2012838

Collaborative Research: Adaptive Multivariate Sampling to Accelerate Discovery

12/01/2019

Program Code:1271

Funding Opportunity Number: PD 16-1271

Leland Jameson

Declined 09/27/2020

Cognizant Program Officer Comments

PIs: Fred Hickernell, Yuhan Ding and James Hyman

Proposals: 2012834 and 2012838

Institutions: Illinois Institute of Technology and Tulane University

Title: Collaborative Research: Adaptive Multivariate Sampling to Accelerate Discovery

PANEL REVIEW: The proposal was reviewed by one of five panels organized by the Computational Mathematics Management Team which met in Spring 2020 at the National Science Foundation. Each of these panels was comprised of between 12 and 20 panelists who are experts in various aspects of computational mathematics. The panel was asked to review the proposals on the basis of the two main NSF review criteria: (1) Intellectual Merit and (2) Broader Impact. Each proposal was reviewed by at least three members of the panel. Another panelist was appointed by the Managing Program Officer as a scribe to write a summary of the panel's discussion of the proposal.

The set of proposals receiving no review rating higher than Good was presented to the panel at the start of deliberations. Panelists were given the opportunity to identify proposals in this set that merited further discussion; the remainder were not discussed further and did not receive panel summaries, and were placed in the category "Not Discussed by Panel". For each proposal discussed in detail, the panel was asked to place the proposal into one of the following three categories: (I) Competitive, (II) Not Competitive, and (III) Not Ranked. The panel was also asked to rank (if possible) proposals within the first category "Competitive". In addition to being reviewed by the Computational Mathematics panels, some proposals were also submitted to other NSF programs for co-review, and some were sent for further review.

Panel letter grades:

E/V, V/G, G

Panel ranking:

Line 7. Line 7 is the lowest line in the Competitive category.

Intellectual Merit:

The first reviewer writes, "This is a good proposal based on the recent developments on the subject but it needs reassessment of the methodology of the initial sampling step." The third reviewer comments that the proposal is well-written and that the PI's are well qualified yet also writes, "Weakness: The examples show the need for the sufficient samples in the exploration stages. More details about how to efficiently obtain sufficient samples in the exploration and how to overcome the challenges using the theory of adaptive algorithms and the RKHS/Kriding will make the proposal stronger."

Broader Impacts:

This project has many strong potential broader impacts such as, "1. As noted above, the planned applications are significant to society (climate change, sexually transmitted diseases). 2. The research will support students and undergraduate research, and the PI's have a successful record of mentoring students. 3. The proposal bridges disciplines and there are plans for dissemination. 4. The proposal will produce open source software of interest to the scientific community."

E/V Review:

The reviewer who gave the highest letter grade writes, "This is an very good/excellent proposal which develops several interesting ideas for better adaptive sampling algorithms. There are specific plans supported by multiple collaborations for meaningful data applications, and the broader impacts are very strong." Yet, a few weaknesses were pointed out by this reviewer, "1. A more thorough development of how active subspaces would be incorporated into the methodology would make the proposal stronger, i.e. expanding Sec. 2.4. 2. Note: the proposed heuristic for selecting \sigma(x) is very related to the adaptive scaling in self-tuning spectral clustering (see Zelnik-Manor and Perona, 2005). However this work is not referenced."

Summary:

As noted, the PI's are well-qualified and the project is well written. Also, the PI's are prominent and well-known scientists. However, a few perceived weaknesses were pointed out such as, "Panelists were concerned that the proposal didn't adequately address potential challenges for the high dimensional case and were not persuaded that the presented methodology would be successful for the noted applications. Already existing methodologies are not cited." After a great deal of deliberation and comparison to other projects reviewed by this panel, this project was ultimately placed in Line 7 of the competitive category. Regretfully, at this level the project falls just outside of the funding range for the computational mathematics program this year and will unfortunately be recommended for declination.

Recommendation:

Decline

Leland Jameson

Computational Mathematics

Review Information

Please note: The Sponsored Projects Office (or equivalent) at the submitting organization is NOT given the capability to read the below review information.

