# Surrogate Modelling of the Tritium Breeding Ratio

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UCL CDT DIS

UK Atomic Energy Authority

# Project Background

Nuclear fusion – the energy of the future!

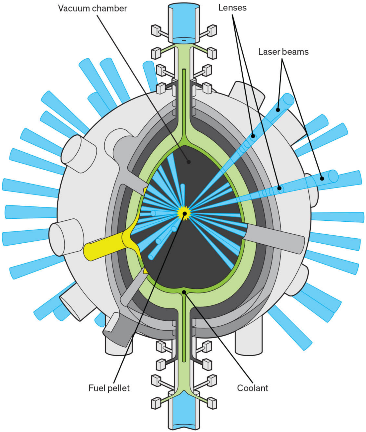



Illustration by Chris Philpot, courtesy of IEEE Spectrum.

- Designing next-generation Inertial Confinement Fusion (ICF) facility.
- Search for optimal reactor design.
- Fueling – important for viability.
- Require fuel of 2 varieties:
  - Deuterium $^2$H – abundant in naturally-sourced water.
  - Tritium $^3$H – 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$^{\dagger}$ | $[0, 1]$ |
| | Breeder $^{6}\mathrm{Li}$ enrichment fraction | $[0, 1]$ |
| | Breeder material | $\{Li_2TiO_3, Li_4SiO_4\}$ |
| | Breeder packing fraction | $[0, 1]$ |
| | Coolant fraction$^{\dagger}$ | $[0, 1]$ |
| | Coolant material | $\{D_2O, H_2O, He\}$ |
| | Multiplier fraction$^{\dagger}$ | $[0, 1]$ |
| | Multiplier material | $\{Be, Be_{12}Ti\}$ |
| | Multiplier packing fraction | $[0, 1]$ |
| | Structural fraction$^{\dagger}$ | $[0, 1]$ |
| | Structural material | $\{$SiC, eurofer$\}$ |
| | Thickness | $[0, 500]$ |
| First wall | Armour fraction$^{\ddagger}$ | $[0, 1]$ |
| | Coolant fraction$^{\ddagger}$ | $[0, 1]$ |
| | Coolant material | $\{D_2O, H_2O, He\}$ |
| | Structural fraction$^{\ddagger}$ | $[0, 1]$ |
| | Structural material | $\{$SiC, eurofer$\}$ |
| | Thickness | $[0, 20]$ |

Groups marked$^{\dagger\ddagger}$ required to sum to 1.

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

Decoupled training approach:

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

Adaptive training approach:

1. Collect initial training dataset at random.
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:

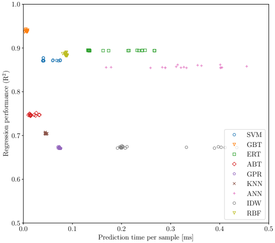
- Support vector machines,
- Gradient boosted trees,
- Extremely randomized trees,
- AdaBoosted decision trees,
- Gaussian process regression,
- $k$ nearest neighbors,
- Artificial neural networks (MLP),
- Inverse distance weighting,
- Radial basis functions.

Performed 4 experiments:

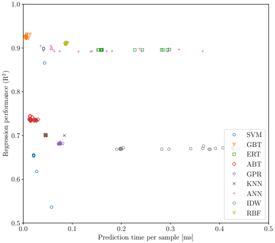
1. Hyperparameter tuning (simplified) – Bayesian optimization, discrete features fixed & withheld.
2. Hyperparameter tuning – same as #1 but with all features.
3. Scaling benchmark – increase training set size.
4. Model comparison – train surrogates for practical use.

# Experiments 1 & 2: Hyperparameter Tuning

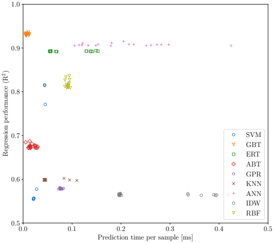
Experiment 1, slice (a)

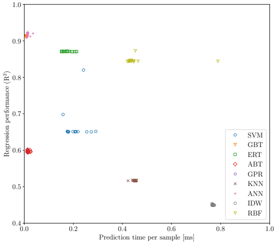



Experiment 1, slice (b)




Experiment 1, slice (c)



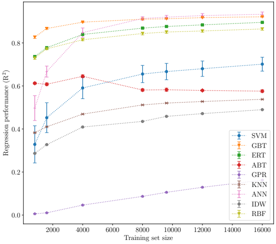




Experiment 2

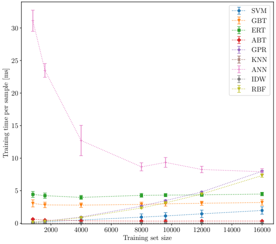
- Showing $\bar{t}_{\text{pred.}}$ vs. $R^2$ for the 20 best surrogates per family (top left $\Leftrightarrow$ fastest, most accurate).
- Omit discrete features $\rightarrow$ negligible performance improvement.
- Dominated by trees (GBTs, ERTs) and neural networks.

