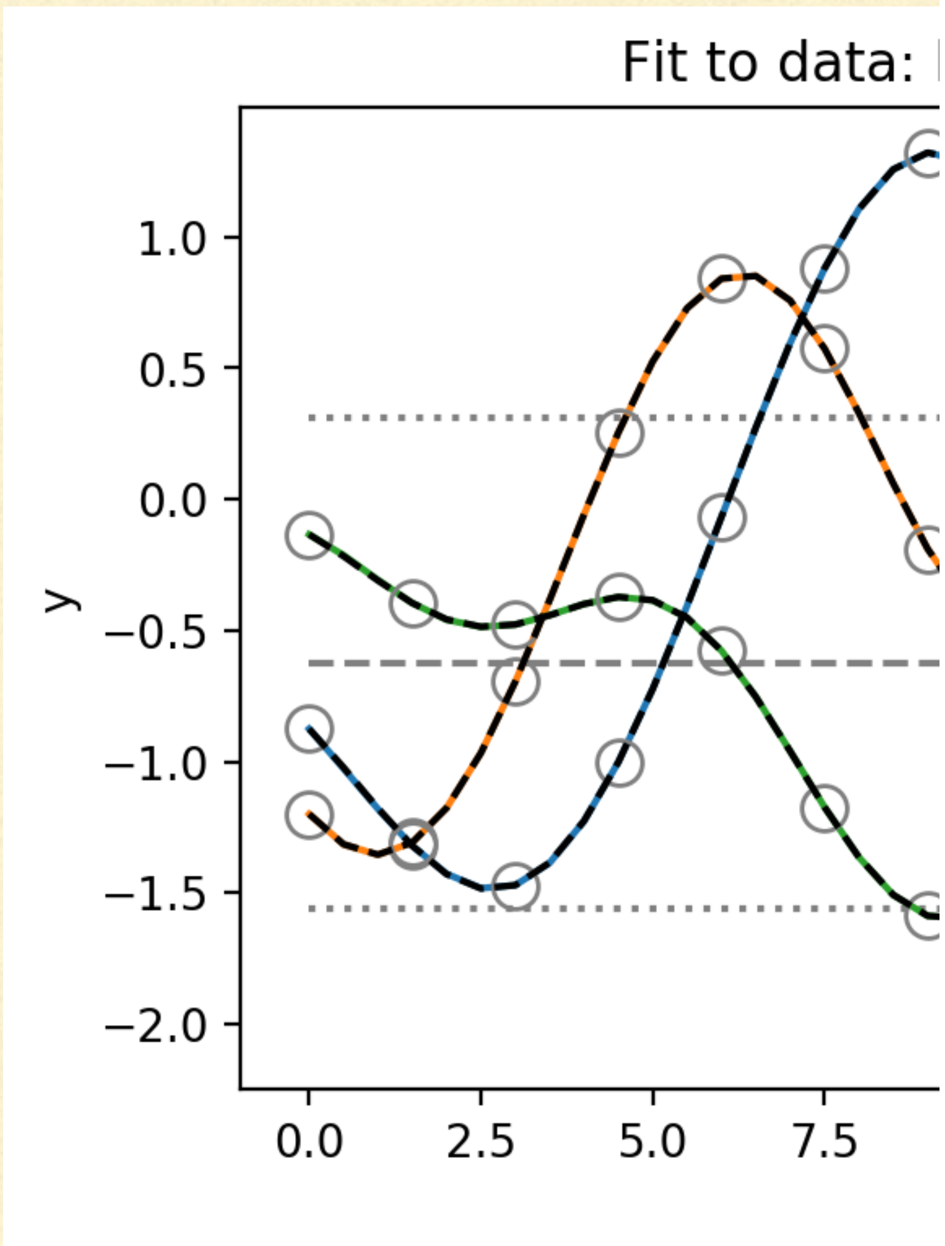
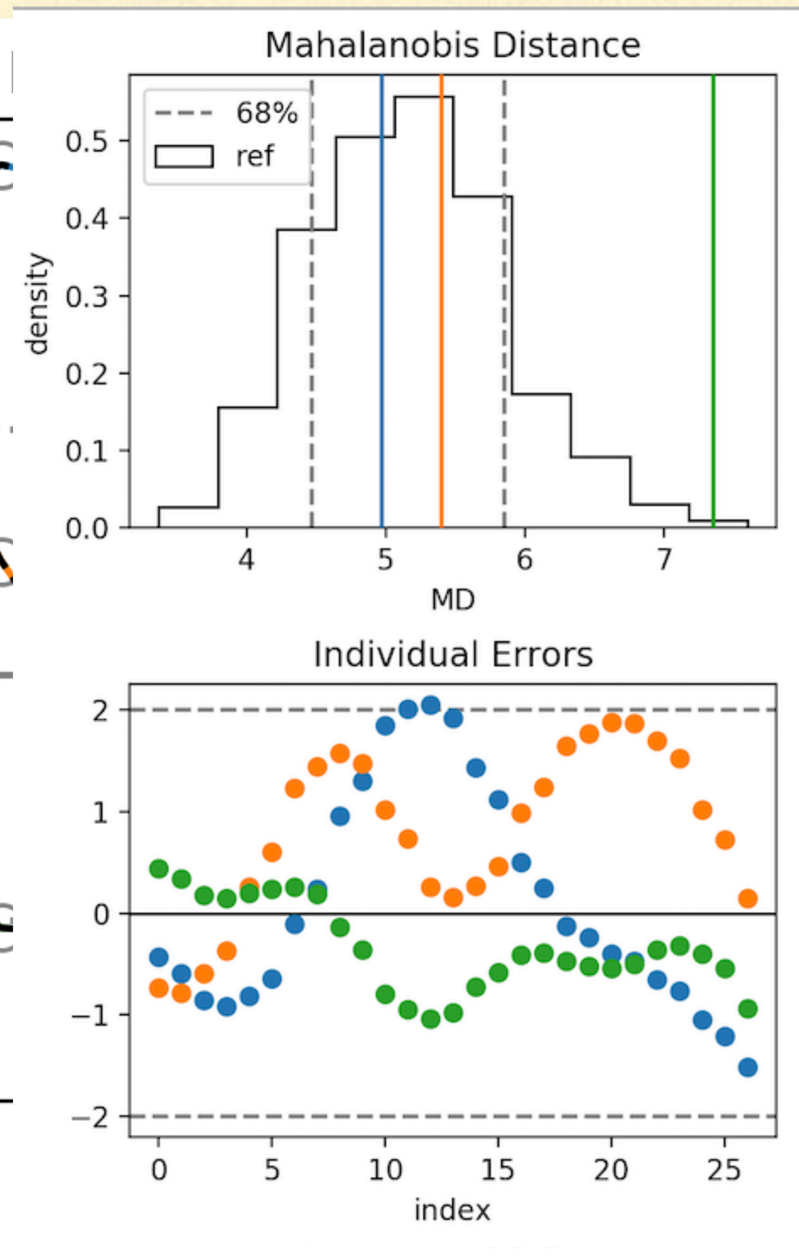
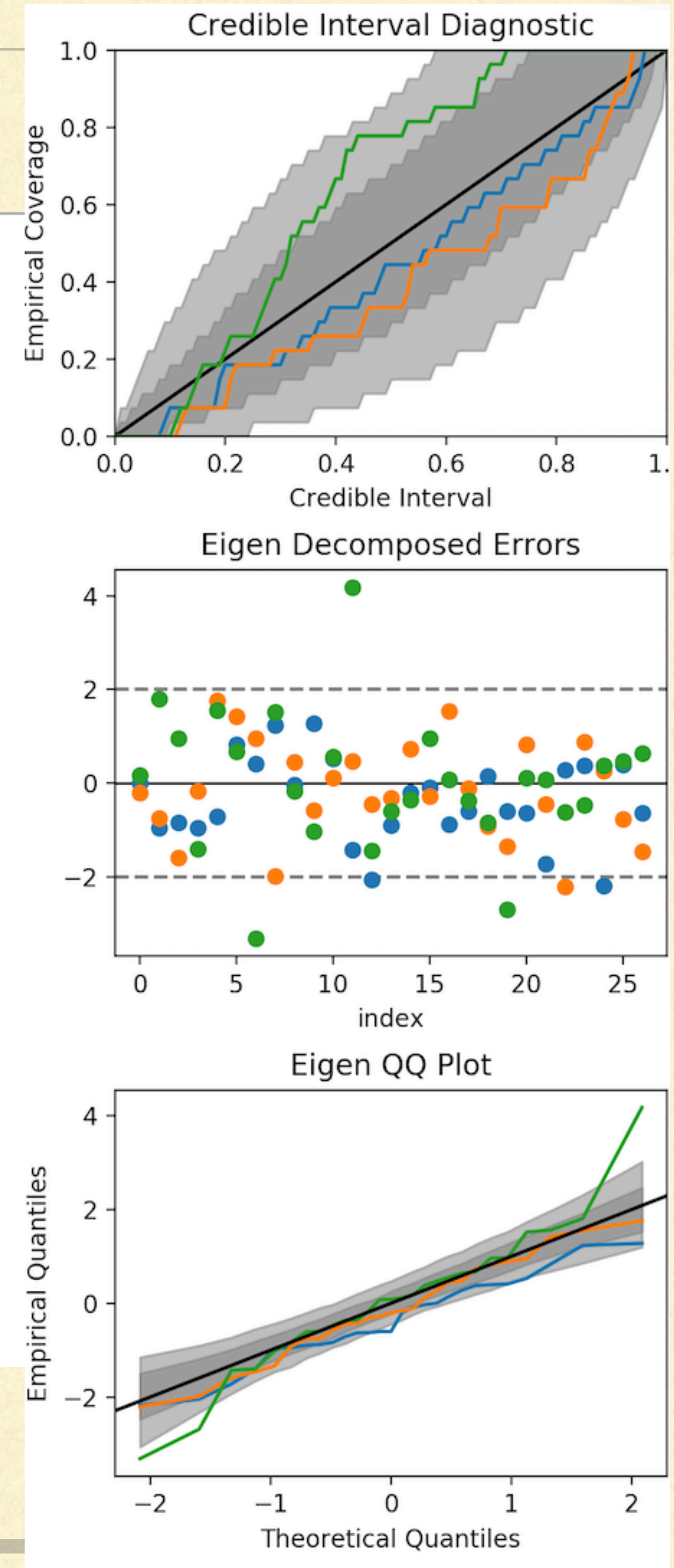
