Calibration, uncertainty quantification, and extrapolation of nuclear reaction models

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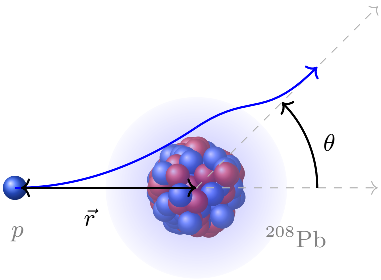
Overview

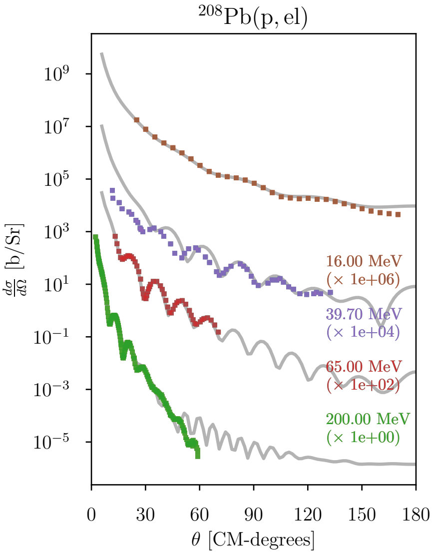
1. Introduction (just a bit of phyics)
2. Calibration (and the software tools enabling it)
3. Extrapolation and uncertainty quantification

Introduction (just a bit of phyics)

Nuclear reactions and the optical potential

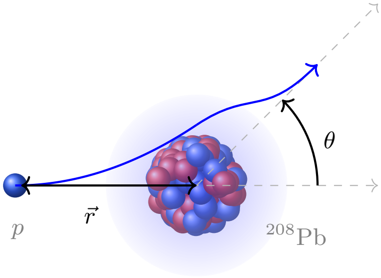
Can you reduce the many-body degrees of freedom of a nuclear reaction problem to few?

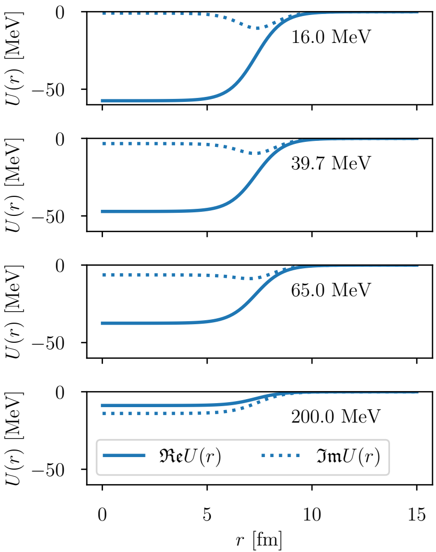




Nuclear reactions and the optical potential

Can you reduce the many-body degrees of freedom of a nuclear reaction problem to few?
Yes, with the optical potential!



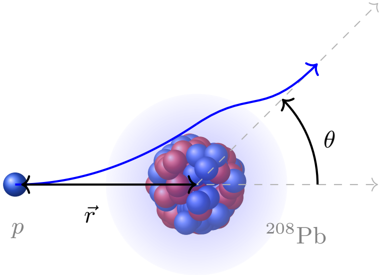


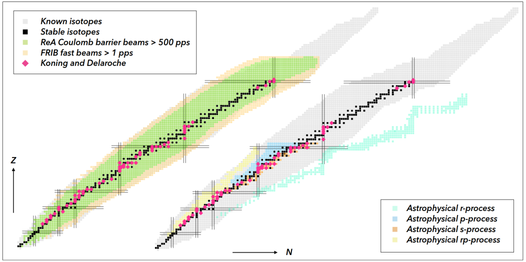
Nuclear reactions and the optical potential

Can you reduce the many-body degrees of freedom of a nuclear reaction problem to few?

Yes, with the optical potential!

...but it requires fitting and extrapolation

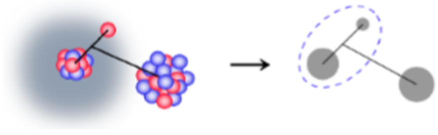




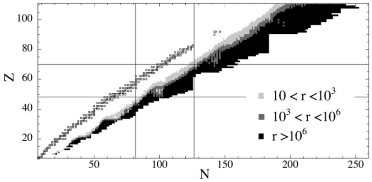
Optical potentials can be fit *locally* or *globally*, but only to stable isotopes[a]

[a] Hebborn et al. 2023, *Journal of Physics G: Nuclear and Particle Physics* 50(6), p. 060501

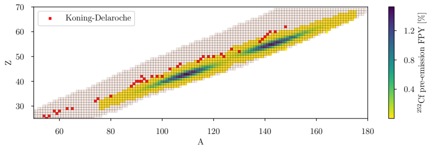
Nuclear reactions on rare isotopes involves extrapolating the optical potential



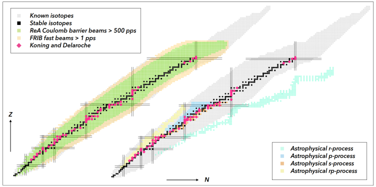
- Extrapolation of global optical potentials are ubiquitous in reaction analyses



(n, γ) rates for r-process [2]



de-excitation of fission fragments [1]



astrophysical processes, rare isotope beam experiments (and more!) [3]

[1] Beyer et al. 2025, *Phys. Rev. C* 112, p. 024604

[2] Goriely and Delaroche 2007, *Physics Letters B* 653(2-4), pp. 178–183

[3] Hebborn et al. 2023, *Journal of Physics G: Nuclear and Particle Physics* 50(6), p. 060501

Extrapolation off the line of stability is constrained by the charge-symmetry of the nuclear force

- Incorporated into the optical potential by Lane[4]

$$
\begin{aligned}
U(r) &= U_0(r) + 4\frac{\boldsymbol{\tau}\cdot\mathbf{T}}{A}U_1(r) \\
&= U_0(r) + \underbrace{4\frac{\tau_3 T_3}{A}U_1(r)}_{(N-Z)/A \text{ dependence in elastic scattering}} + \underbrace{4\frac{\tau_+ T_- + \tau_- T_+}{2A}U_1(r)}_{(p,n) \text{ to isobaric analog}}
\end{aligned}
$$

Goal: improve extrapolation in $(N-Z)/A$ by using $(p,n)_{\text{IAS}}$ as a constraint in a global, uncertainty-quantified optical potential

[4] Lane 1962, *Nuclear Physics* 35, pp. 676–685

(p, n) to the isobaric analog state

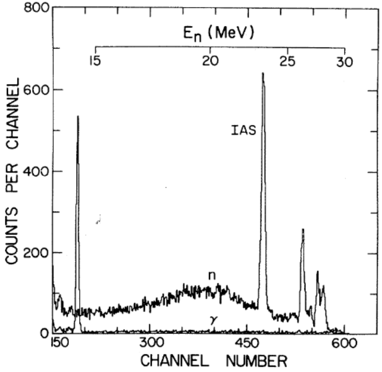
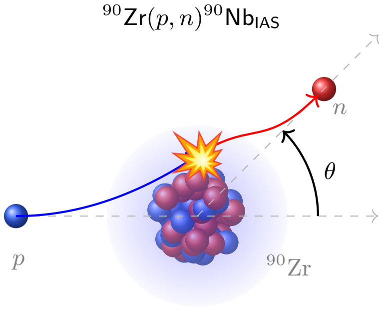


FIG. 1. Neutron (n) and γ-ray (γ) time-of-flight spectra at 0° for 35-MeV protons on ^{90}Zr. Each channel represents 0.1 nsec.