# Experiment 3: Scaling Benchmark

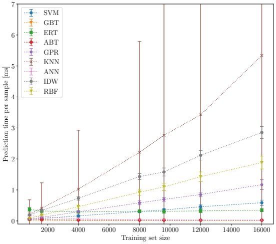
- We observe a hierarchy.
- Trees and neural networks scale the best in $\bar{t}_{\text{pred.}}$.
- Maximizing training set size, neural networks dominate.
- Instance-based surrogates (KNN, IDW) train trivially but have slow lookup.
- Neural networks show inverse scaling due to parallelization.




Regression performance




Training time / sample



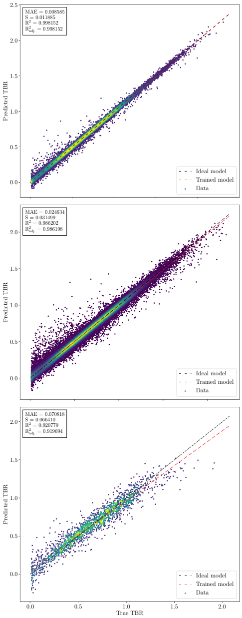

Prediction time / sample

# Experiment 4: Model Comparison

- Trained 8 models for practical use.
- 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.
  - $R^2 = 0.998$, $\sigma = 0.013$,
  - $\bar{t}_{\text{pred.}} = 1.124\,\mu\text{s}$, 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.



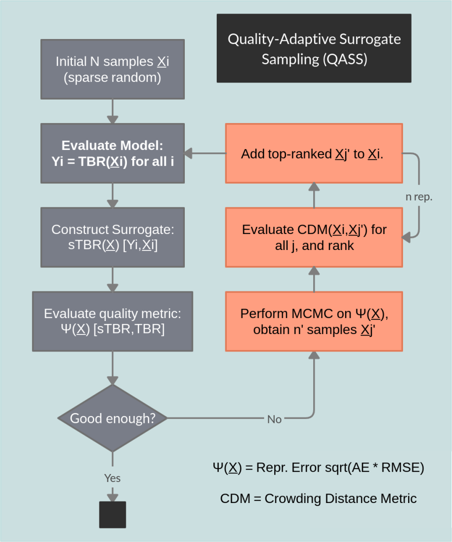
# Adaptive Approach

# Adaptive Sampling: Theory

How 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:

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

(where $C$ enumerates all continuous variables)

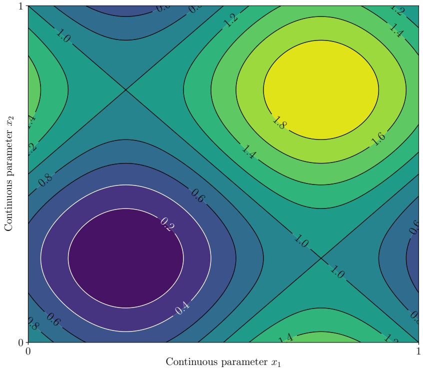
Evaluation set:

- Adaptive samples
- Generated during runtime

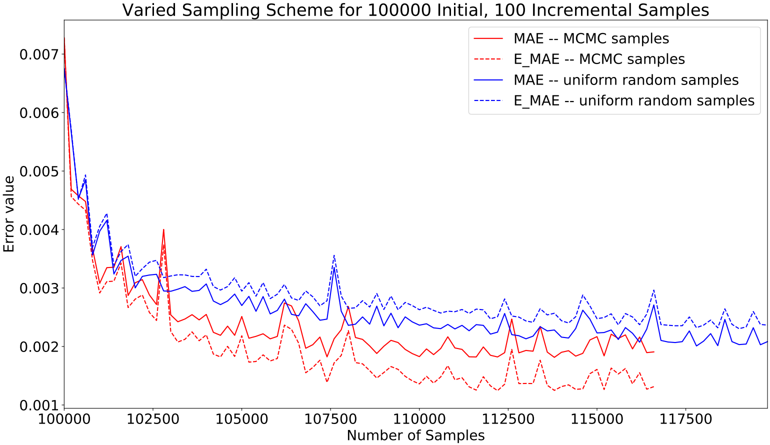
Validation set:

- Uniform random samples
- Generated independently

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



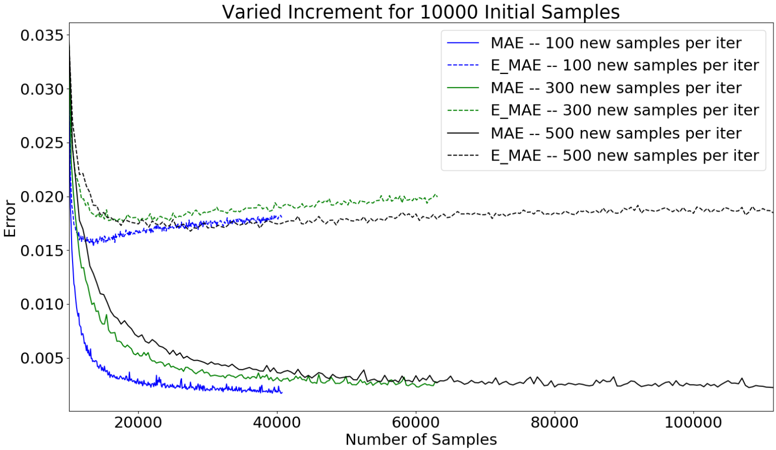
# Adaptive Sampling: Results




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:

- 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 via hyperparameter tuning.

All presented methods portable $\longrightarrow$ 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`