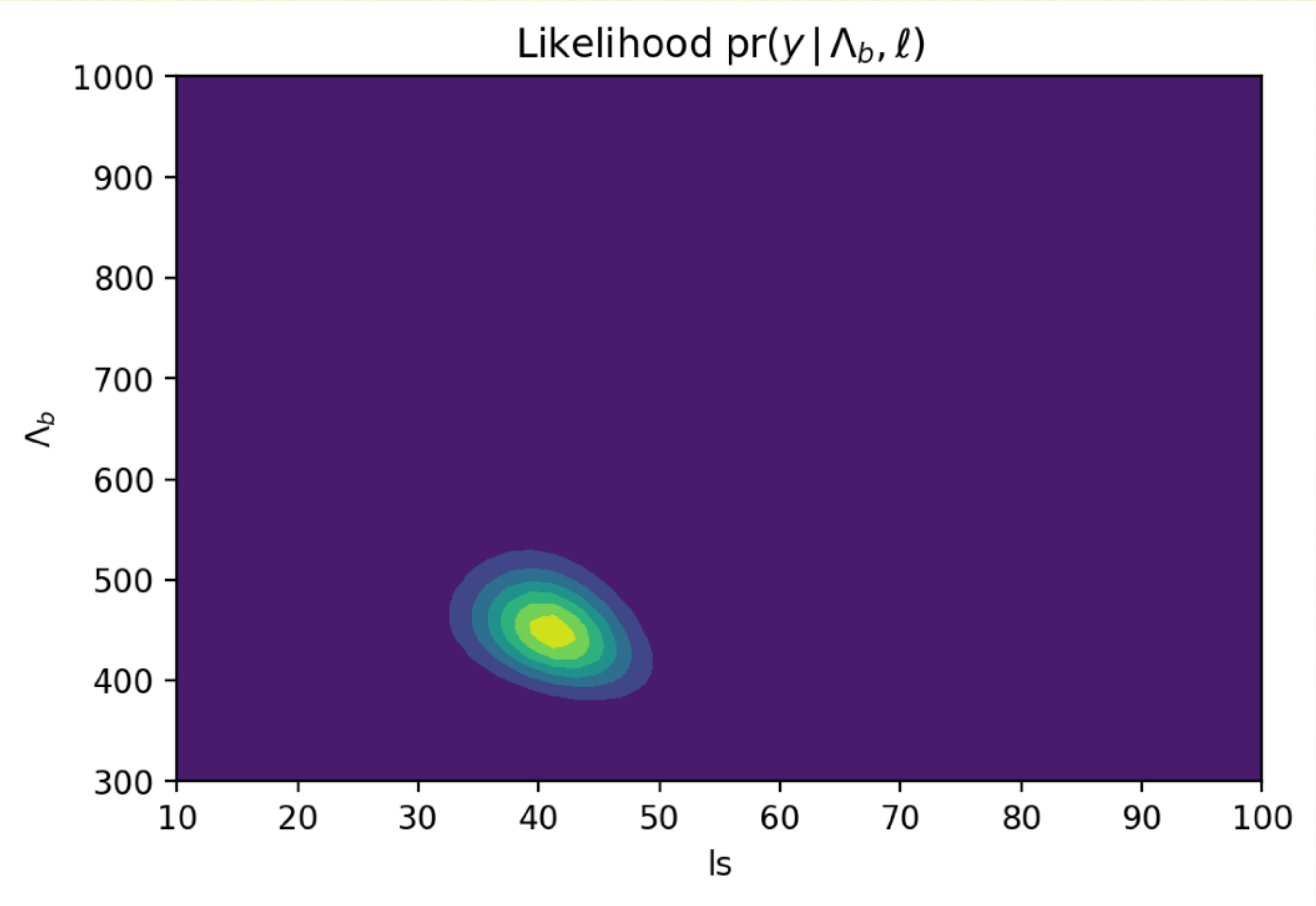






Λ_b and ℓ inference

PRELIMINARY



RKE potential; Λ=500 MeV;
