Discussion on UQ for $0\nu\beta\beta$

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Goal:
To arrive at a reasonable estimate of $0\nu\beta\beta$ transition strengths with a reasonable estimate of their uncertainties within a reasonable timeframe.

Idea:
Use Bayesian model averaging to combine various models with the goal to "average out" some systematic error and develop a collective "error bar".

Notes from last years DBD Topical collaboration meeting (Feb. 2021):
https://users.physics.unc.edu/~engelj/nsf-bb/0vBB_UQ_Workflow.pdf

Bayesian Model Averaging

Basic definitions and equations

We're sorry but equations make the expression of needs easier

$$P(\boldsymbol{X}_p|\boldsymbol{D}_e) = \sum_{m=1}^{n} P(\boldsymbol{X}_p|M_m, \boldsymbol{D}_e)P(M_m|\boldsymbol{D}_e)$$

PDF of **p**redictions given **e**vidence data

PDF of **p**redictions given a **m**odel

Prior for a **m**odel given **e**vidence

model evidence prior $$P(M_m|\boldsymbol{D}_e) = \mathrm{P}(\boldsymbol{D}_e|M_m)/\sum_{m=1}^{n} P(\boldsymbol{D}_e|M_m)$$

marginal likelihood $$P(\boldsymbol{D}_e|M_m) = \int P(\boldsymbol{D}_e|M_m\theta_m)P(\theta_m|M_m)d\theta_m$$

Model Evidence Likelihood

Calibrated Model Parameter Posterior

This integral is the hard part that tools such as emulators and the more robust UQ from BAND will enable. **But we can do something simpler and useful on the short term.**

~~Bayesian~~ Gaussian Model Averaging

Quick And Dirty Version

$$P(\boldsymbol{X}_p|\boldsymbol{D}_e) = \sum_{m=1}^{n} P(\boldsymbol{X}_p|M_m, \boldsymbol{D}_e) P(M_m|\boldsymbol{D}_e)$$

PDF of **p**redictions given **e**vidence data

PDF of **p**redictions given a **m**odel

Prior for a **m**odel given **e**vidence

model evidence prior

$$P(M_m|\boldsymbol{D}_e) = \mathrm{P}(\boldsymbol{D}_e|M_m) \Big/ \sum_{m=1}^{n} P(\boldsymbol{D}_e|M_m)$$

marginal likelihood

$$P(\boldsymbol{D}_e|M_m) \approx f_{\mathcal{N}(\boldsymbol{\mu}_{e,m}, \boldsymbol{\Sigma}_{ee,m})}(\boldsymbol{D}_e)$$

Multivariate Gaussian

$$\boldsymbol{\mu}_m = \begin{pmatrix} \boldsymbol{\mu}_{p,m} \\ \boldsymbol{\mu}_{e,m} \end{pmatrix}$$

$$\boldsymbol{\Sigma}_m = \begin{pmatrix} \boldsymbol{\Sigma}_{pp,m} & \boldsymbol{\Sigma}_{pe,m} \\ \boldsymbol{\Sigma}_{ep,m} & \boldsymbol{\Sigma}_{ee,m} \end{pmatrix}$$

~~Bayesian~~ Gaussian Model Averaging

Quick And Dirty Version

$$P\left(\boldsymbol{X}_p \middle| \boldsymbol{D}_e\right) = \sum_{m=1}^{n} P\left(\boldsymbol{X}_p \middle| M_m, \boldsymbol{D}_e\right) P\left(M_m \middle| \boldsymbol{D}_e\right)$$

PDF of **p**redictions given **e**vidence data

PDF of **p**redictions given a **m**odel

Prior for a **m**odel given **e**vidence

$$\widehat{\boldsymbol{X}}_p = \sum_{m=1}^{n} \widehat{\boldsymbol{X}}_{p,m} P(M_m|\boldsymbol{D}_e)$$

