Surrogate Modelling of the Tritium Breeding Ratio

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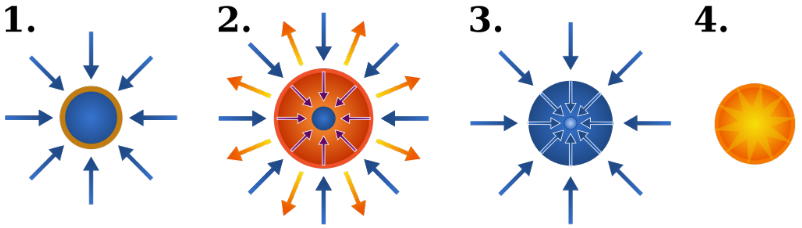
Project Background

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 to tritium fuel:

$$ {}^{1}_{0}\mathrm{n} + {}^{6}_{3}\mathrm{Li} \rightarrow {}^{3}_{1}\mathrm{H} + {}^{4}_{2}\mathrm{He} \qquad {}^{1}_{0}\mathrm{n} + {}^{7}_{3}\mathrm{Li} \rightarrow {}^{3}_{1}\mathrm{H} + {}^{4}_{2}\mathrm{He} + {}^{1}_{0}\mathrm{n} $$

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.

Data Generation

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

Paramak was 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 $^6\mathrm{Li}$ enrichment fraction	$[0, 1]$
	Breeder material	$\{Li_2TiO_3, Li_4SiO_4\}$
	Breeder packing fraction	$[0, 1]$
	Coolant fraction†	$[0, 1]$
	Coolant material	$\{D_2O, H_2O, He\}$
	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:

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

Decoupled Approach

Outline

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

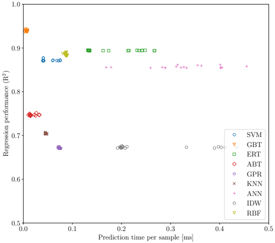
- Support vector machines,
- Gradient boosted trees,
- Extremely randomized trees,
- AdaBoosted decision trees,
- Gaussian process regression,
- *k* nearest neighbors,
- Artificial neural networks (MLP),
- Inverse distance weighting,
- Radial basis functions.

Performed 4 experiments:

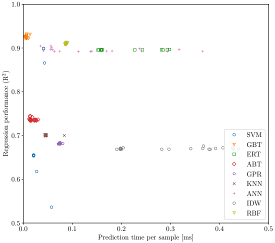
1. Hyperparameter tuning (simplified) – Bayesian optimization, discrete features fixed & withheld.
2. Hyperparameter tuning – same as #1 but with all features.
3. Scaling benchmark – increase training set size.
4. Model comparison – train surrogates for practical use.

Experiments 1 & 2: Hyperparameter Tuning

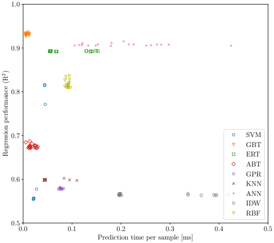
Experiment 1, slice (a)

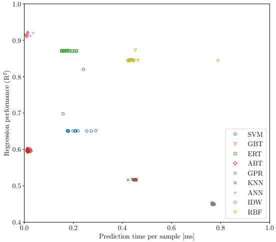


Experiment 1, slice (b)



Experiment 1, slice (c)



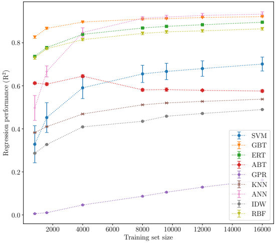


Experiment 2

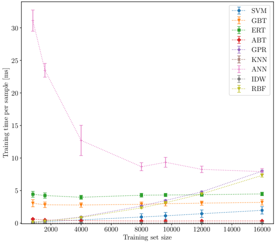
- Plots show $\bar{t}_{\text{pred.}}$ vs. R^2 for 20 best surrogates per family (fastest, most accurate = top left).
- Omitting discrete features yields only a negligible improvement in performance.
- Overall dominated by tree-based surrogates (GBTs, ERTs) and neural networks.

Experiment 3: Scaling Benchmark

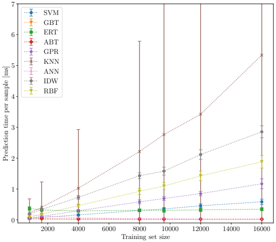
- We observe a hierarchy.
- Best-performing families from the previous experiments also scale the best in $\bar{t}_{\text{pred.}}$.
- More samples: neural networks outperform tree-based models.
- Instance-based surrogates (KNN, IDW) train trivially but have complex lookup.
- Neural networks show inverse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



Regression performance



Training time / sample

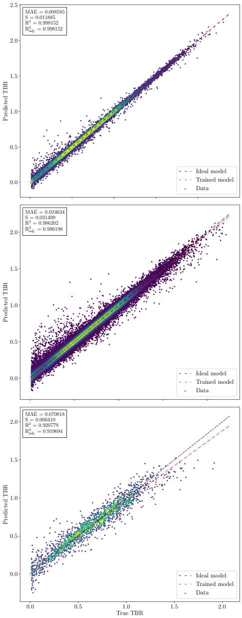


Prediction time / sample

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.

