Fast Regression of the Tritium Breeding Ratio in Tokamak Fusion Reactors

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Abstract. The tritium breeding ratio (TBR) is an essential quantity for the design of modern and next-generation Tokamak nuclear fusion reactors. Representing the ratio between tritium fuel generated in breeding blankets and fuel consumed during reactor runtime, the TBR depends on reactor geometry and material properties in a complex manner. In this work, we explored the training of surrogate models to produce a cheap but high-quality approximation for a Monte Carlo TBR model in use at the UK Atomic Energy Authority. We investigated possibilities for dimensional reduction of its feature space, reviewed 9 families of surrogate models for potential applicability, and performed hyperparameter optimisation. Here we present the performance and scaling properties of these models, the fastest of which, an artificial neural network, demonstrated $R^2 = 0.985$ and a mean prediction time of $0.898\,\mu s$, representing a relative speedup of $8 \cdot 10^6$ with respect to the expensive MC model. We further present a novel adaptive sampling algorithm, Quality-Adaptive Surrogate Sampling, capable of interfacing with any of the individually studied surrogates. Our preliminary testing on a toy TBR theory has demonstrated the efficacy of this algorithm for accelerating the surrogate modelling process.

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1. Introduction

The analysis of massive datasets has become a necessary component of virtually all technical fields, as well as the social and humanistic sciences, in recent years. Given that rapid improvements in sensing and processing hardware have gone hand in hand with the data explosion, it is unsurprising that software for the generation and interpretation of this data has also attained a new frontier in complexity. In particular, simulation procedures such as Monte Carlo (MC) event generation can perform physics predictions even for theoretical regimes which are not analytically tractable. The bottleneck for such procedures, as is often the case, lies in the computational time and power which they necessitate.

Surrogate models, or metamodels, can resolve this limitation by replacing a resource-expensive procedure with a much cheaper approximation [?]. They are especially useful in applications where numerous evaluations of an expensive procedure are required over the same or similar domains, e.g. in the parameter optimisation of a theoretical model. The term "metamodel" proves especially meaningful in this case, when the surrogate model approximates a computational process which is itself a model for a (perhaps unknown) physical process [?]. There exists a spectrum between "physical" surrogates which are constructed with some contextual knowledge in hand, and "empirical" surrogates which are derived purely from samples of the underlying expensive model.

In this project, in coordination with the UK Atomic Energy Authority (UKAEA), we sought to develop a surrogate model for the tritium breeding ratio (TBR) in a Tokamak nuclear fusion reactor. Our expensive model was an MC-based neutronics simulation, *Paramak*‡, which returns a prediction of the TBR for a given configuration of a spherical Tokamak. We took an empirical approach to the construction of this surrogate, and no results described here are explicitly dependent on prior physics knowledge.

For the remainder of Section 1, we will define the TBR and set the context of this work within the goals of the UKAEA. In Section 2 we will describe our datasets generated from the expensive model for training and validation purposes, and the dimensionality reduction methods employed to develop our understanding of the parameter domain. In Section 3 we will present our methodologies for the comparison testing of a wide variety of surrogate modelling techniques, as well as a novel adaptive sampling procedure suited to this application. After delivering the results of these approaches in Section 4, we will give our final conclusions and recommendations for further work.

‡ Provided by collaborator Jonathan Shimwell, at UKAEA.

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Figure 1. Typical single-null reactor configuration as specified by BLUEPRINT [**?**]: 1 — plasma, 2 — breeding blankets

1.1. Problem Description

Nuclear fusion technology relies on the production and containment of an extremely hot and dense plasma. In this environment, by design similar to that of a star, hydrogen atoms attain energies sufficient to overcome their usual electrostatic repulsion and fuse to form helium [**?**]. Early prototype reactors made use of the deuterium (^{2}H, or D) isotope of hydrogen in order to achieve fusion under more accessible conditions, but lead to limited success. The current frontier generation of fusion reactors, such as the Joint European Torus (JET) and the under-construction International Thermonuclear Experimental Reactor (ITER), make use of tritium (^{3}H, or T) fuel for further efficiency gain. Experimentation at JET dating back to 1997 [**?**] has made significant headway in validating deuterium-tritium (D-T) operations and constraining the technology which will be employed in ITER in a scaled-up form.

However, tritium is much less readily available as a fuel source than deuterium. While at least one deuterium atom occurs for every 5000 molecules of naturally-sourced water, and may be easily distilled, tritium is extremely rare in nature. It may be produced indirectly through irradiation of heavy water (D_2O) during nuclear fission, but only at very low rates which could never sustain industrial-scale fusion power.

Instead, modern D-T reactors rely on tritium breeding blankets, specialised layers of material which partially line the reactor and produce tritium upon neutron bombardment, e.g. by

$$^1_0\text{n} + {}^6_3\text{Li} \longrightarrow {}^3_1\text{T} + {}^4_2\text{He} \tag{1}$$

$$^1_0\text{n} + {}^7_3\text{Li} \longrightarrow {}^3_1\text{T} + {}^4_2\text{He} + {}^1_0\text{n} \tag{2}$$

where T represents tritium and ^{7}Li, ^{6}Li are the more and less frequently occurring isotopes of lithium, respectively. ^{6}Li has the greatest tritium breeding cross-section of all tested isotopes [**?**], but due to magnetohydrodynamic instability of liquid lithium in the reactor environment, a variety of solid lithium compounds are preferred.

The TBR is defined as the ratio between tritium generation in the breeding blanket per unit time and tritium fuel consumption in the reactor. The MC neutronics simulations previously mentioned therefore must account for both the internal plasma dynamics of the fusion reactor and the resultant interactions of neutrons with breeding blanket materials. Neutron paths are traced through a CAD model (e.g. Figure 1) of a reactor with modifiable geometry.

The input parameters of the computationally-expensive TBR model therefore fall into two classes. Continuous parameters, including material thicknesses and packing ratios, describe the geometry of a given reactor configuration. Discrete categorical parameters further specify all relevant material sections, including coolants, armours, and neutron multipliers. One notable exception is the enrichment ratio, a continuous

parameter denoting the presence of ^{6}Li. Our challenge, put simply, was to produce a fast TBR function which takes these same input parameters and approximates the MC TBR model with the greatest achievable regression performance.

2. Methodology

3. Results

4. Conclusion

5. Acknowledgements

6. References