

Bayesian Optimization for Subcritical Benchmark Design

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Introduction

- Purpose: optimize a limited number of physical measurement parameters, using Bayesian sampling to reduce the number of design simulations
- Application: subcritical neutron multiplication (M_L) inference benchmark measurements involving the BeRP ball
 - \circ 4.5 kg α -phase plutonium sphere
- Method: maximize the sensitivity of k_{eff} to a specific cross-section or set of cross-sections of interest [1,2]
 - $\,\circ\,$ Sensitivity of k_{eff} is both faster to obtain and proportional to the sensitivity of M_L [3]

Introduction

- Subcritical measurement: any type of SNM in any subcritical configuration
- Benchmark measurement:
 - All physical parameters and uncertainties are well characterized to a high degree of accuracy
 - (Preferably) peer reviewed and compiled with other benchmark experiments into a database
- Subcritical benchmark inferred multiplication measurement: subcritical benchmark measurement that uses time correlations in the measured signal to infer the leakage multiplication of the system

Theory

- Sample a few points equally spaced along the unknown sensitivity curve
 - $_{\odot}$ "Sampling" is completing a KSEN run
- Use Gaussian process (GP) fitting to fit a curve and associated uncertainties to the sample points
- Use a utility function to determine the next point to sample
 Outility function trades off between exploration and exploitation
- Process repeats until a point is found that is higher than all other points in the GP curve
- Maximum of the sensitivity curve can be converged upon intelligently, without having to brute-force sample the entire curve
 - However, complete and exact sensitivity information is not obtained

Results and analysis - SCR α P

- Bayesian optimization algorithm has been tested and shown to quickly converge upon optimized measurement configurations for both the already completed SCRαP benchmark and a BeRP-Mo benchmark
- Applied to a specific portion of SCRαP design process, to determine the configuration at which the sensitivity of k_{eff} to the ⁶³Cu crosssection in the intermediate energy range (0.625eV-100keV) is maximized
- Total possible BeRP reflection thickness of 4"
- Using a combination of HDPE and Cu thicknesses
- Step 1: beginning with 4" of Cu, determine the inches of reflection of Cu which, if replaced by HDPE, yields the maximum sensitivity
- Algorithm required only 15 sampled points to converge, compared to the 99 points generated by the brute-force method

Results and analysis - SCR α P

 Algorithm output an optimized HDPE thickness of 0.4", yielding a maximum sensitivity of 0.0180 (compared to 0.0187 KSEN maximum, at 0.32")



Results and analysis - SCR α P

- In order to be more consistent with the SCRaP benchmark, which included discrete 0.5" thick shells of HDPE and Cu, the optimized thickness was rounded up to 0.5" (corresponding to a sensitivity of 0.0177)
- Step 2: using the optimum HDPE thickness, determine the optimal position of the 0.5" thick HDPE shell within the total 4" reflector thickness
- Algorithm required only 8 sampled points to converge, compared to the 69 points generated by the brute-force method
- Algorithm output an optimized HDPE position of 0" from the BeRP ball, yielding a maximum KSEN output of 0.0180

Results and analysis - SCRαP



- Final result: configuration involving the BeRP ball reflected by an inner layer of 0.5" of HDPE, followed by 3.5" of Cu
 - This is identical to configuration 15 of the benchmark, yields the same maximum sensitivity of 0.018 that was reported in the design process [4,5], and required only 23 KSEN runs as opposed to the 168 runs that would have been required by the brute-force method

Some comments

- Uncertainties of GP curves are inherently larger in regions where fewer sampled points exist
- Noisiness in the underlying brute-force curves and sampled points can create false structure in GP fitted curves
 - Noise can be reduced by running the MCNP inputs for longer, but this will of course increase the overall computation time
 - Trade-off between more precisely fitted sensitivity curves and lower computation time
- If only the maximum or minimum point of the curve is of interest, then the precise shape of the rest of the curve is somewhat irrelevant

- Natural Mo isotopes: 92, 94, 95, 96, 97, 98, and 100
- Applied Bayesian optimization algorithm to BeRP-Mo design process, to determine the configurations at which the sensitivity of k_{eff} to the Mo cross-sections in the intermediate energy range is maximized
- Total possible BeRP reflection thickness of 6"
- Using a combination of HDPE and Mo thicknesses
- Step 1: beginning with 6" of Mo, determine the inches of reflection of Mo which, if replaced by HDPE, yields the maximum sensitivity
- Algorithm required only 15 sampled points per isotope to converge, compared to the 100 points generated for each isotope by the bruteforce method

 Algorithm output an optimized HDPE thickness of 0.4-0.52", yielding maximum sensitivities of 0.0009-0.0059 (compared to 0.0059 KSEN maximum, at 0.6", for isotope 98)



- Again for simplicity, the optimized thickness was rounded up to 0.5" for all isotopes
- Step 2: using the optimum HDPE thickness, determine the optimal position of the 0.5" thick HDPE shell within the total 6" reflector thickness
- Algorithm required an average of only 16 sampled points per isotope to converge, compared to the 137 points generated for each isotope by the brute-force method
- For each isotope the algorithm output an optimized HDPE position of 0.04" (isotopes 92, 94, 96, 98, and 100), 1.52" (isotope 95), or 1.92" (isotope 97) from the BeRP ball, yielding maximum KSEN outputs between 0.0016 and 0.0059

- Configuration 1: BeRP ball reflected by 0.5" of HDPE, followed by 5.5" of Mo
 - Maximizes sensitivity to isotopes 92, 94, 96, 98, and 100 (at 0.0056 for 98, compared to the identical maximum KSEN output of 0.0056 at 0")



- Configuration 2: BeRP ball reflected by 1.5" of Mo, followed by 0.5" of HDPE, and then 4" of Mo
 - Maximizes sensitivity to isotope 95 (at 0.0034 at 1.52", compared to the maximum KSEN output of 0.0039 at 1.64")



- Configuration 3: BeRP ball reflected by 2" of Mo, followed by 0.5" of HDPE, and then 3.5" of Mo
 - Maximizes sensitivity to isotope 97 (at 0.0018 at 1.92" compared to the maximum KSEN output of 0.0020 at 1.68")
- Converging on these 3 configurations required only 217 KSEN runs as opposed to the 1659 runs required by the brute-force method



Conclusions

- A Bayesian optimization algorithm for benchmark experiment design has been developed
- The algorithm was able to converge on optimal measurement configurations that yielded maximized sensitivities to cross-sections of interest
 - \circ For both SCR α P and BeRP-Mo benchmarks
- Convergence is reached using much fewer simulations than the bruteforce method requires
- The Bayesian optimization framework can be applied to various types of experimental design, and is not specific to the subcritical neutron multiplication inference benchmark design presented in this work

Conclusions

- Bayesian optimization is best applied when the design process involves finding the point of maximum or minimum value of a specific parameter over a wide range of values of a small number of measurement design inputs
- The method loses its usefulness when applied to design processes that involve many parameters that are to be tweaked in order to find an optimal combination
 - In this case, an optimization framework such as a genetic algorithm would be more suitable

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