Local Bayesian mixture of different occupations for nuclear mass predictions

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Outline

1. Background
2. Bayesian framework
3. Nuclear models
4. Results
5. Conclusion

Global nuclear mass predictions

Many different theoretical frameworks

- Macroscopic-microscopic finite range droplet model
- Density functional theory
- Empricial microscopic shell models

Important for applications

- Nucleosynthesis, *r*-process

Previous work

Recent use of Bayesian inference

- Bayesian model averaging and uncertainty quantification[1]
  - Find most important/ "best" model
  - Uncertainty of each model
- Bayesian model mixing[2]
  - Localized model importance
  - Improve rms and uncertainty quantification

Could these methods be combined to inform local nuclear properties?

[1] Saito, Y., Dillmann, I., Kruecken, R., Mumpower, M. R., and Surman, R. (2024). Uncertainty quantification of mass models using ensemble bayesian model averaging. *Physical Review C*, 109(5):054301

[2] Kejzlar, V., Neufcourt, L., and Nazarewicz, W. (2023). Local bayesian dirichlet mixing of imperfect models. *Scientific Reports*, 13(1):19600

Bayesian model averaging

- Nuclear space $\mathcal{X} \ni x_i$, data D, masses predicted by models, $\mathcal{M}_1, \ldots, \mathcal{M}_p$
- "Standard" BMA:

$$p(\Delta|D) = \sum_{k=1}^{p} p(\Delta|\mathcal{M}_k, D) p(\mathcal{M}_k|D)$$

- Weights: $w_k = p(\mathcal{M}_k|D) \geq 0$, $\sum w_k = 1$
- Assume normal probability distributions:

$$p(\Delta(x_i)|\mathcal{M}_k, D) = \phi\left(\frac{\Delta(x_i) - m_k(x_i)}{\sigma_k}\right)$$

Local model mixing

- Introduce hyperparameters

$$\boldsymbol{w}(x_i)|\boldsymbol{\alpha}(x_i) \sim \mathrm{Dirichlet}(\boldsymbol{\alpha}(x_i))$$

- Gaussian process gives local dependence:

$$\alpha_k \sim \mathcal{GP}(\mu_k, \mathcal{K}(x_i, x_i'))$$

- $\mathcal{GP}$ depends on parameters $\mu_k, \eta_k, \rho_Z, \rho_N$

Inference procedure

- In total, parameters $\mu_k, \eta_k, \rho_Z, \rho_N, \sigma_k$
- Sample posterior distributions:
  joint posterior $\propto$ likelihood $\cdot$ prior
- We employ PyMC[1] for sampling

[1] Abril-Pla, O., Andreani, V., Carroll, C., Dong, L., Fonnesbeck, C. J., Kochurov, M., Kumar, R., Lao, J., Luhmann, C. C., Martin, O. A., et al. (2023). Pymc: a modern, and comprehensive probabilistic programming framework in python.
PeerJ Computer Science, 9:e1516

Microscopic shell model

- Duflo-Zuker shell model employs two different occupations
  - Natural occupation
  - Particle-hole excitations across HO shell closure
- Intermediate HO excitations of fewer nucleons
- Mixture model of different configurations
  - Particle hole excitations across SO and HO shell closures
- Higher order terms of Hamiltonian
- All fit to binding energy per nucleon for $N, Z \geq 28$

Results - Intermediate HO excitations

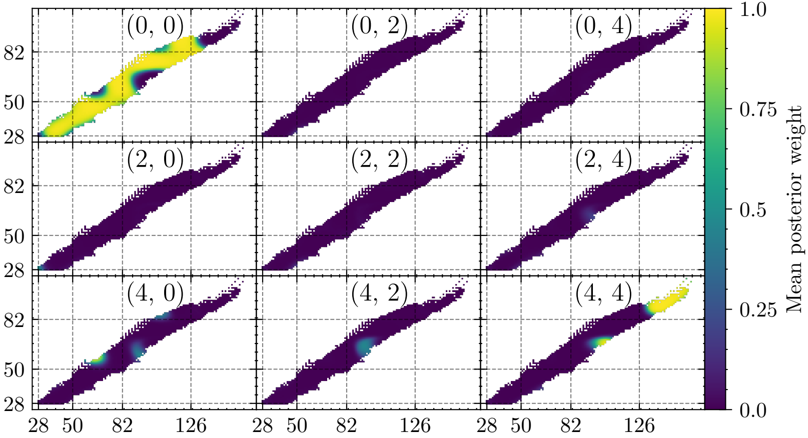


Figure: Posterior weights of mixture with intermediate promotions. Mean RMS: 677 keV, median RMS: 545 keV

Results - SO excitations

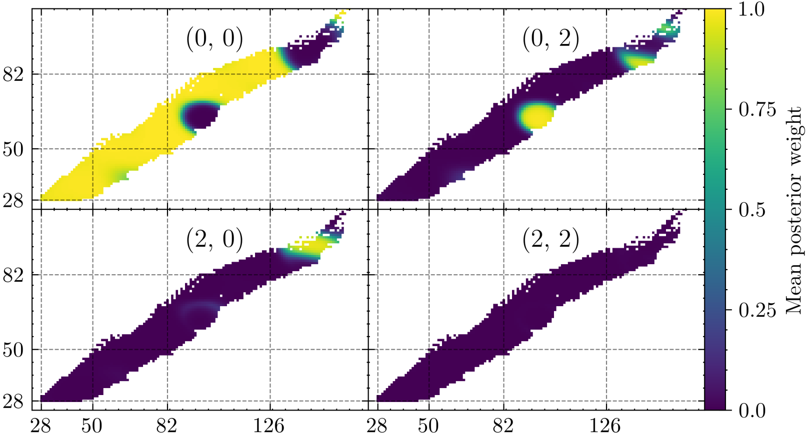


Figure: Posterior weights of mixture with intermediate promotions.

