

Surrogate Modelling of the Tritium Breeding Ratio

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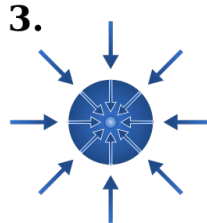
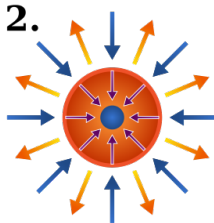
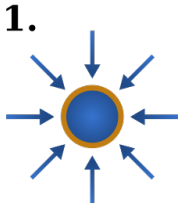
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Nuclear fusion – the energy of the future!

- 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*.



Tritium breeding blankets convert neutron radiation to tritium fuel:



Tritium breeding ratio (TBR) = fuel bred / fuel consumed

- Depends on numerous geometric and material parameters.
- Evaluated precisely by OpenMC neutronics simulation *Paramak*, but is computationally expensive.

Our Challenge:

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

We produced training and test datasets by uniform random sampling over the 7 discrete and 11 continuous parameters of Paramak.

Paramak deployed on UCL's Hypatia cluster:

- Generated 1M samples.
- 27 days of runtime.

2 classes of runs:

- All parameters free.
- Discrete fixed, continuous free.

Groups of fractions marked^{†‡} are required to sum to 1.

	Parameter name	Domain
Blanket	Breeder fraction [†]	[0, 1]
	Breeder ⁶ Li enrichment fraction	[0, 1]
	Breeder material	{Li ₂ TiO ₃ , Li ₄ SiO ₄ }
	Breeder packing fraction	[0, 1]
	Coolant fraction [†]	[0, 1]
	Coolant material	{D ₂ O, H ₂ O, 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 ₂ O, H ₂ O, He}
	Structural fraction [‡]	[0, 1]
	Structural material	{SiC, eurofer}
	Thickness	[0, 20]

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_{adj} .
- Computational complexity: training & prediction time / sample

2 approaches for surrogate training:

- 1 Decoupled – trains models from previously sampled datapoints.
- 2 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:

- 1 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

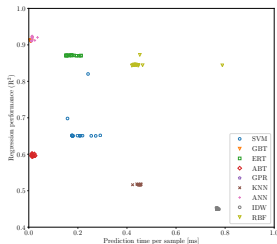
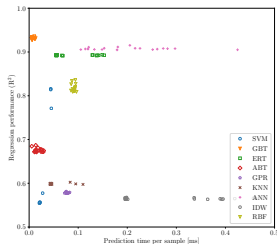
Experiment 1, slice (a)



Experiment 1, slice (b)



Experiment 1, slice (c)

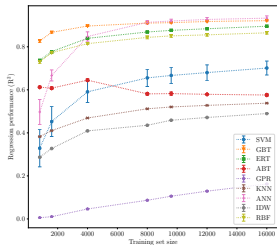


Experiment 2

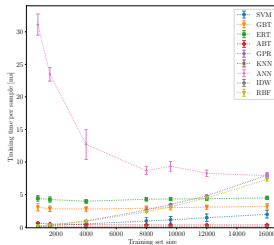
- Plots show $\bar{t}_{\text{pred.}}$ vs. R^2 for 20 best surrogates per family (top left \Leftrightarrow fastest, most accurate).
- Omitting discrete features yields only a negligible improvement in performance.
- Overall dominated by tree-based surrogates (GBTs, ERTs) and neural networks.

Experiment 3: Scaling Benchmark

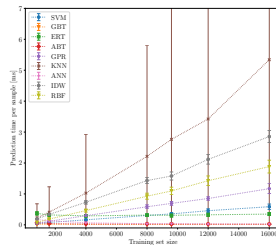
- We observe a hierarchy.
- Best-performing families from the previous experiments also scale the best in $\bar{t}_{\text{pred.}}$.
- More samples: neural networks outperform tree-based models.
- Instance-based surrogates (KNN, IDW) train trivially but have complex lookup.
- Neural networks show inverse scaling due to parallelization.



Regression performance



Training time / sample

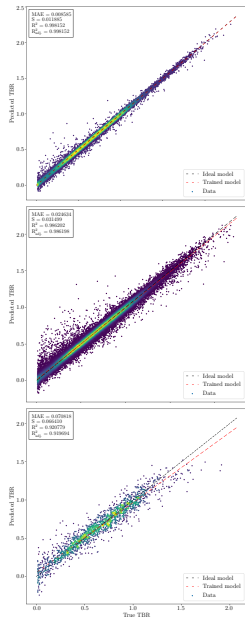


Prediction time / sample

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.
 - $R^2 = 0.998$, $\sigma = 0.013$,
 - $\bar{t}_{\text{pred.}} = 1.124 \mu\text{s}$, $6\,916\,416\times$ faster.
- Model 2 – fastest prediction:[†]
 - ANN (2-layer MLP), 500K samples.
 - $R^2 = 0.985$, $\sigma = 0.033$,
 - $\bar{t}_{\text{pred.}} = 0.898 \mu\text{s}$, $8\,659\,251\times$ faster.
- Model 4 – smallest training set:[†]
 - GBT, 10K samples.
 - $R^2 = 0.913$, $\sigma = 0.072$,
 - $\bar{t}_{\text{pred.}} = 6.125 \mu\text{s}$, $1\,269\,777\times$ faster.

[†] with acceptable regression performance.

