Surrogate Modelling of the Tritium Breeding Ratio

Petr Mánek Graham Van Goffrier

Centre for Doctoral Training in Data Intensive Science
University College London

8th October 2020

Project Background

Nuclear fusion – the energy of the future!

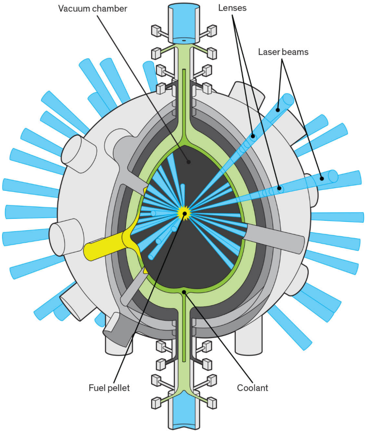


Illustration by Chris Philpot, courtesy of IEEE Spectrum.

- Designing next-generation Inertial Confinement Fusion (ICF) facility.
- Search for optimal reactor design.
- Fueling – important for viability.
- Require fuel of 2 varieties:
  - Deuterium ^2H – abundant in naturally-sourced water.
  - Tritium ^3H – extremely rare.
- Modern reactors can generate tritium during operation.

Problem Description

Tritium breeding blankets convert neutron radiation to ^{3}H fuel:

$$ {}^1_0\mathrm{n} + {}^6_3\mathrm{Li} \to {}^3_1\mathrm{H} + {}^4_2\mathrm{He} \qquad {}^1_0\mathrm{n} + {}^7_3\mathrm{Li} \to {}^3_1\mathrm{H} + {}^4_2\mathrm{He} + {}^1_0\mathrm{n} $$

^{3}H balance described by Tritium Breeding Ratio (TBR) = $\dfrac{\text{fuel bred}}{\text{fuel consumed}}$

- Depends on numerous geometric and material parameters.
- Evaluated by *Paramak* – OpenMC neutronics simulation.
- Slow . . . we want to consider as many reactor designs as possible!

Our Challenge

Produce a *fast* TBR surrogate that strongly approximates Paramak.

Data Generation

Produced datasets by sampling Paramak outputs over its 7 discrete and 11 continuous input parameters at random.

Deployed at UCL's Hypatia cluster:

- Created 1M points.
- 27 days of runtime.

2 classes of runs:

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

	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	$[0, 20]$

Groups of parameters marked†‡ are required to sum to 1.

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 to solution:

Decoupled Approach

1. Collect training dataset.
2. Use data to train a surrogate.

Adaptive Approach

1. Collect initial training dataset.
2. Use data to train a surrogate.
3. Collect more data in regions where surrogate performed poorly.
4. Repeat steps 2 and 3.

Decoupled Approach

Outline

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

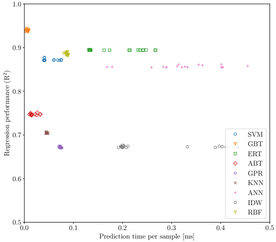
- Support vector machines,
- Gradient boosted trees,
- Extremely randomized trees,
- AdaBoosted decision trees,
- Gaussian process regression,
- *k* nearest neighbors,
- Artificial neural networks (MLP),
- Inverse distance weighting,
- Radial basis functions.

Performed 4 experiments:

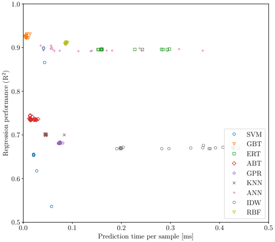
1. Hyperparameter tuning (simplified) – Bayesian optimization, discrete features fixed & withheld.
2. Hyperparameter tuning – same as #1 but with all features.
3. Scaling benchmark – increase training set size.
4. Model comparison – train surrogates for practical use.