From measurements at MSU Cyclotron Lab [a]



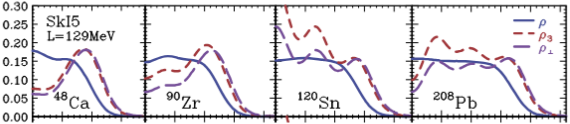
- replace a single neutron in the target with the incident proton
- probe of N, Z symmetry energy and neutron skins in nuclei

[a] Doering et al. 1975, *Physical Review C* 12(2), p. 378

The East Lansing Model

$$U(r;E,A,Z) = U_0(r;E,A) + \left(\frac{N-Z}{N+Z}\right) U_1(r;E,A)$$

- 24 parameters (compared to 22 for CHUQ, 48 for KDUQ)
- Lane-consistent, spherical, global, energy dependent
- Coulomb correction to all orders
- relationship between (p,n), isovector/neutron skins, and symmetry energy by Danielewicz et al[5]
- **Does this mean we can predict other observables, like neutron-skins and charge radii? Can we use other measurements of them as constraints?**



visitlearn.msu.edu/resources/facility-for-rare-isotope-beams
photos.msu.edu

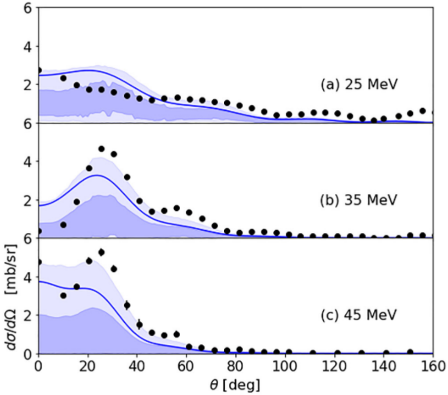
github.com/beykyle/elm

[5] Danielewicz et al. 2017, *Nuclear Physics A* 958, pp. 147–186

Calibration (and the software tools enabling it)

Progress on uncertainty quantification and extrapolation of the optical potential

- traditionally frequentist, least-squares fitting, a few parameters at a time
- parameter ambiguities (multi-modality) [6]
- state-of-the-art: 50 parameter model fit with computational steering, local/global hierarchy [7]
- Bayesian calibration and UQ with local potentials [8]
- first global Bayesian calibration demonstrates scattering on stable isotopes poorly constrains isovector potential[9]
- hence, large uncertainties for (p, n)[10] and for reactions on highly asymmetric isotopes [11]
- systematic errors, model discrepancy have been ignored



^{48}Ca (p,n)^{48}Sc$_{\text{IAS}}$

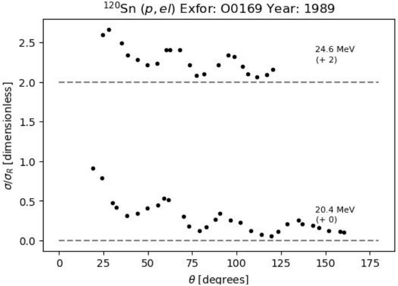
[6] Satchler et al. 1964, *Physical Review* 136(3B), B637
[7] Koning and Delaroche 2003, *Nuclear Physics A* 713(3-4), pp. 231–310
[8] Catacora-Rios et al. 2021, *Phys. Rev. C* 104, p. 9; Lovell et al. 2017, *Physical Review C* 95(2), p. 024611
[9] Pruitt et al. 2023, *Physical Review C* 107(1), p. 014602
[10] Smith et al. 2024, *Physical Review C* 110(3), p. 034602
[11] Goriely and Delaroche 2007, *Physics Letters B* 653(2-4), pp. 178–183

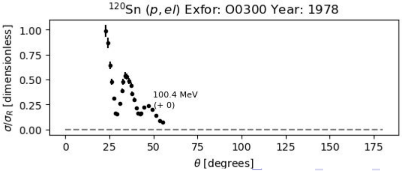
Curation of a body of experimental data

- $\sim$ 100 EXFOR entries, ~ 10K data points
- $40 \leq A \leq 208$
- $10 \text{ MeV} < \text{E}_{\text{lab}} < 200 \text{ MeV}$
- $d\sigma/d\Omega$ and A_y from elastic (p,p), (n,n)
- $d\sigma/d\Omega$ with clean $\Delta J^\pi = 0^+$ from $(p,n)_{\text{IAS}}$
- manual ID & cleaning of outliers
- types of error reported inconsistent

github.com/beykyle/exfor_tools

```python
all_entries_pp = exfor_tools.get_exfor_differential_data(
    target=target,
    projectile=proton,
    quantity="dXS/dA",
    product="EL",
    energy_range=[10, 200],  # MeV
)
```



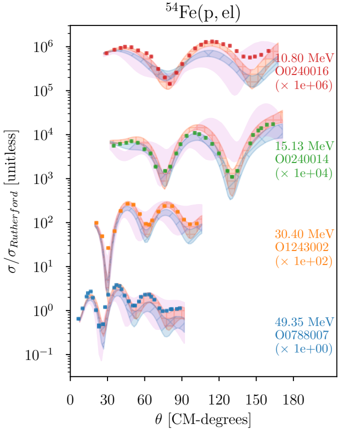


jit$\mathcal{R}$ allows for global calibration without needing emulators

philosophy:

Modular library for building workspaces which take in interaction models and spit out reaction observables

- calculable $\mathcal{R}$-matrix on Lagrange mesh [a]
- modular python library
- precompute everything you can
- `numba` just-in-time compilation, heavy `numpy` vectorization
- **2 orders of magnitude faster than comparable fortran codes**, just as fast as emulators [b] in UQ setting



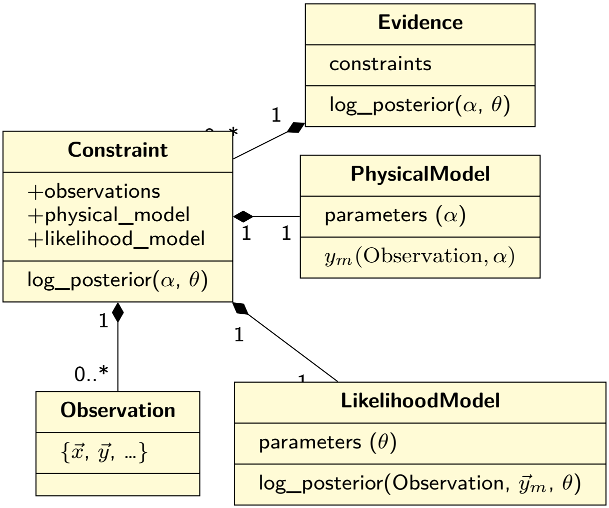
[a] Baye 2015, *Physics reports* 565, pp. 1–107
[b] Odell et al. 2024, *Physical Review C* 109(4), p. 044612

Open source, part of BAND framework [a]