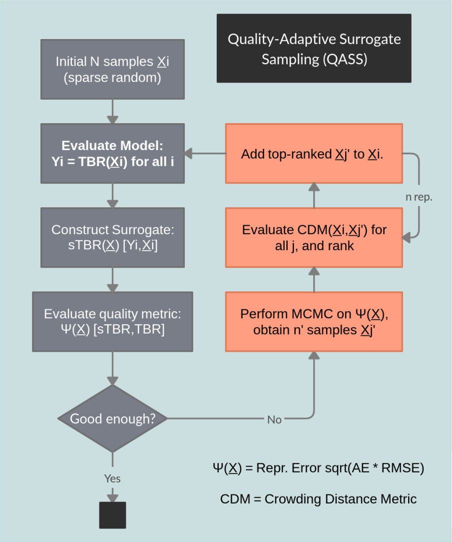
Adaptive Approach

Adaptive Sampling: Theory

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!



Application on Toy Theory

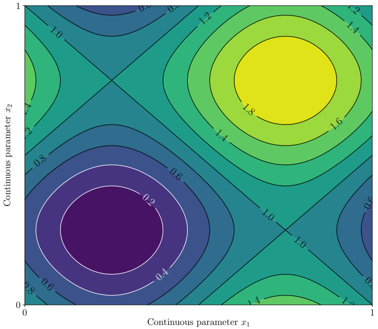
Toy functional TBR theory with wavenumber n, and qualitatively comparable ANN performance to Paramak:

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

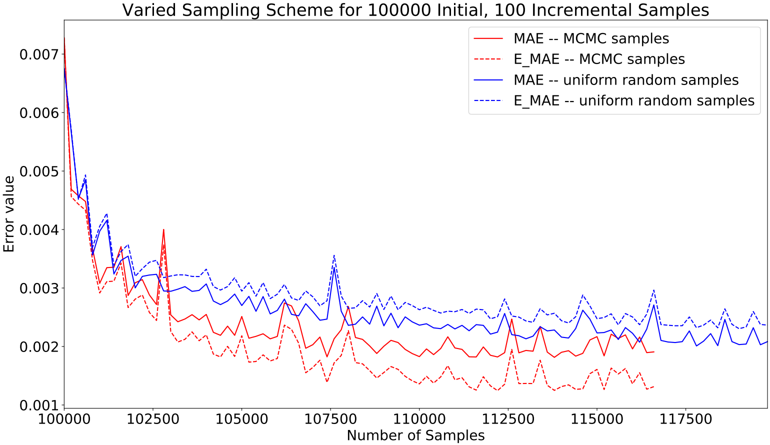
Two evaluation sets:

- Adaptively-sampled dataset
- Independent random dataset

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



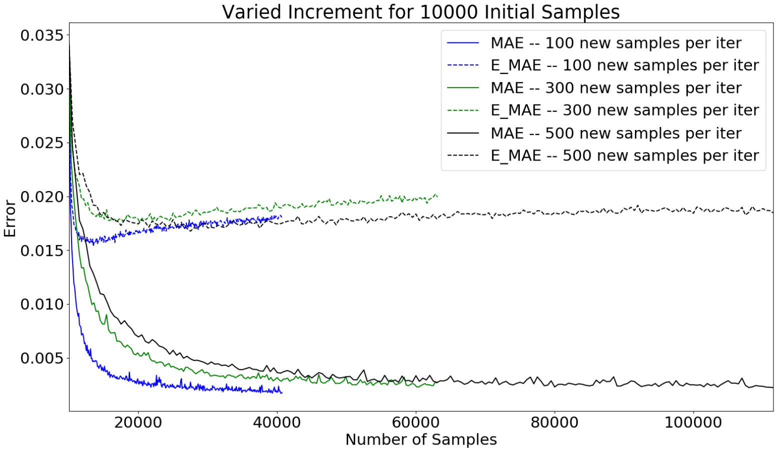
Adaptive Sampling: Results



60% decrease in MAE for independent evaluation (dashed)

Equivalently, 6% decrease in samples needed for same accuracy

Adaptive Sampling: Results



Fewer incremented samples can lead to better accuracy!

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

Conclusion

Decoupled approach:

- Tuned and compared surrogates from 9 state-of-the-art families.
- Found heuristic: GBTs for $< 10^4$ samples, ANNs for $\geqslant 10^5$ samples.
- Fastest found surrogate predicts TBR with standard deviation of error 0.033 in $0.898\,\mu s$, 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 through hyperparameter optimization.

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`