Total cross section only

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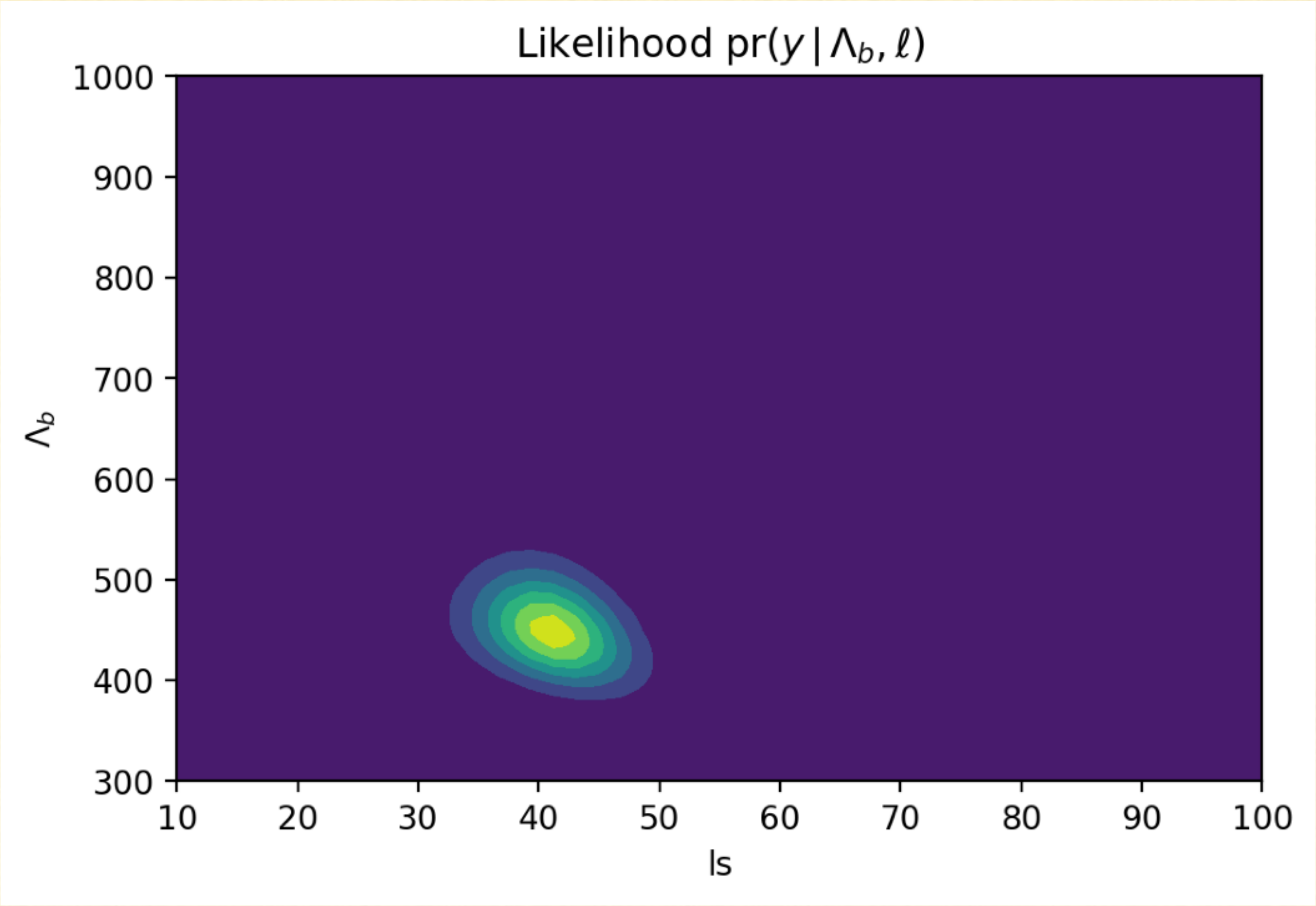