[a] Beyer et al. 2023, (Version 0.3.0)

`rxmc`: spotlight on the body of evidence and the likelihood

- curating a body of evidence from multiple constraints
- Bayesian calibration with flexible likelihood models
- designed with `jit`$\mathcal{R}$ and `exfor-tools` in mind
- built-in MCMC, or just calculate the log posterior as input to another MCMC package (e.g. `surmise`)
- handles parametric likelihood models with Gibbs sampling
- alpha stage: https://github.com/beykyle/rxmc/



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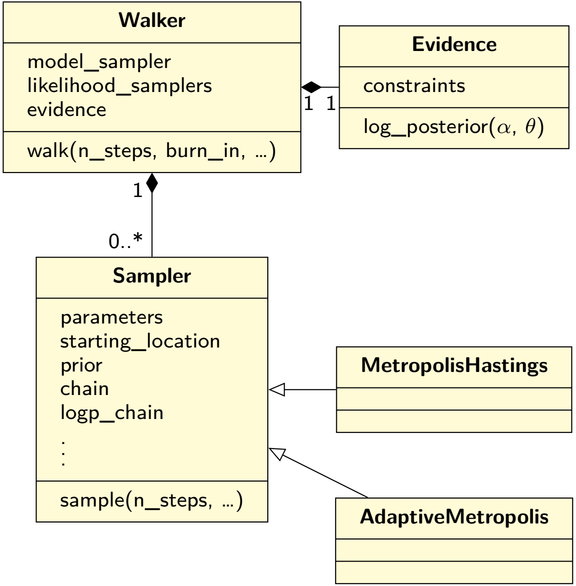
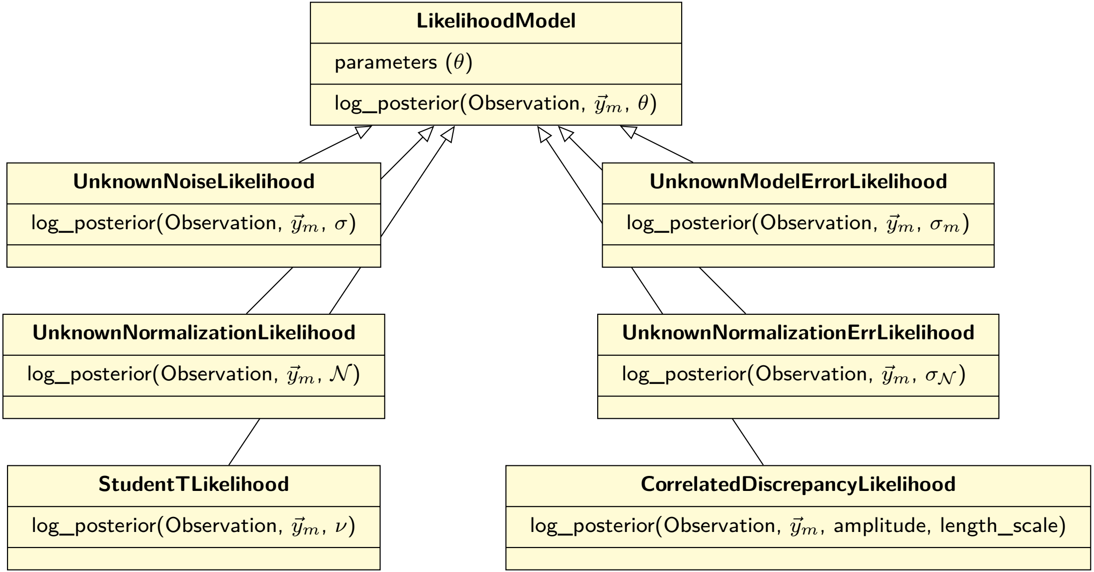


`rxmc`: spotlight on the body of evidence and the likelihood



Statistical model for ELM

$$\underbrace{p(\boldsymbol{\alpha}|\mathcal{D},\mathcal{M})}_{\text{posterior}} \propto \underbrace{p(\mathcal{D}|\boldsymbol{\alpha},\mathcal{M})}_{\text{likelihood}} \underbrace{p(\boldsymbol{\alpha})}_{\text{prior}}$$

Likelihood model:

$$\ln p(\mathcal{D}|\boldsymbol{\alpha},\mathcal{M}) = -\frac{1}{2}\left(\boldsymbol{\Delta}^\top \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{\Delta} + \ln\left((2\pi)^k\,|\boldsymbol{\Sigma}|\right)\right)$$
$$\Delta_i(\alpha) = y_{\mathcal{M}}(x_i,\boldsymbol{\alpha}) - y_i$$
$$\Sigma_{ij}(\alpha) = \delta_{ij}\left(\sigma^2_{exp,i} + \sigma^2_{UU,i}\right)$$

- $\boldsymbol{\Sigma}$ approximated as diagonal
- unaccounted-for-uncertainty is a free parameter

$$\sigma_{UU,i} \equiv \frac{1}{2}\epsilon(y_{\mathcal{M}}(x_i,\boldsymbol{\alpha}) + y_i)$$

Prior model

- estimated from posterior of prior calibrations w/out (p,n) [a]

[a] Pruitt et al. 2023, *Physical Review C* 107(1), p. 014602

Calibration

- Adaptive Metropolis-Hastings in Gibbs with `rxmc`
- Goodman-Weare from `emcee`[a]
- massively parallel computation

[a] Foreman-Mackey et al. 2013, *PASP* 125(925), p. 306; Goodman and Weare 2010, *Communications in applied mathematics and computational science* 5(1), pp. 65–80

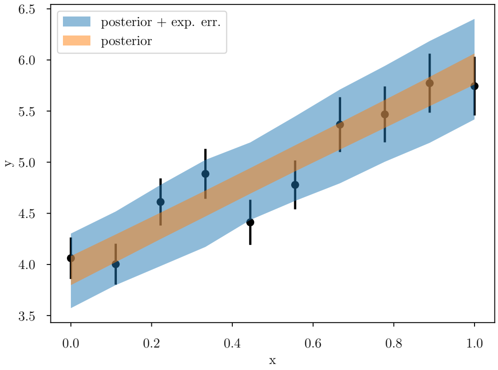
To re-scale or not to re-scale the log-likelihood? Are we overconfident if posterior credible intervals are narrow?

