Bayesian Evaluation Framework for Imperfect Differential and Integral Data or Models
ORNL ND10 Task FY 2022 Report
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Technical Program Review Meeting,
Motivation and Overview

• ORNL ND-10 Task:
  – advance UQ methods for NCSP
  – Differential Nuclear Data and Integral Benchmarks

• FY 2022 activities:
  – Documentation
  – Conference Presentations and Proceedings

• High level overview of the framework

Note: everything else being the same, consistency with Bayes' theorem in this framework improves the likelihood of success. Reliability of a given evaluations still depends on evaluator’s skill/expertise.
Common assumptions used in Bayesian ND evaluations

1. **Linearity:**
   - all models are linear

2. **Normality:**
   - all probability distribution functions are normal, i.e., Gaussian

3. **Perfection:**
   a) The model provides a perfect description of the measured data
   b) The data are perfect and complete *(including the covariances)*
These assumptions can now be selectively removed or enforced

- **Linearity** and **Normality**:  
  - e.g. Metropolis Hastings Monte Carlo (MHMC); known as Bayesian Monte Carlo

- **Perfection**:  
  - Evaluator can remove this assumption by specifying posterior expectation values and covariance of deviations between the model and data

**Note:** everything else being the same, consistency with Bayes' theorem in this framework improves the likelihood of success. Reliability of a given evaluation still depends on evaluator's skill/expertise.
Illustrating a mechanism behind small evaluated uncertainties

• Example: suppose a large number (“N”) of identical measurements
  – Suppose measurements are identical in value as well as uncertainty
    • This enables focus on evaluated covariance/uncertainty since the mean values are unaffected
  – Suppose that the correlation among measurements is set to 0
  – Bayes’ theorem then yields uncertainty $\rightarrow$ 0 as $N \rightarrow$ infinity (illustrated below)
    • Unrealistically small evaluated uncertainties are rectified by inflating them until reasonable
  – The uncertainties are underestimated less apparently for any value of $N$

• Our Bayesian framework provides tools to address this problem.
Conventional evaluation workflow is not completely Bayesian:

1. Evaluator uses expert judgment to align measured data sets before the evaluation
2. Bayesian evaluation is performed (implicitly) assuming *perfect* data and model
3. Unrealistically small uncertainties are inflated manually afterwards
New framework enables completely Bayesian evaluations:

1. Evaluator estimates the effect of imperfections by setting Bayesian posterior expectation values of deviations as well as their covariances
   - Deviation is defined as a difference between the evaluated data and model
   - Evaluators’ expert judgment (or intuition) now formally recognized within Bayes’ theorem!

2. Bayesian evaluation is now determined by the deviations defined in 1.
   - No need to manually inflate evaluated uncertainties as in Step 3. previously
Illustration cont’d.:

By virtue of setting **NON-zero** constraints on the posterior covariance matrix of deviations between the model and data.
Benefits of a generalized form of the Bayes’ Theorem (BT):

• It could improve evaluations of any data, separately or jointly
  – differential cross sections (SAMMY),
  – integral benchmarks (TSURFER/SAMPLER), …

• Enables *Bayesian Monte Carlo* evaluation of *large data sets*
  – Useful for, e.g., TSL evaluations of SNS data, RRR, …

• Enables *Bayesian* evaluation of:
  – *inconsistent* data sets, and/or
  – *defective* model

• Conventional BT is recovered when imperfections made to vanish
  – A seamless connection to the BT in SAMMY/TSURFER/SAMPLER

• API implementation in the SCALE code system
Promising new applications of our Bayesian framework:

• Foundation for the next generation of Bayesian evaluation tools:
  – TSL: ORNL ND-11
  – TSL + RRR: ORNL ND-9
  – TSL + RRR + IBE: NSR&D

• Machine Learning (ML):
  – revisiting UQ of Bayesian Neural Networks to address small uncertainties!
  – ORNL SEED Money project 2022-23 for nuclear data

• UQ for ML in Proliferation Detection
  – DNN R&D 2024 FOA: Data Science whitepaper submitted…
ORNL ND10 FY2022 Publication summary:

• ORNL/TM-2022/2448 Technical Report

• ANS Winter Meeting 2022:

• ND 2022:
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