Comments on paper
Fast Regression of the Tritium Breeding Ratio in Fusion Reactors

By:
P. Mánek, G. Van Goffrier, V. Gopakumar, N. Nikolau, J. Shimwell and I. Waldmann

Proposed for publication on:
Nuclear Fusion

The paper presents a comparison of different families of surrogate methods for the calculation of the Tritium Breeding Ration (TBR) in a fusion reactor, claiming major focus to be on Inertial Confinement. In the paper, a "surrogate" method is defined as a cheaper approximation of a much expensive calculation procedure like, for example, a Monte Carlo calculation. Often surrogate methods involve using Artificial Intelligence techniques like, e.g., Artificial Neural Networks.

The paper compares different families of surrogate methods checking both accuracy and computational complexity, and presents a novel adaptive method for sampling the relevant parameter space, called Quality-Adaptive Surrogate Sampling (QASS), aiming at optimizing the prediction accuracy for a given size of the sampling set or, alternatively, minimizing the number of training points required for a given accuracy. If finally shows that the QASS method is effective at improving the efficiency of a large variety of surrogate methods.

Although I found the paper interesting to read and acknowledge it can produce a valuable contribution to the development of future fusion technologies, I feel it to be a bit out of the scope of the *Nuclear Fusion* journal. Numerical techniques are obviously a mission-critical for the development of a scientific and technological task as complex as controlled tehrmonuclear fusion, but a paper with such a strong pitch on computational sciences should be directed more properly, I would suggest, to a journal like, e.g., *Journal of Computational Physics* or *Computer Physics Communications*, to which I would recommend to re-direct the submission. I understand, however, that it is up to the editor to take a final decision on the paper acceptability based upon its subject. In the following, I will list my comments as if the paper were to be processed by *Nuclear Fusion*: I hope they could be useful to improve its quality, whatever journal it will finally be submitted to.

1. **Title**
   I think the title is a bit misleading. At least to me, it generated first the feeling that the paper were to discuss predictions of the TBR in fusion reactors. I think something more descriptive could be *Fast Regression Methods for the Evaluation of the Tritium Breeding Ratio in Fusion Reactors*, or something similar.
2. **Page 2, line 29, left column**
   It is stated that the paper presents *an empirical surrogate model for the tritium dreeding ratio (TBR) in an inertial confinement fusion (ICF) reactor.*.
   This sentence is puzzling to me. If I read correctly the paper later, it compares a family of

surrogate methods and develop a strategy for adaptive sampling (QASS). I suspect this is what really the sentence refers to. If it is so, I think the authors should change the sentence, pointing more clearly to QASS.

3. **Page 2, line 53, left column**
   It is stated that the energy distribution for the neutrons considered in the paper is the one called *Miur*. Actually, a quick serach revealed that this is just a gaussian distribution with certain free parameters. I guess it would be more informative rewording this sentence as *a gaussian energy distribution with some user-selected free parameters*, re-directing to the relevant literature for more details.

4. **Page 2, line 24, right column**
   While commenting figure 1, it is stated that the geometry of the system were intentionally left adjustable. I suspect that the free parameters are those listed later in Table 1, but this is not stated explicitly. I would appreciate if an explicit comment on which parameters are actually left adjustable could be made at this point.

5. **Page 2, line 45, right column**
   At this point, the paper mentions *a novel adaptive sampling procedure suited to this application*. I suspect this is what was previously meant (see my comment 2). I think the authors should try to resolve as much as possible this ambiguity between *novel surrogate method* and *novel sampling procedure*.

6. **Page 3, line 6, left column**
   It is stated that nuclear fusion technology *relies on the production and containement of an extremely hot and* ***dense*** *plasma containing enriched Hydrogen isotopes*.
   While this is certainly true for ICF applications, it is not true for magnetic confinement applications, where the fuel density is approximately 10^{-5} the atmospheric level. It is true that the paper claims to focus on ICF applications, which would make the statement correct. However, in the next few lines it discusses explicitly JET and ITER, which are magnetic fusion experiments. In these few lines there is an oscillation between inertial and magnetic fusion experiments, which make this paper segment ambiguous. I would appreciate if the authors could resolve such ambiguity.

7. **Page 3, line 25, left column**
   It is stated that *modern D-T reactors rely on tritium breeding blanket*.
   This sentence seem to be linked to the previous mentioning of JET and ITER. I would appreciate if the authors could be a bit more explicit and precise. It should be noted that JET does *not* have a blanket, while only test modules will be installed in ITER. It is true that such component is expected to be eventually installed in a reactor. Maybe, an example taken from ICF technology could also be added.