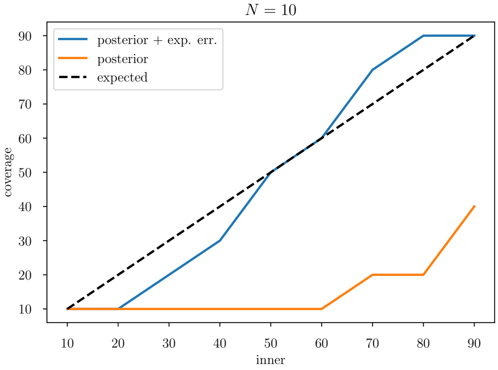
Pruitt et al[12] re-scaled the log likelihood by k/N (# of free parameters / # of experimental data points):

$$\ln p(\mathcal{D}|\boldsymbol{\alpha}, \mathcal{M}) \to -\left(\frac{k}{N}\right)\frac{1}{2}\left(\boldsymbol{\Delta}^{\top}\cdot\boldsymbol{\Sigma}\cdot\boldsymbol{\Delta} + \ln\left((2\pi)^{k}\,|\boldsymbol{\Sigma}|\right)\right)$$

[12] Pruitt et al. 2023, *Physical Review C* 107(1), p. 014602

Empirical coverage and the fallacy of overconfidence





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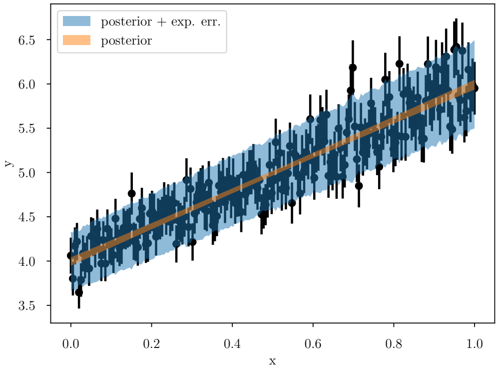
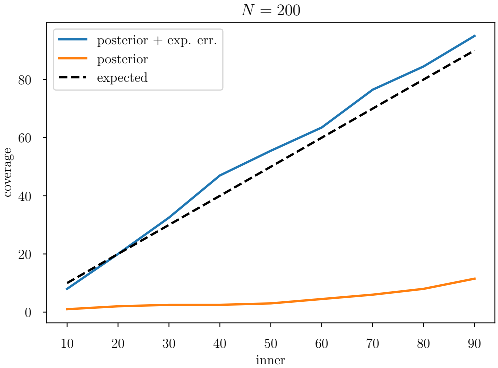
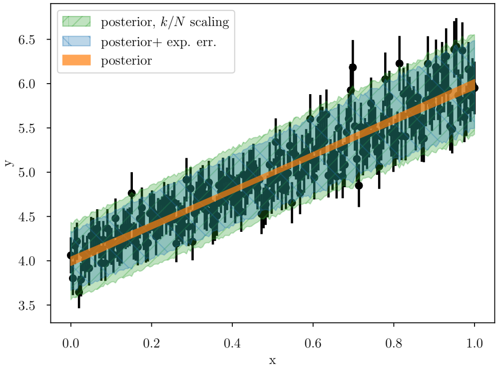
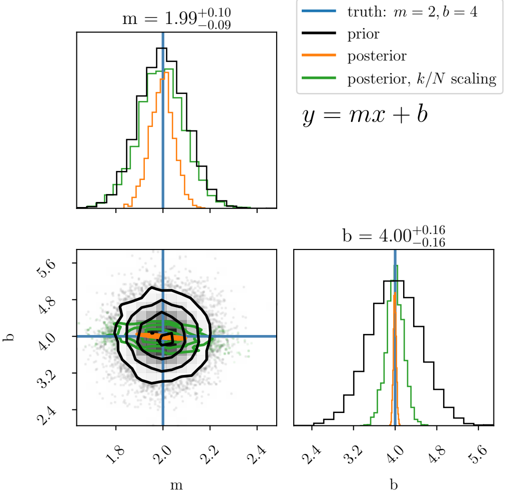




Re-normalizing the covariance leads to over-emphasis of the prior





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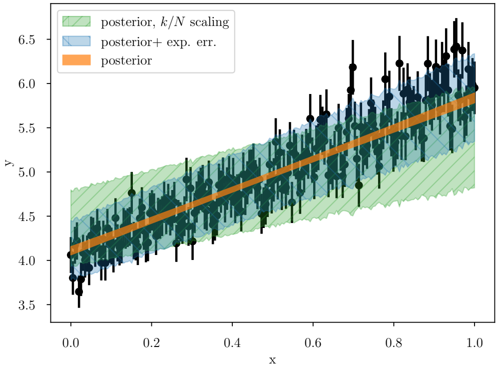

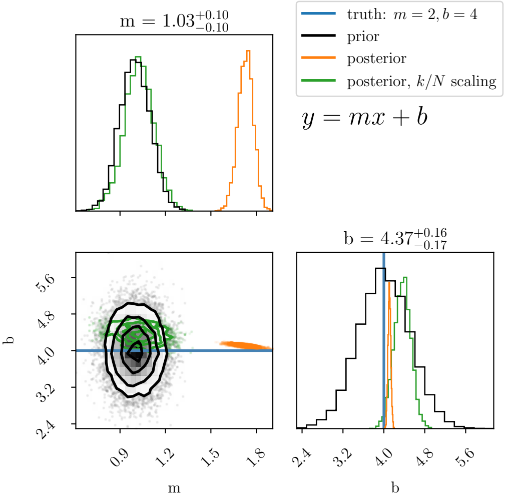

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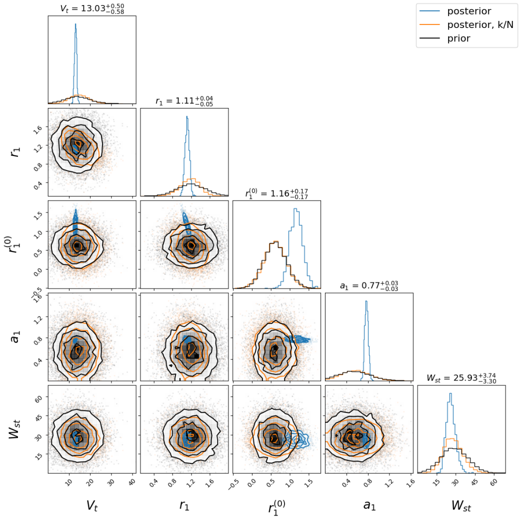
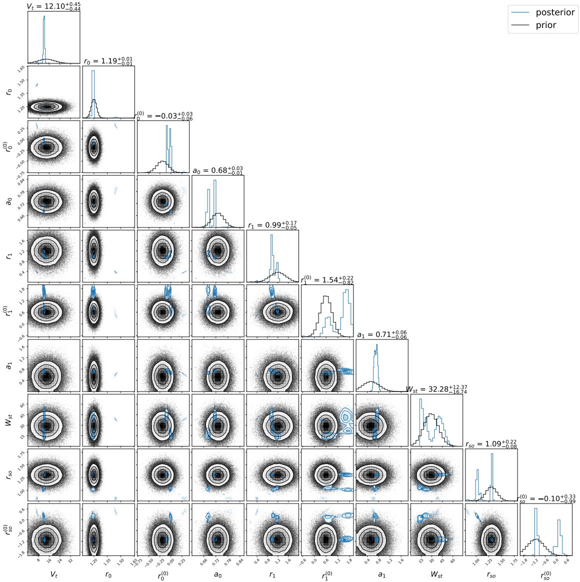