Panel Summary

Panel Summary Release Date

Panel Summary #1 08/17/2020

Proposal Review Summary of All Reviews

Review Release Date

Proposal Review #3 08/17/2020

Proposal Review #2 08/17/2020

Proposal Review #1 08/17/2020

Context Statement

Computational Mathematics Program

Proposal Review Context, 2020

Proposals handled by the Computational Mathematics Program are evaluated using mail and panel reviews. The number and type of reviews used for each project depend on the complexity of the proposal and the areas of expertise required. A recommendation for declination or award is not considered until three or more substantive reviews are received. When reading reviews, please keep in mind that reviewers address their comments chiefly to the NSF, not necessarily to the investigators. Some reviews may contain irrelevant, insubstantial, or erroneous statements that were not used for making the recommendation.

While reviewers' ratings are considered, the content of their reviews is more important in assessing the merits of each proposal. Different reviewers may offer insights into different aspects of a proposal (issues related to problem formulation and approach, relevant work in other areas of mathematics, perspectives on the importance of a particular problem within a subarea of computational mathematics or in a broader context, or relevance to applications or other disciplines). Reviewers' comments are considered in the context of other reviews they have provided. Thus, the average rating is not the determining factor; rather, a clear and detailed picture of each proposal's strengths and likely impact is used for deriving a recommendation.

Decisions about particular proposals are often difficult and may be reached by using factors other than reviewer comments and ratings. For renewal proposals, program directors often have additional information not available to reviewers, for example, progress reports. Appropriate balance among subfields, the balance between new investigators and those previously supported, contribution to particular initiatives or to interdisciplinary efforts, effect on education and human resource development, the availability of other funding, the total amount of funds available to the program for new and renewal proposals, and NSF policies are other important factors used for arriving at a decision.

The hallmark of a successful proposal is one or more salient strengths. Usually this is reflected in high ratings, although not all reviewers give bold but risky proposals the highest marks. It has long been impossible to fund all the meritorious proposals. Proposals recommended for award, are distinguished from other high quality proposals, by having a strong potential for impact in the field or more broadly in science. Taken collectively, funded proposals represent a balance across the dynamic and essential areas of the discipline. This means that factors other than a simple rank ordering of proposals are used for making recommendations for declination or award.

This year the computational mathematics program expects to review over 300 competing proposals, many of them of an interdisciplinary or group nature, and to fund less than one third of them. As always, this will include a substantial number of awards that do not provide sufficient salary support for the investigators.

Proposal Panel 1 : 2012838

Brief Summary of Project:

The proposal explores several approaches to improving sequential adaptive sampling using a surrogate model.

Intellectual Merit:

Strengths: The proposal is well-written. The proposal does a nice job summarizing open challenges. Appropriate/Compelling applications have been discussed. Figures are helpful. Los Alamos and other interested parties will get involved.

Weakness: Panelists were concerned that the proposal didn't adequately address potential challenges for the high dimensional case and were not persuaded that the presented methodology would be successful for the noted applications. Already existing methodologies are not cited.

Broader impact:

The applications were deemed very good in terms of relevance/broader impacts and the network of collaborators who would contribute.

RECOMMENDATION

Although the topic was interesting and applications appropriate/compelling, the panel was concerned about missing relevant work and whether the proposed framework would succeed in the high-dimensional case.

The panel placed this proposal in the category: competitive.

This summary was read by/to the panel and the panel concurred that the summary accurately reflects the panel discussion.

PANEL RECOMMENDATION: Competitive

Proposal Review 2 : 2012838

Rating:Multiple Rating: (Excellent/Very Good)

Summary

In the context of the five review elements, please

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

STRENGTHS:

1. This proposal did a nice job summarizing a complicated subject area and outlining the current open challenges: generally the acquisition function depends only on x (or when it depends on y next samples tend to be close to existing points); correctly selecting the length scale \sigma(x) for the MLS kernel is challenging; methods have poor scalability in high dimensions.

2. The proposal explores several interesting and innovative approaches to improving adaptive sampling, including a more rigorous understanding of bandwidth selection, data-driven kernels which allow for more variation in certain data regions, and avoiding the curse of dimension by utilizing active subspace. Figures 2 and 3 are very helpful in communicating the main ideas.

3. The applications of the methodology are well planned and highly meaningful, and involve collaborations with multiple experts (e.g. collaborating with Los Alamos for modeling sea ice, collaborations at Tulane for modeling sexually transmitted disease).