8. **Page 3, line 32-39, right column**
   The authors mention *a fast TBR function which takes these same input parameters and approximates the MC model....* It is not clear, to me, what the term *function* means here. I feel there is again the ambiguity between *surrogate methods* and *sampling technique*. Could the authors resolve it?

9. **Page 4, line 52, left column**
   The authors state that they track *relative measures that are better suited for comparison*

between this work and others, because they are invariant...
I think it would be better to mention explicitly which ones are the relative metrics and the absolutes (mentioned a few lines earlier).

10. **Page 5, line 5, right column**
The definition given the for standard deviation does not correspond to the one usually reported in statistics. Could the authors please check it?

11. **Page 5, line 51, left column**
... to better characterize the relationship of each family between sample count and the metrics of interest... This sentence is a bit obscure to me. Maybe the authors could re-phrase it?

12. **Figure 5**
The font-size of the labels is really small and makes it difficult to read. Could the authors increase it?

13. **Page 6, lines 25-31, right column**
The authors comment the results displayed in figure 3. I understand that the figure was produced by keeping fixed some discrete parameters, but I have no clue which one (or which ones, in case different parameters were kept fixed for different subsets of the data shown). Could the authors explicitly show which one(s)?

14. **Page 6, lines 34, right column**
It is stated that *ERTs, SVMs, and ANNs also achieved satisfactory results with respect to both examined metrics*, where I understand the considered metrics are regression performance and prediction time per sample. Actually, the figure suggests that ANNs could be relatively slow. Could the authors elaborate a bit more on that?

15. **Page 6, lines 43, right column**
It is stated that *GBTs, ANNs and ERTs ... are known to be capable of capturing relationships involving mixed feature types that were deliberately withheld in the first experiment.*
I think it would be appropriate to add a reference to the relevant literature to substantiate this statement.

16. **Page 7, lines 30-37, right column**
Following both hyperparameter tuning experiments, we conclude that while domain restrictions employed in the first case have proven effective in improving the regression performance of some methods, their performance fluctuates considerably depending on the selected slices.
The mentioned fluctuations are not obvious to me. Maybe the authors could elaborate a bit more on this to make them more apparent to the reader.

17. **Page 7, lines 54, right column**
Commenting the dependence of the performance of the surrogate method families on the dataset size, it is stated that:
While such families achieve nearly comparable performance on the largest dataset, in the opposite case tree-based ensemble approaches clearly outperform ANNs.
To me, this sentence is only partially meaningful, because it should be complemented by a comment on the accuracy level that can be attained by whatever methods on the smallest dataset. If it appeared that the achievable accuracy is too low for practical applications, even the speed advantage would be useless. Could the authors add a line of comment/clarification on that?

18. **Page 8, right column**
    The figures inserted in the column are a bit too large. They cover the margin of the left column and some words are chopped. Could the authors fix this?
19. **Page 9, lines 8 and 12, left column**
    The speedups obtained with the surrogate methods are written as $\omega = 6916416\times$ and $\omega = 8659251\times$. I think that writing the acceleration obtained using standard scientific notation 6.92×10^6 and 8.66×10^6 would be far more immediate to read.
20. **Page 9, line 41, left column**
    The authors introduce a sinusoidal theory as an alternative to the expensive MC Paramak model used to assess the efficiency of the surrogate methods and sampling techniques they analyze. They qualify this theory as *robust*. It is by far not clear to be what the word *robust* means in this context. Could the authors clarify this?
21. **Page 10, line 4**
    The best-performing method(s) under each are highlighted in bolt
    I do not fully understand this sentence. Perhaps a word is missing (*under each ... what ... ?*)
22. **Page 10, figure 7 and 8**
    They are too large and covers some letters of the opposite left column. I think they should be resized.
23. **Page 11, line 7, left column**
    An increase in initial sample size was observed to also ***resolve precision*** *in these smooth regions...*
    I do not understand what the wording *resolve precision* means in this context. Maybe the authors could elaborate a bit more on that?
24. **Page 11, line 26-31, left column**
    The authors claim they developed *fast and high-quality surrogates for the Paramak TBR model.*
    I suspect that here again there is an ambiguity between *surrogate models* and *sampling strategies*. If the authors really developed a novel surrogate model, this is not clear to me. Could the authors elaborate more on that?
25. **Page 12, line 32, left column**
    When following the url reported in the citation, I reach a publication with title *The components of the Wired Spanning Forest are recurrent*, which looks different from the declared one. Maybe is the link wrong?

Should the submitted paper continue its pipeline to be published on Nuclear Fusion, I would be happy to ha a look at the revised version.