Results - SO promotions

- Mean RMS: 520 keV, median RMS: 505 keV.
- Mean σ_k:
  - (0, 0): 4.4 keV
  - (0, 2): 2.3 keV
  - (2, 0): 2.2 keV
  - (2, 2): 10 keV (corresponds to prior)

  Individual uncertainties for each model!

Uncertainty Quantification

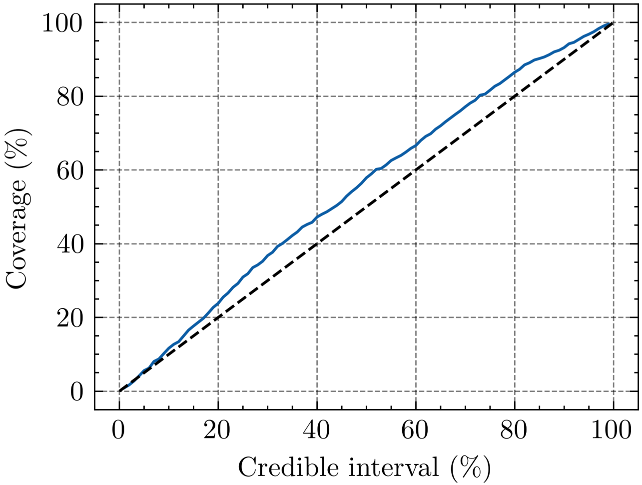


Figure: Credible intervals of posterior distributions vs coverage of experimental data, for the SO promotion model.

Conclusion

- Combination of Bayesian frameworks for local evaluation of models
- Can potentially be used to fit models with location dependent terms
- Demonstration of lower rms by local selection of models
- Uncertainty intervals correlate well with observed model coverage

Thank you!

Questions?

More on model setup

- Prior distributions:

$$\begin{aligned} \boldsymbol{\sigma} &\overset{\text{iid}}{\sim} \text{Gamma}(10, 1), \\ \mu_k &\sim \mathcal{N}(0, 1), \\ \eta_k &\sim \text{Gamma}(10, 2), \\ \rho_Z, \rho_N &\overset{\text{iid}}{\sim} \text{Gamma}(5, 2) \end{aligned}$$

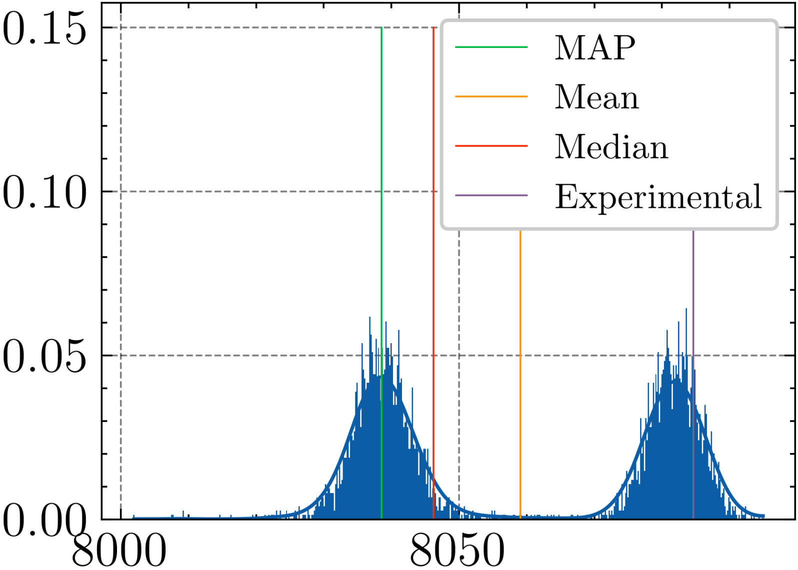
- No-U-Turn Sampler (NUTS) [1]
- Hilbert Space Gaussian Process approximation [2] implemented in PyMC.
- Covariance function

$$\mathcal{K}(x_i, x_i') = \eta_k \exp\left[-\frac{(Z - Z')^2}{2\rho_Z^2} - \frac{(N - N')^2}{2\rho_N^2}\right]$$

[1] Hoffman, M. D., Gelman, A., et al. (2014). The no-u-turn sampler: adaptively setting path lengths in hamiltonian monte carlo.
J. Mach. Learn. Res., 15(1):1593–1623

[2] Riutort-Mayol, G., Bürkner, P.-C., Andersen, M. R., Solin, A., and Vehtari, A. (2023). Practical hilbert space approximate bayesian gaussian processes for probabilistic programming.
Statistics and Computing, 33(1):17

Mean, median and MAP



Inferred existence probabilities