WEAKNESSES:

1. A more thorough development of how active subspaces would be incorporated into the methodology would make the proposal stronger, i.e. expanding Sec. 2.4.

2. Note: the proposed heuristic for selecting \sigma(x) is very related to the adaptive scaling in self-tuning spectral clustering (see Zelnik-Manor and Perona, 2005). However this work is not referenced.

In the context of the five review elements, please

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

STRENGTHS:

1. As noted above, the planned applications are significant to society (climate change, sexually transmitted diseases).

2. The research will support students and undergraduate research, and the PI’s have a successful record of mentoring students.

3. The proposal bridges disciplines and there are plans for dissemination.

4. The proposal will produce open source software of interest to the scientific community.

WEAKNESSES: I didn’t notice any weaknesses.

Please evaluate the strengths and

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

applicable

Summary Statement

This is an very good/excellent proposal which develops several interesting ideas for better adaptive sampling algorithms. There are specific plans supported by multiple collaborations for meaningful data applications, and the broader impacts are very strong.

Proposal Review 3 : 2012838

Rating: Good

Summary

In the context of the five review elements, please

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

The project proposes a sequential adaptive sampling approach in which after the initial sampling, a surrogate model is formed to predict the model response and then each new sample is chosen based on the variation of the model and its consistency with the observed data. The approach is reasonable but there are a few problems that are not addressed properly. The most serious one is that in the initial step the suggested sampling uses a space-filling methodology that is prohibitive in high dimensions. This immediately raises questions about feasibility of using this methodology for the first mentioned application (p. 11), namely the Sea-Ice Model that features 39 dimensional setup. Such problems could be avoided if a substantial dimension reduction in the initial sampling is possible but the suggested method from [16] is very unlikely to be successful.

The description of the method features one dimensional or low dimensional sampling (even mentions the arcsin distribution on p. 1). Later in 2.4 (p. 9 and 10,) the problem is partially addressed by mentioning coordinate ordering and weights, as well as active subspaces. These are standard remedies to slightly expand the scope of possible applications but such a fix is far from being enough. The rest of the methodology is fine and the entire approach is likely to produce (very) good results in (very) low dimensional settings.

The results from prior NSF support are more than satisfactory.

In the context of the five review elements, please

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

The software produced under the grant would be implemented in libraries on open source repositories.

The educational and outreach activities are perfectly outlined in the broader impact section.

Please evaluate the strengths and

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

applicable

Summary Statement

This is a good proposal based on the recent developments on the subject but it needs reassessment of the methodology of the initial sampling step.

**Proposal Review 1:**

**Summary**

In the context of the five review elements, please   
evaluate the strengths and weaknesses of the proposal with respect to intellectual merit.   
  
Topic: The proposal plans to develop adaptive multivariate sampling methods for large-scale simulations. The proposed methods have explore and   
exploit with surrogate models two stages. The surrogate models include the trend model with the moving least squares (MLS) and a variation model   
With reproducing kernel Hilbert space (RKHS) and Kriging. The PIs proposed different ways to overcome two challenges in MLS and also use data-based inferred kernel for surrogate   
variation models. Several applications are proposed.   
  
  
Intellectual Merit:    
  
Strengths: The proposal is well-organized and well-written. The PI is well qualified. The proposed work includes the algorithm design and theoretical justification for the algorithms, applications, and software.   
  
  
Weakness: The examples show the need for the sufficient samples in the exploration stages. More details about how to efficiently obtain   
sufficient samples in the exploration and how to overcome the challenges using the theory of adaptive algorithms and the RKHS/Kriding   
will make the proposal stronger.   
  
  
In the context of the five review elements, please   
evaluate the strengths and weaknesses of the proposal with respect to broader impacts.   
  
Broader Impacts:   
  
Strengths: Mentor junior scholars; provide research experiences for undergraduate and high school students. Prepare students for academic and industry careers.   
Creating softwares.    
  
  
Please evaluate the strengths and   
weaknesses of the proposal with respect to any additional solicitation-specific review criteria, if   
applicable   
  
  
  
Summary Statement   
  
Results from Prior NSF Support: The PI were productive under prior NSF support. (Producing several papers and   
mentoring graduate students)