Removing subset of parameters and constraints removes multimodality



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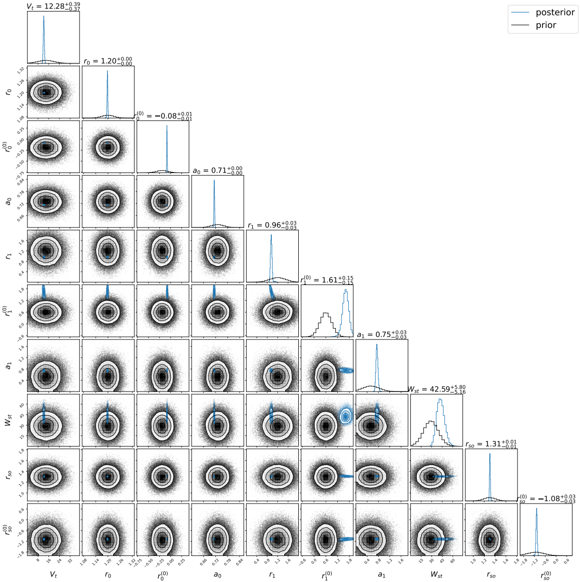
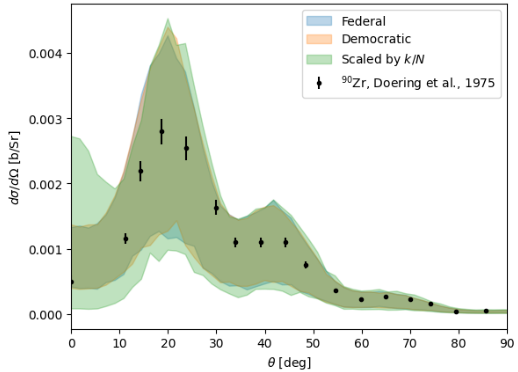
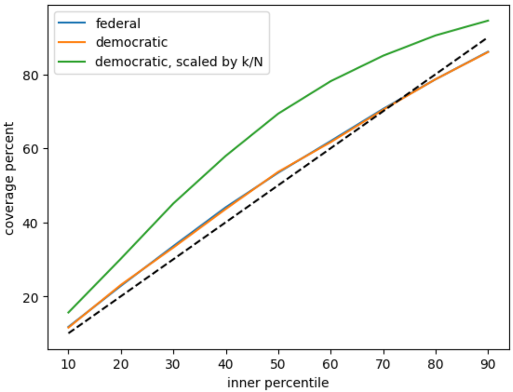


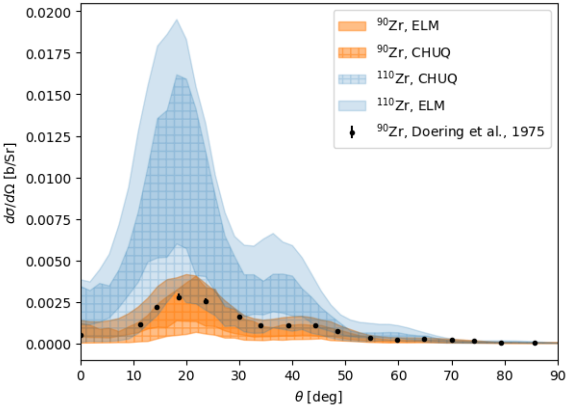
Predictive posteriors and empirical coverage





Extrapolation and uncertainty quantification

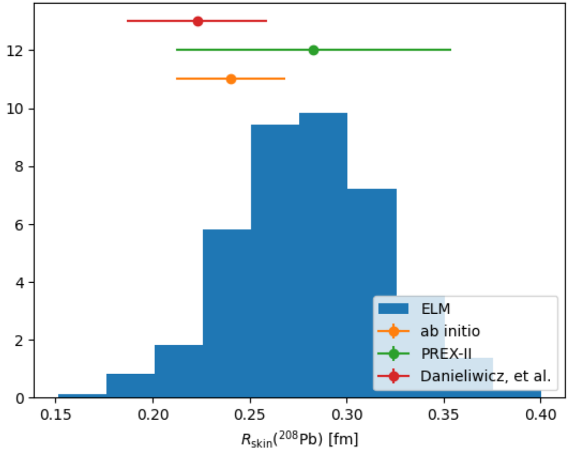
Extrapolation in $(N-Z)/A$



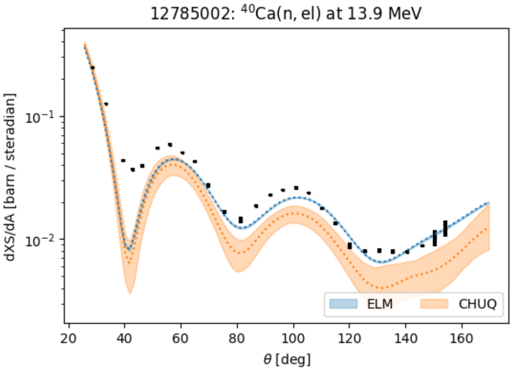
Problem: Model is function of $(N-Z)/A$, but model discrepancy model has no dependence on input space at all!

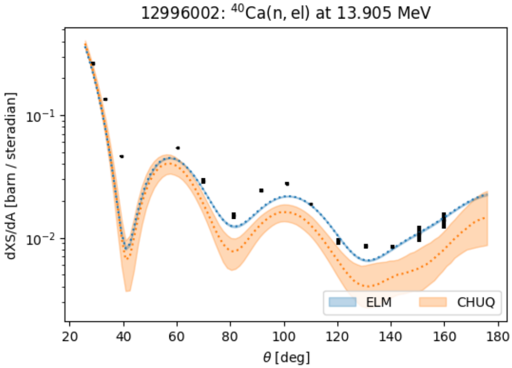
Reaching for another observable: neutron skins

Preliminary ...



Challenges in calbration





Aside: systematic error in the likelihood

Common approach is to introduce a normalization parameter $\mathcal{N}$:

$$\chi^2(\alpha) = \sum_i \frac{(y_i - \mathcal{N} y_m(x_i;\alpha))^2}{\sigma_i^2} + \frac{(\mathcal{N}-1)^2}{\sigma_\mathcal{N}^2} \tag{1}$$

This is incorrect! The correct approach is actually[13]:

$$\chi^2(\alpha) = \sum_i \frac{(\mathcal{N} y_i - y_m(x_i;\alpha))^2}{(\mathcal{N}\sigma_i)^2} + \frac{(\mathcal{N}-1)^2}{\sigma_\mathcal{N}^2} \tag{2}$$

One can implicitly marginalize over $\mathcal{N}$, which requires use of a non-diagonal covariance[14]. This relates to Peelle's Pertinent Puzzle in nuclear data evaluation[15].

[13] Giulio D'Agostini (1994). "On the use of the covariance matrix to fit correlated data". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 346.1-2, pp. 306–311; Ian J Thompson and Filomena M Nunes (2009). *Nuclear reactions for astrophysics: principles, calculation and applications of low-energy reactions*. Cambridge University Press.

[14] Roger Barlow (2021). "Combining experiments with systematic errors". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 987, p. 164864.

[15] R Frühwirth et al. (2012). "Peelle's pertinent puzzle and its solution". In: *EPJ Web of Conferences*. Vol. 27. EDP Sciences, p. 00008; Denise Neudecker et al. (2012). "Peelle's pertinent puzzle: A fake due to improper analysis". In: *Nuclear science and engineering* 170.1, pp. 54–60.

