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Proposal Review 1: 2152988

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Agency Name: **National Science Foundation**

Agency Tracking Number: 2152988

Organization:

NSF Program: CDS&E-MSS

PI/PD: Hickernell, Fred

Application Title: Collaborative Research: Quasi-Monte Carlo for Efficient Simulation

Multiple Rating: (Very Good/Good) Rating:

Review

Summary

In the context of the five review elements, please

evaluate the strengths and weaknesses of the proposal with respect to intellectual merit.

Intellectual Merits (IM):

The proposed work will focus on developing the open source package QMCPy along with addressing methodological and theoretical issues associated with QMC. The proposed methods will be applied to two important applications: big data analysis; and expensive Bayesian modeling. If successful, the proposal will significantly advance statistics and will provide computational tools for dealing with big-data challenges.

The resource is adequate and available to PIs to carry out the proposed work.

Strengths of IM:

- 1. The LD sequence generators including higher-order digital sequence will be implemented in the package. These generators are not yet available in popular libraries.
- 2. The code will be speed up with re-writing critical Python code in C.
- 3. The code will provide user-friendly interface for interfacing with other libraries such as SciPy, TensorFlow.
- 4. The proposal will also tackle theoretical issues which include: a). determining theoretically and empirically under what conditions adaptive importance sampling makes significant improvement in computation times; b). proving the convergence error; c). provide theoretical guarantee of approximation error of multilevel QMC to function being inferred.

5. The proposal will scale up the machine learning algorithms in big data analysis by a new "data squashing" method, and speed up sampling posterior distribution in Bayesian modeling by developing a new LD posterior sampling.

Weaknesses of IM:

Some of the plans for addressing some of the theoretical difficulties miss details. The proposal can be strengthened if the PIs can compare the proposed QMC algorithms with other methods (e.g. Hamiltonian MC) to show strength and limitations of the proposed work.

In the context of the five review elements, please

evaluate the strengths and weaknesses of the proposal with respect to broader impacts.

Broader Impacts (BI):

Implementation of the open source QMC software will provide research groups an easy-to-use platform for testing new ideas. The PIs will also expand the scope of QMC applications. Students supported by this project will learn to write clean, efficient code and software engineering tools. The PIs will make efforts to attract students from underrepresented minorities and women. The work will be presented at conferences.

Strengths of BI:

- 1. Pls have a successful track recording in mentoring students from underrepresented minorities and women.
- 2. The plan for the software development is solid.

Weaknesses of BI:

The educational component of the proposal focuses on the software development. It would be nice to see elements in advancing students' theoretical understandings of aspects of the proposal work.

Please evaluate the strengths and

weaknesses of the proposal with respect to any additional solicitation-specific review criteria, if applicable

NSF Prior Support:

PIs have prior NSF support.

Results of NSF Prior Support:

Many publications, and have students' support.

Data Management Plan:

Adequate

Post-Doctoral Mentoring Plan: N/A

Summary Statement

The work aims to develop quasi-Monte Carlo methos in variation/variance reduction methods, automatic stopping criteria, big data subsampling methods and low-discrepancy Bayesian sampling. The open source package QMCPy will be further developed through a well-thought plan. The proposal will train graduate students.

The proposal is among middle one third of the proposals the reviewer has reviewed.



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