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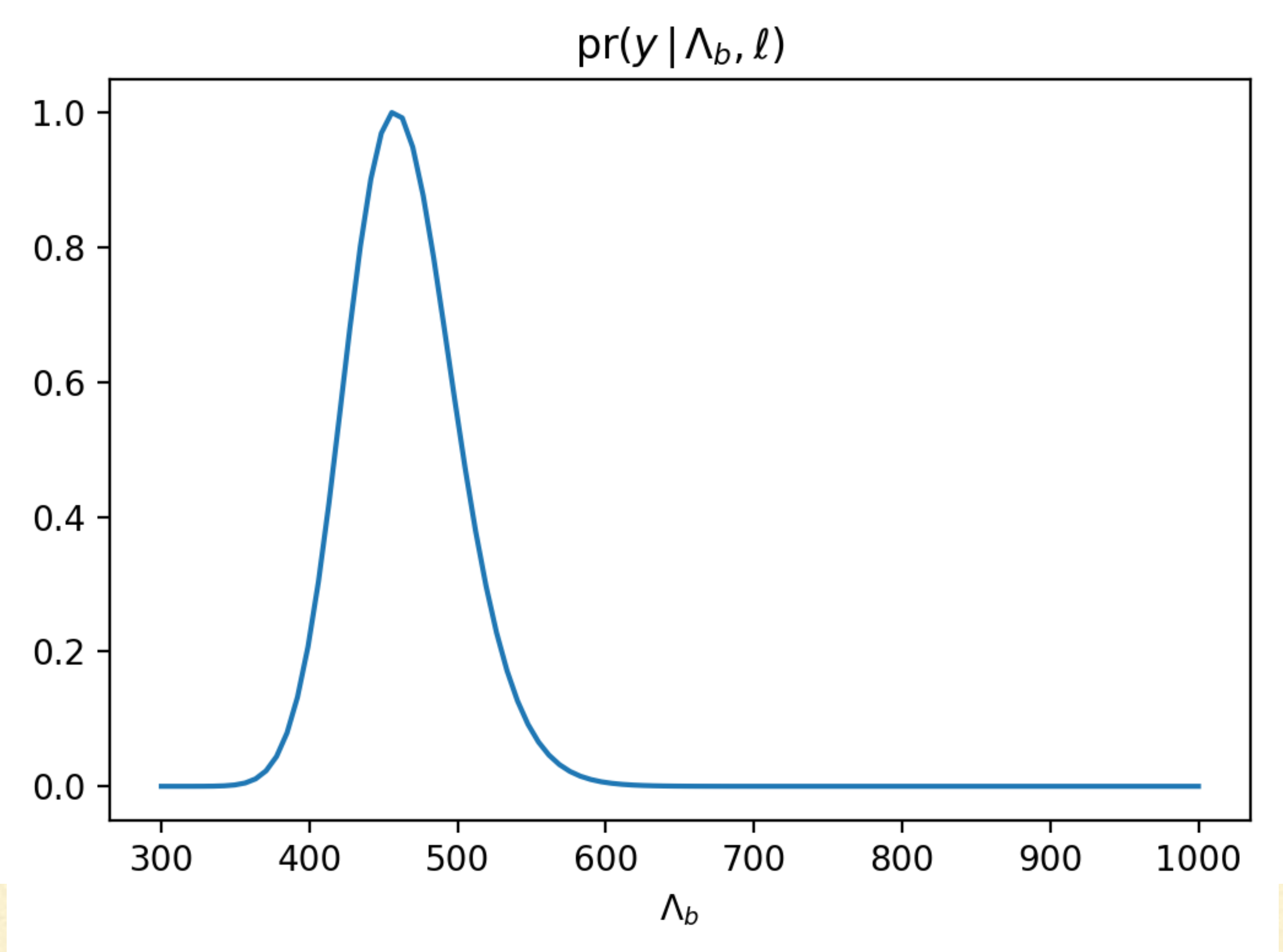