Handling multiple constraints with systematic errors

- statistical only:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2$$

- statistical error is fit parameter:

$$\Sigma_{ij} = \delta_{ij}(\eta\, y_m(x_i;\alpha))^2$$

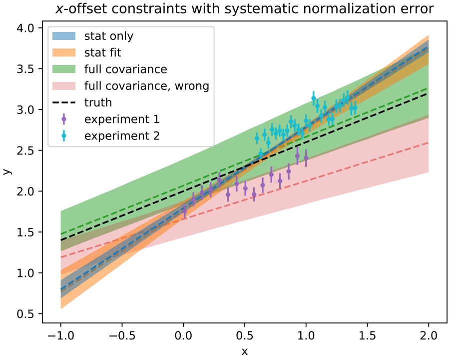
- full covariance:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2 + \sigma_N^2 y_m(x_i;\alpha) y_m(x_j;\alpha)$$

- full covariance, wrong:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2 + \sigma_N^2 y_i y_j$$

We have a high-schooler working on calibrating optical potentials accounting properly for systematic error!



https://github.com/beykyle/rxmc/blob/main/examples/systematic_err_demo.ipynb

Summary and outlook

ELM2025 coming soon!

- reasonable posteriors without re-scaling, prediction of $R_{\text{skin}}(^{A}Z)$
- an open-source software ecosystem for reaction phenomenology has been developed

Statistics outlook

- need model discrepancy model that is function of input space
- multi-modality in full model calibration? What orthogonal constraints can we fold in?
- handle errors in angle and narrow diffraction peaks
- handle systematic errors
- model mixing

Thank you for your time!

In collaboration with Filomena Nunes and the Few Body Reactions Group

BAND Bayesian Analysis of Nuclear Dynamics

MICHIGAN STATE UNIVERSITY

FRIB

Few Body Reactions Group

References I

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References II

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Extra slides: ELM physical model

$$U(r,E,A,Z) = U_0(r,E,A) \pm \frac{N-Z}{N+Z} U_1(r,E,A) + V_C$$

$$\begin{aligned}
U_0(r,E,A) = {} & V_0(E) f((r - R_0(A))/a_0) + iW_0(E) f((r - R_w(A))/a_w) \\
& - 4ia_w W_{s,0}(E) \frac{d}{dr} f((r - R_w(A))/a_w) + 2\,(\boldsymbol{\sigma} \cdot \boldsymbol{\ell})\ V_{so} \frac{1}{r} \frac{d}{dr} f((r - R_{so}(A))/a_{so}) \\
U_1(r,E,A) = {} & V_1(E) f((r - R_1(A))/a_1) - 4ia_w W_{s,1}(E) \frac{d}{dr} f((r - R_w(A))/a_w)
\end{aligned}$$

$$f(x) = \frac{1}{1+\exp(x)} \qquad R_i(A) = r_{i,0} + r_{i,A} A^{1/3} \qquad E_C = 6Z\alpha\hbar c/5R_C$$

$$\begin{aligned}
V_{0(1)}(E) &= V_{0(1)} - \alpha(E - E_C) \\
W(E) &= W \bigg/ \left(1 + \exp\left(\frac{\eta_W - (E - E_C)}{\lambda_W}\right)\right) \\
W_{s,0(1)}(E) &= W_{s,0(1)} \bigg/ \left(1 + \exp\left(\frac{(E - E_C) - \eta_s}{\lambda_s}\right)\right)
\end{aligned}$$

Extra slides: ELM statistical model and calibration

- Goodman-Weare [16] affine-invariante stretch move sampler from `emcee`[17], using default step-size ($a = 2$)
- 256 chains, 200,000 samples each
- massively parallel calibration requires ~ 3 days to run
- priors taken from CHUQ posterior
- priors for r_1^0, r_1^A and a_1 taken from Danielewicz[18]
- each data sector re-scaled to be equally important
- fractional uncertainties reasonably consistent with CHUQ: $\frac{d\sigma^{(n,n)}}{d\Omega}$: 35%, $\frac{d\sigma^{(p,p)}}{d\Omega}$: 44%, $A_y^{(n,n)}$: 140%, $A_y^{(p,p)}$: 155%, $\frac{d\sigma^{(p,n)}}{d\Omega}$: 55%

[16] Goodman and Weare 2010, *Communications in applied mathematics and computational science* 5(1), pp. 65–80
[17] Foreman-Mackey et al. 2013, *PASP* 125(925), p. 306
[18] Danielewicz et al. 2017, *Nuclear Physics A* 958, pp. 147–186

To re-scale or not to re-scale (the likelihood)

Pruitt et al[19] re-scaled the log likelihood by k/N (# of free parameters / # of experimental data points):

$$\ln p(\mathcal{D}|\boldsymbol{\alpha}, \mathcal{M}) = -\frac{k}{N}\frac{1}{2}\left(\boldsymbol{\Delta}^{\top} \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{\Delta} + \ln\left((2\pi)^{k}\,|\boldsymbol{\Sigma}|\right)\right)$$

We do not re-scale for ELM

[19] CD Pruitt et al. (2023). "Uncertainty-quantified phenomenological optical potentials for single-nucleon scattering". In: *Physical Review C* 107.1, p. 014602.

Charge exchange to isobaric analog states

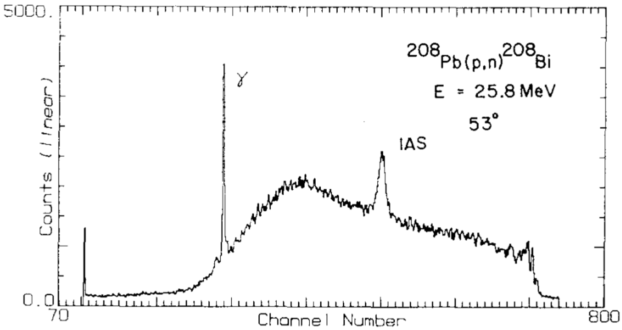
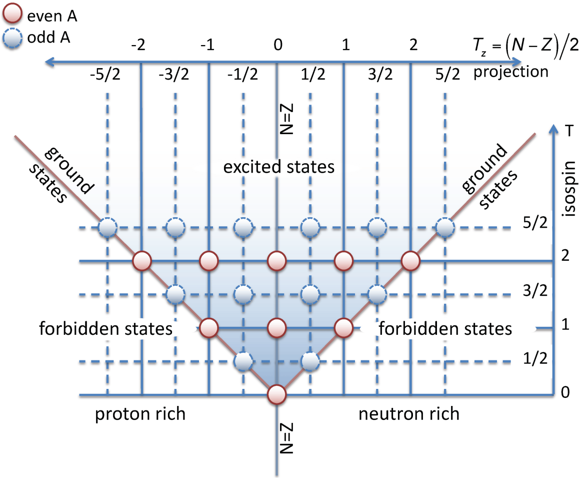


Fig. 1. Time-of-flight neutron spectrum for the reaction ^{208}Pb(p, n)^{208}Bi at 25.8 MeV showing the broad peak of the isobaric analogue state (IAS) and a narrow peak caused by incomplete rejection of γ-rays. The abscissa gives the time with units of 0.50 nsec per channel; higher energy neutrons are to the right in the spectrum. The flight path was approximately 9 m.

Reprinted from[20]

[20] SD Schery et al. (1974). "The (p, n) reaction to the isobaric analogue state of high-Z elements at 25.8 MeV". In: *Nuclear Physics A* 234.1, pp. 109–129.