Experiments 1 & 2: Hyperparameter Tuning

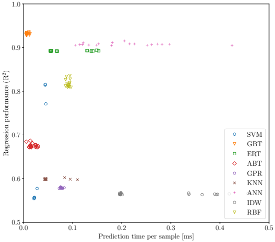
Experiment 1, slice (a)

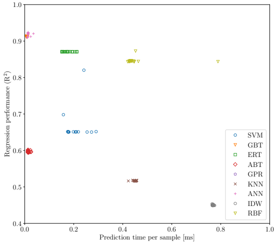


Experiment 1, slice (b)



Experiment 1, slice (c)



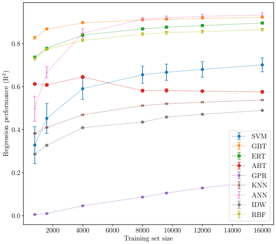


Experiment 2

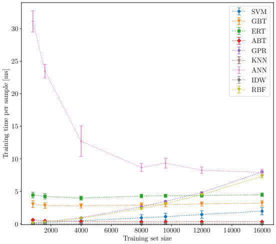
- Showing $\bar{t}_{\text{pred.}}$ vs. R^2 for the 20 best surrogates per family (top left $\Leftrightarrow$ fastest, most accurate).
- Omit discrete features $\rightarrow$ negligible performance improvement.
- Dominated by trees (GBTs, ERTs) and neural networks.

Experiment 3: Scaling Benchmark

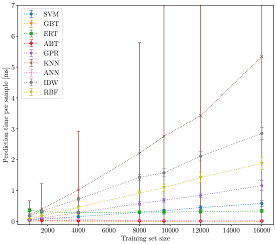
- We observe a hierarchy.
- Trees and neural networks scale the best in $\bar{t}_{\text{pred.}}$.
- Maximizing training set size, neural networks dominate.
- Instance-based surrogates (KNN, IDW) train trivially but have slow lookup.
- Neural networks show inverse scaling due to parallelization.



Regression performance



Training time / sample



Prediction time / sample

Experiment 4: Model Comparison

Trained 8 models for practical use.

Model 1, best regression performance

- ANN (4-layer MLP), 500K samples.
- $R^2 = 0.998$, $\sigma = 0.013$,
- $\bar{t}_{\text{pred.}} = 1.124\,\mu\text{s}$, speedup $6\,916\,416\times$

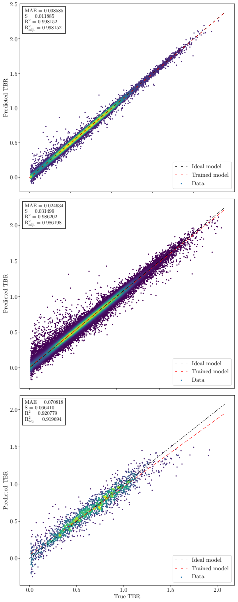
Model 2, fastest prediction†

- ANN (2-layer MLP), 500K samples.
- $R^2 = 0.985$, $\sigma = 0.033$,
- $\bar{t}_{\text{pred.}} = 0.898\,\mu\text{s}$, speedup $8\,659\,251\times$

Model 4, smallest training set†

- GBT, 10K samples.
- $R^2 = 0.913$, $\sigma = 0.072$,
- $\bar{t}_{\text{pred.}} = 6.125\,\mu\text{s}$, speedup $1\,269\,777\times$

† with acceptable regression performance.



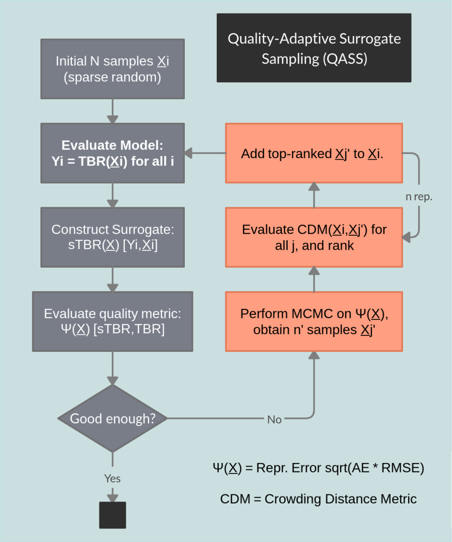
Adaptive Approach

Adaptive Sampling: Theory

How to use information *during training* to reduce sample quantity?

