

Surrogate Modelling of the Tritium Breeding Ratio

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Project Background



Nuclear fusion – the energy of the future!

- Must produce and contain an extremely hot and dense plasma
 - Magnetic Confinement Fusion (MCF): toroidal circulation
 - Inertial Confinement Fusion (ICF): spherical compression
- Modern designs require enriched Hydrogen fuel of two varieties:
 - Deuterium (²H) abundant in naturally-sourced water
 - Tritium (³H) extremely rare, but can be produced *in-reactor*



Problem Description



Tritium breeding blankets convert neutron radiation from the fusion plasma into a steady supply of tritium fuel.

$${}_0^1{\rm n} + {}_3^6{\rm Li} \rightarrow {}_1^3{\rm H} + {}_2^4{\rm He} \\ {}_0^1{\rm n} + {}_3^7{\rm Li} \rightarrow {}_1^3{\rm H} + {}_2^4{\rm He} + {}_0^1{\rm n}$$

However, the tritium breeding ratio (TBR) depends on numerous geometric and material parameters.

TBR evaluation *Paramak* achieves very accurate results by OpenMC Monte Carlo neutronics simulation, but is computationally expensive.

Our Challenge:

Produce a fast TBR function that strongly approximates Paramak, making use of the latest in surrogate modelling techniques.

Data Generation



We designed the Approximate TBR Evaluator (ATE) package to generate training and test datasets from Paramak.

UCL's Hypatia cluster provided the multithreading power for us to produce one million TBR samples, representing 27 days of runtime.

These runs included full evaluations on the 18 continuous and discrete parameters of Paramak, and "slice" evaluations with all discrete parameters frozen.

	Parameter name	Domain
Blanket	Breeder fraction [†]	[0, 1]
	Breeder ⁶ Li enrichment fraction	[0, 1]
	Breeder material	$\{Li_2TiO_3, Li_4SiO_4\}$
	Breeder packing fraction	[0, 1]
	Coolant fraction [†]	[0, 1]
	Coolant material	$\{\mathrm{D_2O},\mathrm{H_2O},\mathrm{He}\}$
	Multiplier fraction [†]	[0, 1]
	Multiplier material	$\{Be, Be_{12}Ti\}$
	Multiplier packing fraction	[0, 1]
	Structural fraction [†]	[0, 1]
	Structural material	${SiC, eurofer}$
	Thickness	[0, 500]
First wall	Armour fraction [‡]	[0, 1]
	Coolant fraction [‡]	[0, 1]
	Coolant material	$\{D_2O, H_2O, He\}$
	Structural fraction [‡]	[0, 1]
	Structural material	{SiC, eurofer}
	Thickness	[0, 20]

Methodology



Conventional regression task – search for a cheap surrogate $\hat{f}(x)$ that minimizes dissimilarity with an expensive function f(x):

- Regression performance: mean absolute error, σ of error, R^2 , $R^2_{\text{adj.}}$
- Computational complexity: training & prediction time / sample.

2 approaches for surrogate training:

- Decoupled trains models from previously sampled datapoints.
- Adaptive repeats sampling & model training, increases sampling density in low-performance regions.



Decoupled Approach



Compared 9 state-of-the-art surrogate families:

- Support vector machines,
- Gradient boosted trees,
- Extremely randomized trees,
- AdaBoosted decision trees,
- Gaussian process regression,

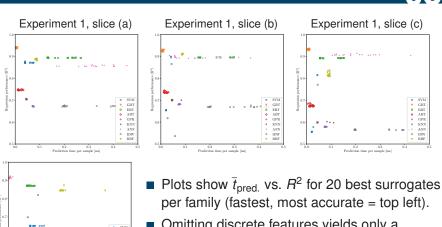
- k nearest neighbors,
- Artificial neural networks (MLP),
- Inverse distance weighting,
- Radial basis functions.

Performed 4 experiments:

- Hyperparameter tuning (simplified) Bayesian optimization, discrete features fixed & withheld.
- 2 Hyperparameter tuning same as #1 but with all features.
- 3 Scaling benchmark increase training set size.
- 4 Model comparison train surrogates for practical use.