Charge exchange to isobaric analog states



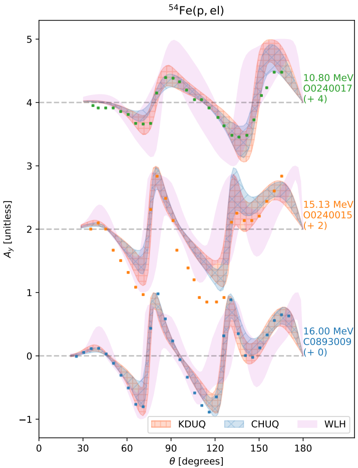
Reprinted from[21]

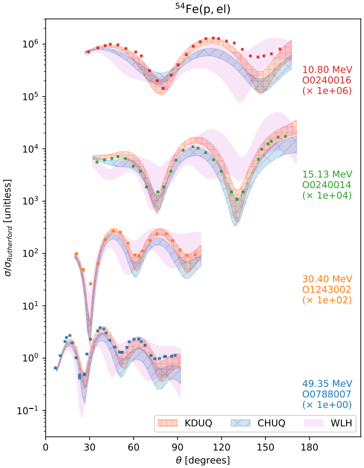
[21] Michael A Bentley (2022). "Excited States in Isobaric Multiplets—Experimental Advances and the Shell-Model Approach". In: *Physics* 4.3, pp. 995–1011. ISSN: 2624-8174. DOI: 10.3390/physics4030066. URL: https://www.mdpi.com/2624-8174/4/3/66.

jit$\mathcal{R}$ demos and tutorials: built-in optical potentials

```
[2]: from jitr.optical_potentials import chuq, kduq, wlh
```

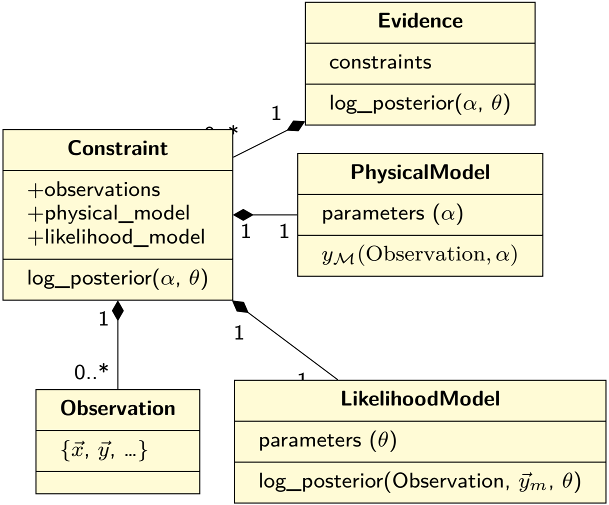
https://github.com/beykyle/jitr/blob/main/examples/notebooks/builtin_omps_uq.ipynb





`rxmc`: spotlight on the body of evidence and the likelihood

- curating a body of evidence from multiple constraints
- Bayesian calibration with flexible likelihood models
- designed with `jit`$\mathcal{R}$ and `exfor-tools` in mind
- built-in MCMC, or just calculate the log posterior as input to another MCMC package (e.g. `surmise`)
- handles parametric likelihood models with Gibbs sampling
- alpha stage: https://github.com/beykyle/rxmc/



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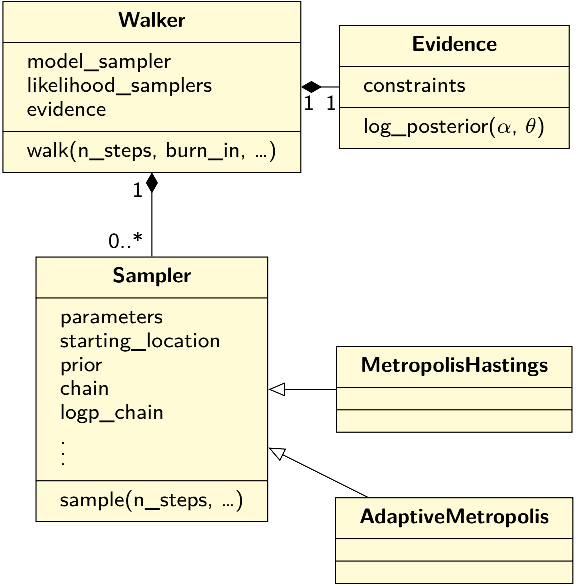
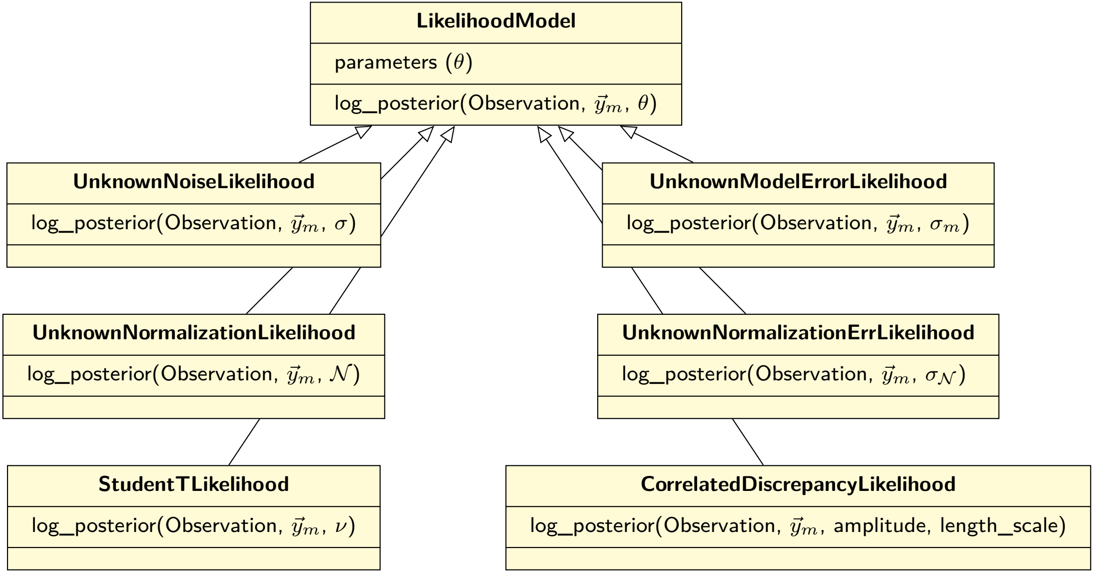


rxmc: spotlight on the body of evidence and the likelihood



Aside: systematic error in the likelihood

Common approach is to introduce a normalization parameter $\mathcal{N}$:

$$\chi^2(\alpha) = \sum_i \frac{(y_i - \mathcal{N} y_{\mathcal{M}}(x_i;\alpha))^2}{\sigma_i^2} + \frac{(\mathcal{N}-1)^2}{\sigma_{\mathcal{N}}^2} \tag{3}$$

This is incorrect! The correct approach is actually[22]:

$$\chi^2(\alpha) = \sum_i \frac{(\mathcal{N} y_i - y_{\mathcal{M}}(x_i;\alpha))^2}{(\mathcal{N}\sigma_i)^2} + \frac{(\mathcal{N}-1)^2}{\sigma_{\mathcal{N}}^2} \tag{4}$$

One can implicitly marginalize over $\mathcal{N}$, which requires use of a non-diagonal covariance[23]. This relates to Peelle's Pertinent Puzzle in nuclear data evaluation [24].

