Uncertainty quantification of an empirical shell-model interaction

using principal component analysis

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Progress in *Ab Initio* techniques in Nuclear Physics @ TRIUMF

March 5, 2020

Recent UQ in Nuclear Theory

- Jordan M. R. Fox, Calvin W. Johnson, and Rodrigo Navarro Perez.
  Uncertainty quantification of an empirical shell-model interaction using principal component analysis.
  (arXiv e-prints, page arXiv:1911.05208, November 2019.)
- Sota Yoshida, Noritaka Shimizu, Tomoaki Togashi, and Takaharu Otsuka.
  Uncertainty quantification in the nuclear shell model.
  (Phys. Rev. C, 98:061301, Dec 2018.)
- R. Navarro Pérez, J. E. Amaro, and E. Ruiz Arriola.
  Uncertainty quantification of effective nuclear interactions.
  (International Journal of Modern Physics E, 25(05):1641009, 2016.)
- J. D. McDonnell, N. Schunck, D. Higdon, J. Sarich, S. M. Wild, and W. Nazarewicz.
  Uncertainty quantification for nuclear density functional theory and information content of new measurements.
  (Phys. Rev. Lett., 114:122501, Mar 2015.)
- J Dobaczewski, W Nazarewicz, and PG Reinhard.
  Error estimates of theoretical models: a guide.
  (Journal of Physics G: Nuclear and Particle Physics, 41(7):074001, 2014.)
- R J Furnstahl, D R Phillips, and S Wesolowski.
  A recipe for EFT uncertainty quantification in nuclear physics.
  (Journal of Physics G: Nuclear and Particle Physics, 42(3):034028, feb 2015.)
- Silas R. Beane, William Detmold, Kostas Orginos, and Martin J. Savage.
  Uncertainty Quantification in Lattice QCD Calculations for Nuclear Physics.
  (J. Phys., G42(3):034022, 2015.)

...and many more!

Sensitivity analysis for effective interactions

Effective interactions treat single-particle energies and two-body matrix elements as *parameters* ($\boldsymbol{\lambda}$).

$$\hat{\mathcal{H}} = \sum_{rs} T_{rs} \hat{a}_r^\dagger \hat{a}_s + \frac{1}{4} \sum_{rstu} V_{rs,tu} \hat{a}_r^\dagger \hat{a}_s^\dagger \hat{a}_u \hat{a}_t$$

where $\{T_{rs}, V_{rs,tu}\} \equiv \boldsymbol{\lambda}$.

Our goals:

- Understand sensitivity with respect to data $\rightarrow$ **parameter covariance**
- Propagate uncertainty $\rightarrow$ **distributions of observables**

We study the **USDB** interaction [1], but these methods are general.

Details of Sensitivity analysis method

See poster.

Principle component analysis

Our sensitivity analysis approximates the parameter covariance matrix $C^{\boldsymbol{\lambda}}$ where

$$C^{\boldsymbol{\lambda}}_{ii} = \sigma^2(\lambda_i) \text{ , and } C^{\boldsymbol{\lambda}}_{ij} = \langle(\lambda_i - \langle\lambda_i\rangle)(\lambda_j - \langle\lambda_j\rangle)\rangle$$

Rather than interpret $C^{\boldsymbol{\lambda}}$, we perform a PCA transformation to get "PCA-parameters" $\boldsymbol{\mu}$ where

$$WC^{\boldsymbol{\lambda}}W^T = C^{\boldsymbol{\mu}} \text{ is diagonal. } (\boldsymbol{\mu} = W\boldsymbol{\lambda})$$

So, we obtain linear-combinations of matrix elements with no cross-correlations.

Principle component analysis

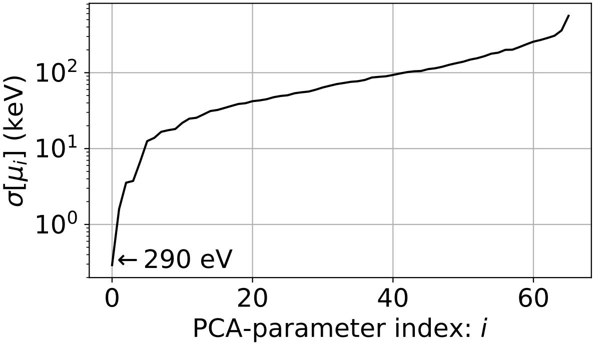

Figure: Ordered 1σ uncertainties of PCA-parameters. The most sensitive PCA-parameter is restricted to within 290 eV, while the majority are much less sensitive.

Uncertainty propagation

Since $C^{\boldsymbol{\mu}}$ is diagonal, we can sample the PCA-parameter distribution:

$$\boldsymbol{\mu}' \sim \mathcal{N}(\boldsymbol{\mu}, C^{\boldsymbol{\mu}})$$

and evaluate an observable using the parameterization $\boldsymbol{\lambda}' = W^T \boldsymbol{\mu}'$. We perform $\mathcal{O}(1000)$ perturbations to generate good statistics.