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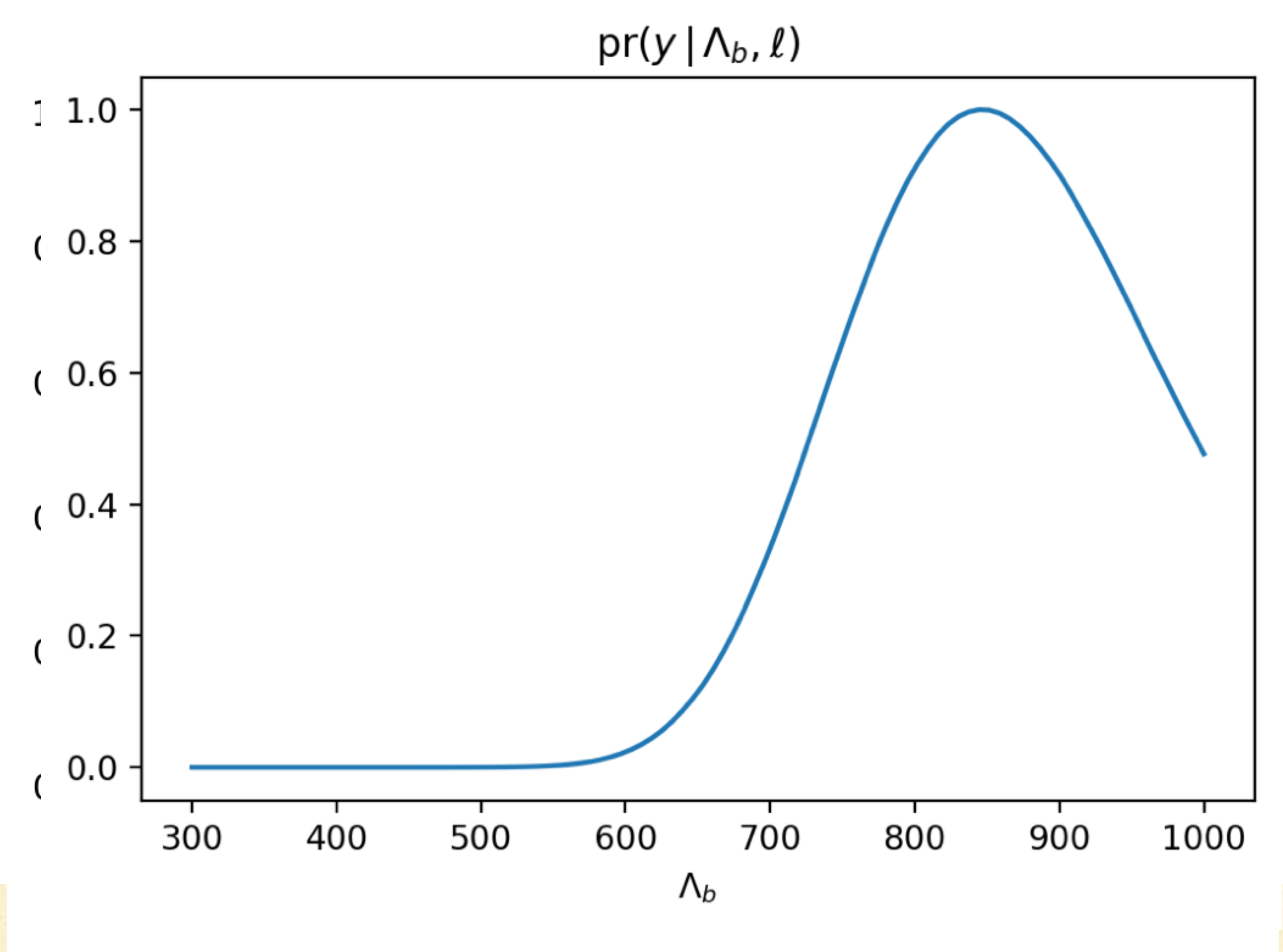

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