[22] D'Agostini 1994, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 346(1-2), pp. 306–311; Thompson and Nunes 2009

[23] Barlow 2021, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 987, p. 164864

[24] Frühwirth et al. 2012, vol. 27, p. 00008; Neudecker et al. 2012, *Nuclear science and engineering* 170(1), pp. 54–60

`rxmc` demos and tutorials: handling multiple constraints with systematic errors

- statistical only:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2$$

- fit (fractional) statistical error:

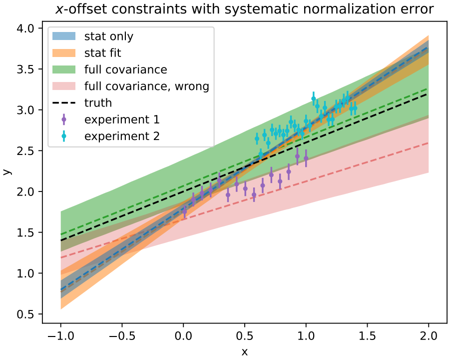
$$\Sigma_{ij} = \delta_{ij}(\eta\, y_{\mathcal{M}}(x_i;\alpha))^2$$

- full covariance:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2 + \sigma_N^2 y_{\mathcal{M}}(x_i;\alpha) y_{\mathcal{M}}(x_j;\alpha)$$

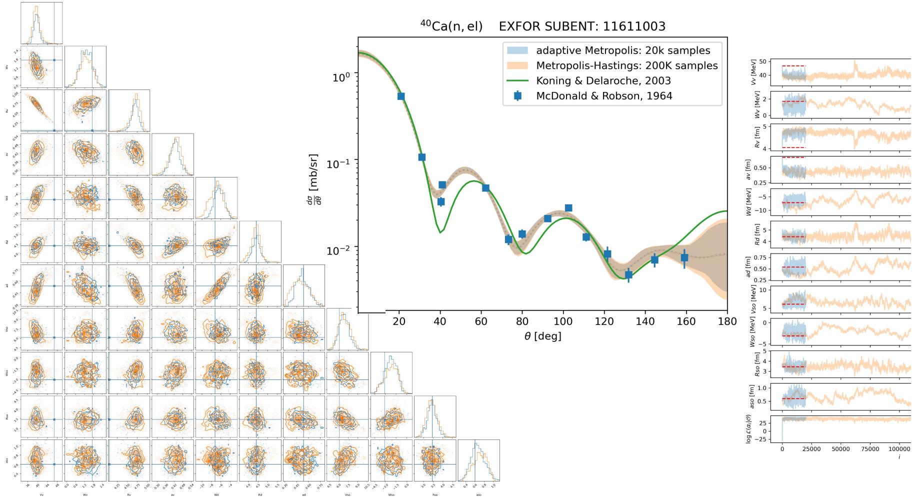
- full covariance, wrong:

$$\Sigma_{ij} = \delta_{ij}\sigma_i^2 + \sigma_N^2 y_i y_j$$



https://github.com/beykyle/rxmc/blob/main/examples/systematic_err_demo.ipynb

`rxmc` demos and tutorials: compare sampling algorithms for fitting an optical potential



https://github.com/beykyle/rxmc/blob/main/examples/fitting_an_optical_potential.ipynb

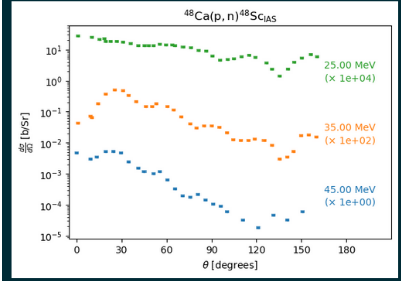
Curating a body of evidence

```
: entry_pn = ExforEntry(
      entry="00178",
      reaction=ca48_pn,
      quantity="dXS/dA",
      vocal=True,
      parsing_kwargs={
          "statistical_err_labels": ["DATA-ERR"],
          "systematic_err_labels": ["ERR-1"],
      },
  )
```

```
Found subentry 00178006 with the following columns:
['ERR-1', 'ERR-2', 'ERR-3', 'ERR-4', 'EN', 'Q-VAL', 'ANG-ERR', 'DATA-ERR', 'ANG-CM', 'DATA', 'ERR-T']
Found subentry 00178007 with the following columns:
['ERR-1', 'ERR-2', 'ERR-3', 'ERR-4', 'EN', 'Q-VAL', 'ANG-ERR', 'DATA-ERR', 'ANG-CM', 'DATA', 'ERR-T']
Found subentry 00178008 with the following columns:
['ERR-1', 'ERR-2', 'ERR-3', 'ERR-4', 'EN', 'Q-VAL', 'ANG-ERR', 'DATA-ERR', 'ANG-CM', 'DATA']
```

```
: fig, ax = plt.subplots(1, 1, figsize=(6, 4))
  entry_pn.plot(
      ax, offsets=100, label_kwargs={"label_xloc_deg": 165, "label_offset_factor": 0.0001}
  )
  ax.set_xlim([-5, 210])
  ax.set_title(ax.title.get_text() + r"$_\text{IAS}$")
```

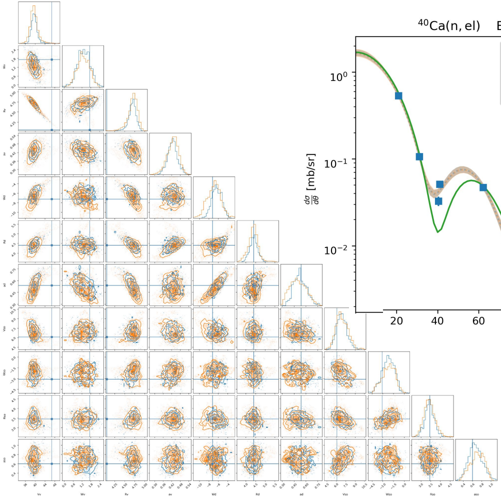
```
: Text(0.5, 1.0, '$^{48} \\rm{Ca}(p,n)^{48} \\rm{Sc}$$_\\text{IAS}$')
```

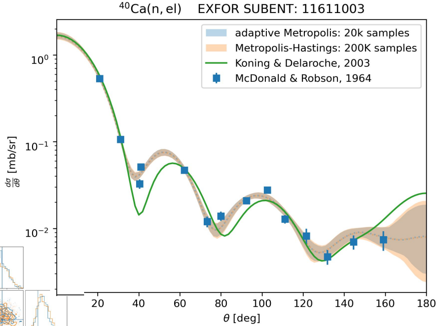


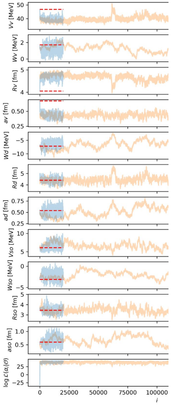
https://github.com/beykyle/exfor_tools

- reproducible curation
- systematically improvable with new evaluations

Comparison of sampling algorithms for fitting an optical potential







https://github.com/beykyle/rxmc/blob/main/examples/fitting_an_optical_potential.ipynb