Our novel 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:

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

(where C enumerates all continuous variables)

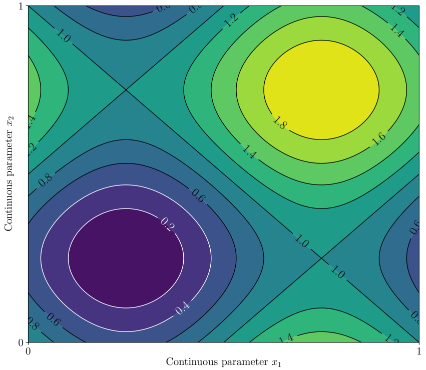
Evaluation set:

- Adaptive samples
- Generated during runtime

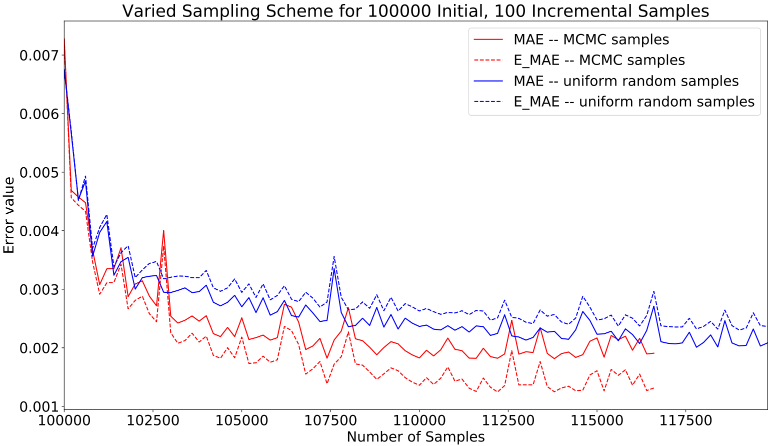
Validation set:

- Uniform random samples
- Generated independently

Placebo comparison – incremental uniform-random samples, no MCMC.



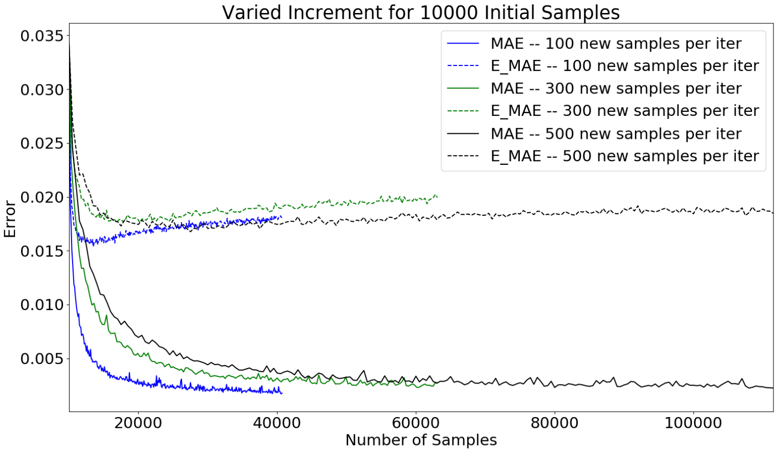
Adaptive Sampling: Results



60% decrease in MAE for validation set (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

- Heuristic: GBTs for $< 10^4$ samples, ANNs for $\geqslant 10^5$ samples.
- Fastest found surrogate evaluates TBR in $0.898\,\mu s$ with error 0.033. This is roughly $8 \cdot 10^6 \times$ faster than Paramak.
- Found surrogates with comparable properties with $\approx$10K samples.

Adaptive Approach

- New theoretical approach QASS developed, based on MCMC.
- 60% decrease in evaluation MAE demonstrated.
- 6% decrease in expensive TBR samples needed.

- Portable methods $\rightarrow$ cheap approximation of any simulation.
- Article in IOP Journal of Nuclear Fusion (pending).
- Included as a benchmark in the SciML Collaboration.

Thank you for listening!

Petr Mánek .... petr.manek.19@ucl.ac.uk
Graham Van Goffrier .... graham.vangoffrier.19@ucl.ac.uk

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`