Experiments 1 & 2: Hyperparameter Tuning





Experiment 2

RBF

- Omitting discrete features yields only a
- negligible improvement in performance.
- Overall dominated by tree-based surrogates (GBTs, ERTs) and neural networks.

Experiment 3: Scaling Benchmark



- We observe a hierarchy.
- Best-performing families from the previous experiments also scale the best in \overline{t}_{pred} .
- More samples: neural networks outperform tree-based models.

- Instance-based surrogates (KNN, IDW) train trivially but have complex lookup.
- Neural networks show inverse scaling due to parallelization.







Regression performance

Training time / sample

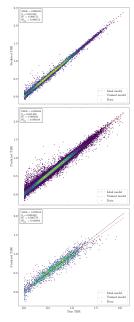
Prediction time / sample

Experiment 4: Model Comparison



- Trained 8 models for practical use.
- Plots show true vs. predicted TBR by Models 1, 2 & 4, coloured by density.
- Model 1 best regression performance:
 - ANN (4-layer MLP), 500K samples.
 - $R^2 = 0.998$, $\sigma = 0.013$,
 - $\bar{t}_{pred.} = 1.124 \, \mu s, 6916416 \times faster.$
- Model 2 fastest prediction:[†]
 - ANN (2-layer MLP), 500K samples.
 - $R^2 = 0.985$, $\sigma = 0.033$,
 - $\bar{t}_{pred.} = 0.898 \, \mu s, \, 8659 \, 251 \times \text{ faster.}$
- Model 4 smallest training set:[†]
 - GBT, 10K samples.
 - \blacksquare $R^2 = 0.913$, $\sigma = 0.072$,
 - $\bar{t}_{pred.} = 6.125 \,\mu s$, 1 269 777× faster.

with acceptable regression performance.





Adaptive Approach

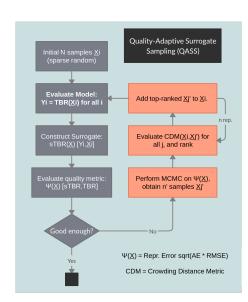
Adaptive Sampling: Theory



Adaptive sampling takes advantage of surrogate information content *during training* to reduce sample quantity.

We developed a technique which is novel in the literature:

- Construct surrogate quality distribution by nearestneighbour interpolation.
- Draw candidate samples by quality using MCMC.
- Include samples with high crowding distance.
- Repeat!



Application on Toy Theory

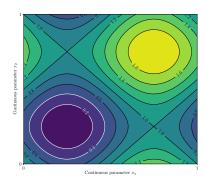


Toy functional TBR theory with wavenumber n, and similar ANN performance to Paramak:

TBR =
$$\frac{1}{|C|} \sum_{i \in C} [1 + \sin(2\pi n(x_i - 1/2))]$$

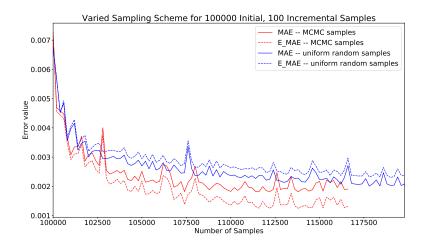
Evaluation performed both on the adaptively-sampled dataset and on a baseline uniform-random dataset.

An baseline scheme with incremental but uniform-random samples used as a placebo comparison.



Adaptive Sampling: Results





Conclusion



Decoupled approach:

- Tuned and compared surrogates from 9 state-of-the-art families.
- Found heuristic: GBTs for $< 10^4$ points and ANNs for $\ge 10^5$ points.
- Fastest found surrogate predicts TBR with standard deviation of error 0.033 in 0.898 μ s, which is 8 · 10⁶× faster than Paramak.
- While this used 500K datapoints, we found surrogates with comparable properties with as little as 10K datapoints.

Adaptive approach:

- TODO
- TODO
- TODO
- TODO

Presented methods portable \rightarrow can be used as cheap approximation of any simulation or black box function.



Thank you for listening!

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Further reading:

- Single page abstract (available online).
- Journal article, currently in internal pre-submission review (available online):
 Fast Regression of the Tritium Breeding Ratio in Fusion Reactors.
- Industry group project final report (available online).
- All models, plots, training data, source code and technical documentation.
 https://github.com/ucl-tbr-group-project