Restricted domain

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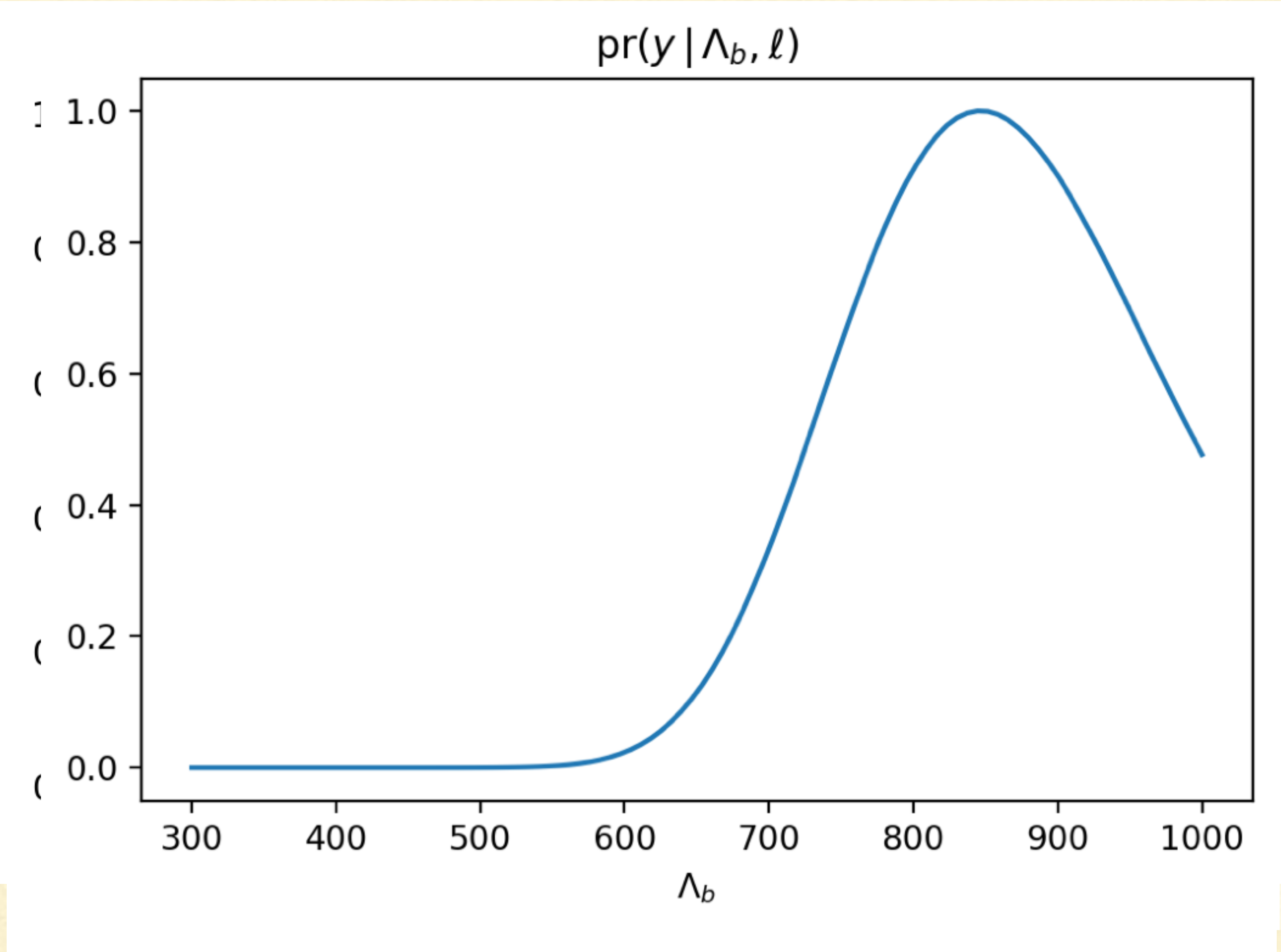

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To do:

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