Conditioned mean vector of model outputs

$$\widehat{\boldsymbol{\Sigma}}_{pp} = \sum_{m=1}^{n} \left(\widehat{\boldsymbol{\Sigma}}_{p,m} + \widehat{\boldsymbol{X}}_{p,m}\widehat{\boldsymbol{X}}_{p,m}^{\intercal}\right) P(M_m|\boldsymbol{D}_e) - \widehat{\boldsymbol{X}}_p\widehat{\boldsymbol{X}}_p^{\intercal}$$

Conditioned covariance matrix of model outputs

$$\widehat{\boldsymbol{X}}_{p,m} = \boldsymbol{\mu}_{p,m} + \boldsymbol{\Sigma}_{pe,m}\boldsymbol{\Sigma}_{ee,m}^{-1}\left(\boldsymbol{D}_e - \boldsymbol{\mu}_{e,m}\right)$$

$$\widehat{\boldsymbol{\Sigma}}_{pp,m} = \boldsymbol{\Sigma}_{pp} - \boldsymbol{\Sigma}_{pe,m}\boldsymbol{\Sigma}_{ee,m}^{-1}\boldsymbol{\Sigma}_{ep,m}$$

Poor-man's ansatz: hierarchical ~~Bayesian~~ Gaussian model averaging

1. Compute observables needed
   - Ab initio *(too expensive to fully quantify covariances w/o emulators)*
   - Other models (directly estimate covariances)

2. Apply Quick and Dirty BMA on each method separately *(for ab initio)*
   - Compute mean vectors and covariance matrices conditioned on some subset of evidence data.
   - Compute Gaussian BMA weights on subset of evidence data
   - Compute BMA means and covariances

3. Compute mean vectors and covariance matrices conditioned on some global (all methods and models) full set of evidence data.

4. Compute Gaussian BMA weights on a subset of evidence data

5. Compute BMA means and covariances

Everything needed for Q&D BMA is a needed input for robust UQ down the road!
This is a way to offer useful preliminary predictions to experimental collabs ASAP!

Poor-man's ansatz: hierarchical ~~Bayesian m~~ Gaussian model averaging

1. Compute observables needed
   - Ab initio models *(too expensive to fully quantify covariances w/o emulators)*
   a) Compute observables for an many chiral interactions as possible. Non-converged results with an estimate of convergence uncertainty are better than not computing anything.
   b) Estimate systematic uncertainties
      - Method uncertainties
      - Convergence error
   c) When possible, estimate 1-σ uncertainties and covariances.
   - Other models *(directly estimate covariances)*
   a) Compute observables
   b) Estimate 1-σ uncertainties and covariances.

Data and pseudo-data to be computed

In the DBD candidates ^{48}Ca, ^{76}Ge, ^{130}Te, ^{136}Xe:

- Single β-decay rates in nearby nuclei, e.g., intermediate nucleus in decay
- β^- strength distribution from initial nucleus
- β^+ distribution from final nucleus
- $2\nu\beta\beta$ matrix elements
- Magnetic moments and M1's in three nuclei involved in decay
- E2 to lowest 2^+ state in initial and final nuclei
- Energies of lowest few excited states
- Charge radii
- Synthetic data, e.g., $nn \rightarrow ppe^-e^-$ transition amplitude
- 100MeV transfer scale OBS

Other heavy nuclei, not necessarily experimental candidates, would also be useful.
With ab initio methods, we should use 3-4 interactions:

- 1.8/2.0 (EM)
- N3LO L-NL
- N3LO GO, N2LO$_{sat}$, others?

With the phenomenological shell model, a few different interactions could be employed.

Poor-man's ansatz: hierarchical ~~Bayesian~~ Gaussian model averaging

2. Apply Quick and Dirty BMA on each method separately *(for ab initio)*
   - Compute mean vectors and covariance matrices conditioned on some subset of evidence data.
   - Compute Gaussian BMA weights on subset of evidence data
   - Compute BMA means and covariances
   - Low model/space fidelity is more than adequate for estimating covariances

What sort of data and pseudo-data to be should be used to build ab initio covariances?

Many computations are involved: emulators will be valuable!

How sophisticated do they need to be compared to what is needed for BAND?