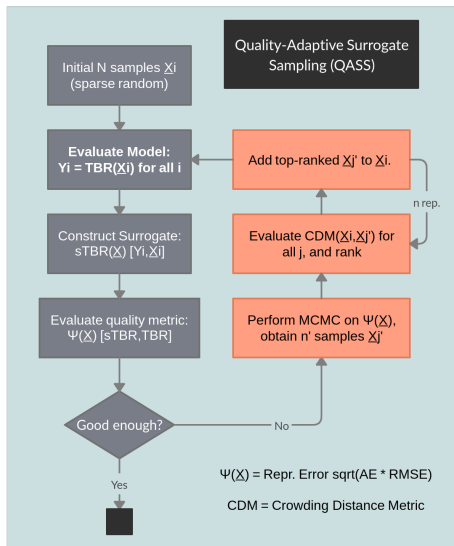


Adaptive Approach

How can we take advantage of surrogate information content *during training* to reduce sample quantity?

We developed a new technique:

- 1 Construct surrogate quality distribution by nearest-neighbour interpolation.
- 2 Draw candidate samples by quality using MCMC.
- 3 Include samples with greatest separation from neighbours.
- 4 Repeat!



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

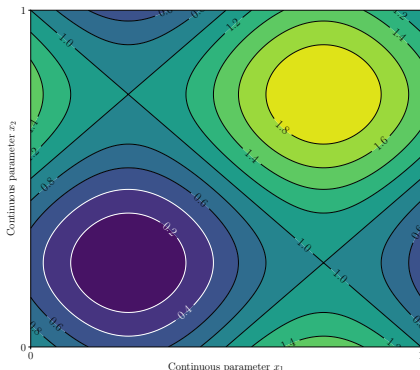
$$\text{TBR} = \frac{1}{|C|} \sum_{i \in C} [1 + \sin(2\pi n(x_i - 1/2))]$$

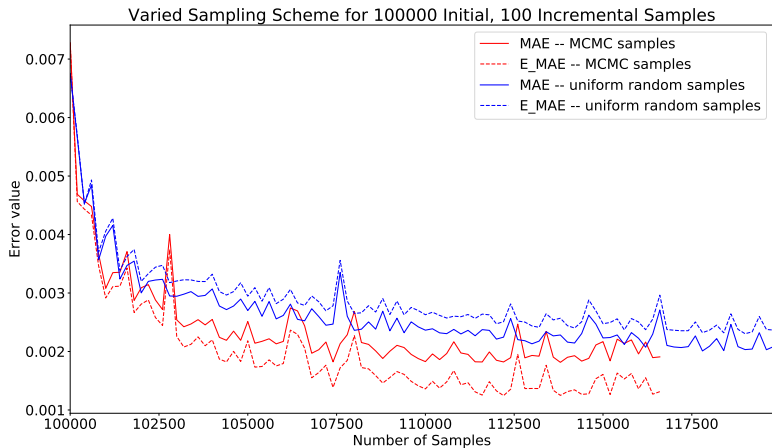
(where C is the set of variable indices)

2 evaluation sets:

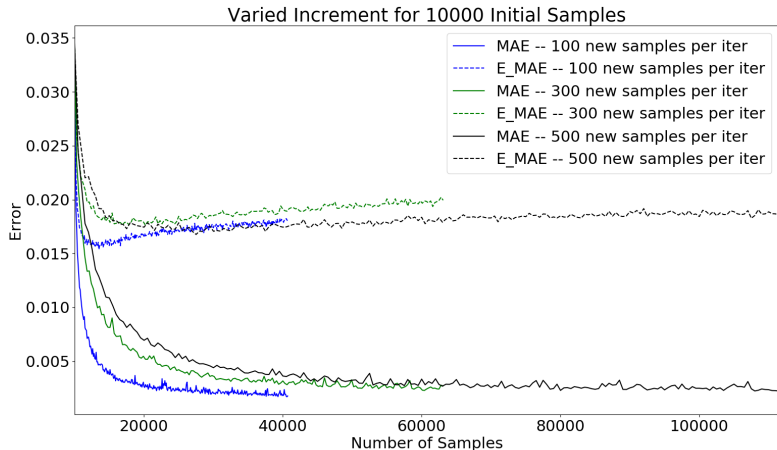
- Adaptively-sampled dataset
- Independent random dataset

Placebo comparison – a baseline scheme without MCMC, incremental uniform-random samples.





60% decrease in MAE for independent evaluation (dashed)
Equivalently, 6% decrease in samples needed for same accuracy



Fewer incremented samples can lead to better accuracy!

But depends on initial samples, specific model – further study needed.

Decoupled approach:

- Tuned and compared surrogates from 9 state-of-the-art families.
- Found heuristic: GBTs for $< 10^4$ samples, ANNs for $\geq 10^5$ samples.
- Fastest found surrogate predicts TBR with standard deviation of error 0.033 in $0.898 \mu\text{s}$, which is $8 \cdot 10^6 \times$ faster than Paramak.
- While this used 500K samples, we found surrogates with comparable properties with as little as 10K samples.

Adaptive approach (on toy theory):

- New theoretical approach QASS developed, based on MCMC.
- 60% decrease in evaluation MAE demonstrated.
- 6% decrease in expensive TBR samples needed.
- Strong potential for further reduction via hyperparameter tuning.

All 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>