Observables of interest: reduced transition strengths $B(\mathrm{E2})$, $B(\mathrm{M1})$, $B(\mathrm{GT})$.

$$B(\mathcal{O}) = |\langle \Psi : J_f | \mathcal{O} | \Psi : J_i \rangle|^2 / (2J_i + 1) \text{ where } |\Psi\rangle = |\Psi(\boldsymbol{\lambda}')\rangle$$

Results: Electric quadrupole transitions

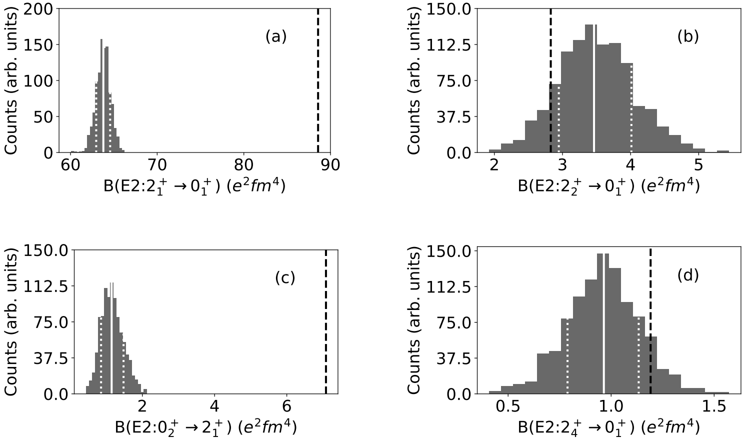

Figure: E2 transition strengths for ^{26}Mg. Black dashed line shows experimental value [2]. The the median values and uncertainty interval are highlighted in white.

Results: Magnetic dipole transitions

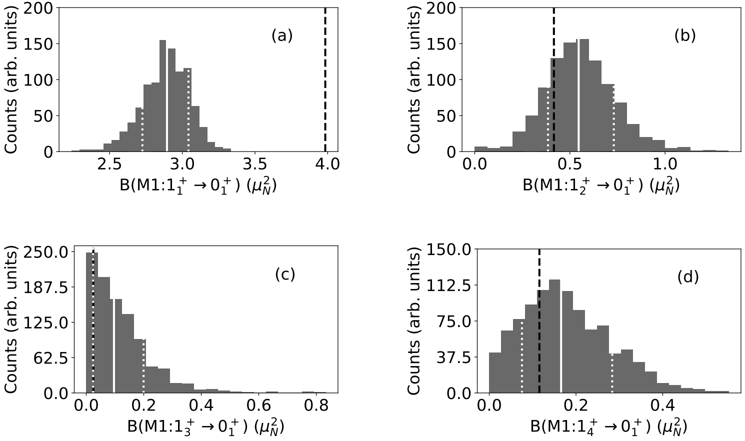

Figure: M1 transition strengths for ^{26}Al. Black dashed line shows experimental value [2]. The uncertainty interval is highlighted in white.

Results: Gamow-Teller transitions

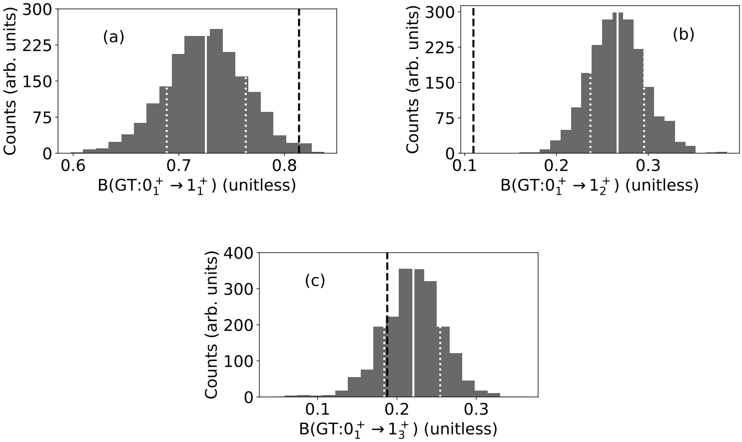

Figure: Gamow-Teller transition strengths for β^--decay of ^{26}Ne to ^{26}Na. Black dashed line shows experimental value [3]. The uncertainty interval is highlighted in white.

Thank you for listening!

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Sensitivity analysis procedure

Assuming errors are normally distributed, the parameter distribution is

$$P(\boldsymbol{\lambda}|D) \approx \frac{|H|^{1/2}}{(2\pi)^{k/2}} \exp\left[-\frac{1}{2}(\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\text{MAP}})^T H(\boldsymbol{\lambda} - \boldsymbol{\lambda}_{\text{MAP}})\right],$$

where H is the Hessian matrix,

$$H_{ij} = \frac{1}{2}\frac{\partial^2}{\partial\lambda_i\partial\lambda_j}\chi^2$$

where χ^2 is the sum of squared residuals,

$$\chi^2(\boldsymbol{\lambda}) = \sum_{\alpha=1}^{N}\left(\frac{E_\alpha^{SM}(\boldsymbol{\lambda}) - E_\alpha^{exp}}{\Delta E_\alpha}\right)^2.$$

Thus, finding parameter sensitivity is tantamount to computing H.