Surrogate Modelling of the Tritium Breeding Ratio

Petr Mánek   Graham Van Goffrier
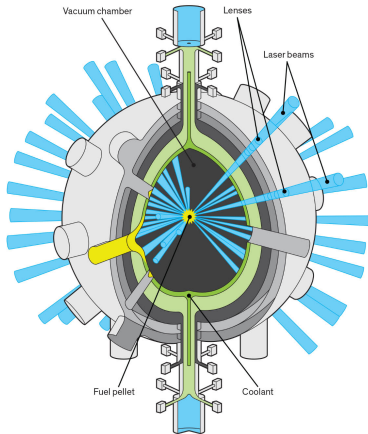
Centre for Doctoral Training in Data Intensive Science
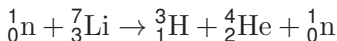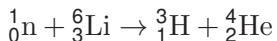University College London

8th October 2020

UK Atomic
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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.

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

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

^{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.

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}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.

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 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

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.
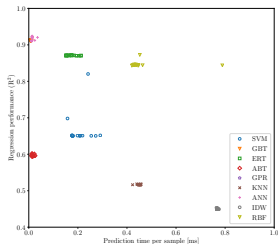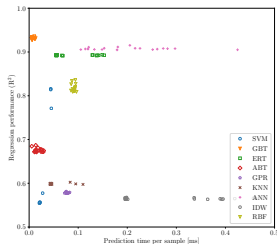4. Model comparison – train surrogates for practical use.

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.
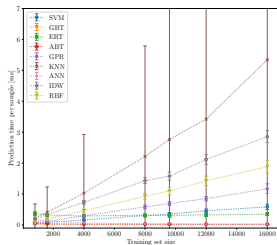
- Dominated by trees (GBTs, ERTs) and neural networks.

- 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.
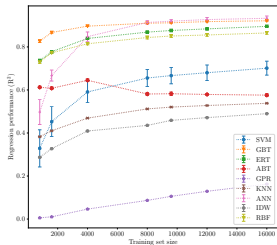
Regression performance
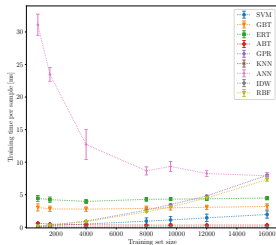
Training time / sample

Prediction time / sample

Experiment 4: Model Comparison

Trained 8 models for practical use.

Model 1, best regression performance

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

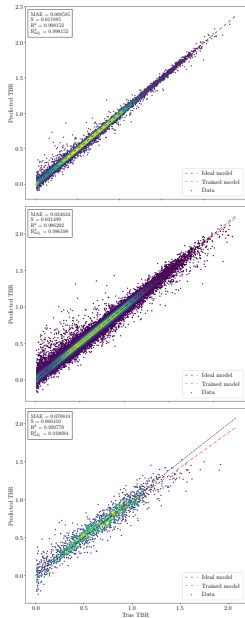## Model 2, fastest prediction[†]

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

Model 4, smallest training set[†]

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

[†] with acceptable regression performance.

Adaptive Approach

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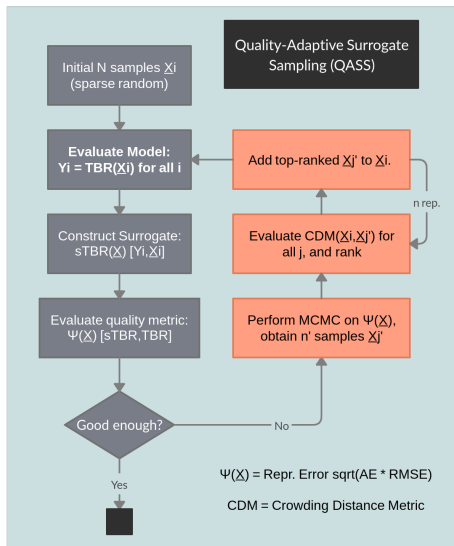
How can we take advantage of surrogate information content *during training* to reduce sample quantity?

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!

Quality-Adaptive Surrogate Sampling (QASS)

Initial N samples $\underline{X}_i$ (sparse random)

Evaluate Model: $Y_i = TBR(\underline{X}_i)$ for all i

Construct Surrogate: $sTBR(\underline{X})$ [$Y_i, \underline{X}_i$]

Evaluate quality metric: $\Psi(\underline{X})$ [sTBR,TBR]

Good enough?

Add top-ranked $\underline{X}_j'$ to $\underline{X}_i$.

n rep.

Evaluate CDM($\underline{X}_i, \underline{X}_j'$) for all j, and rank

Perform MCMC on $\Psi(\underline{X})$, obtain n' samples $\underline{X}_j'$

No

Yes

$\Psi(\underline{X})$ = Repr. Error sqrt(AE * RMSE)

CDM = Crowding Distance Metric

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

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

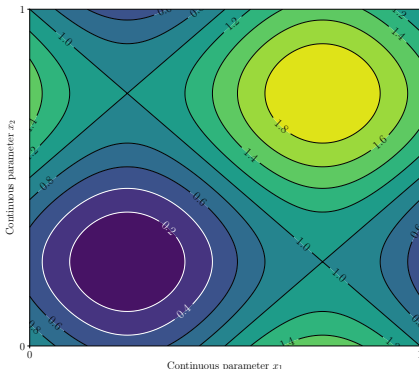(where C enumerates all continuous variables)
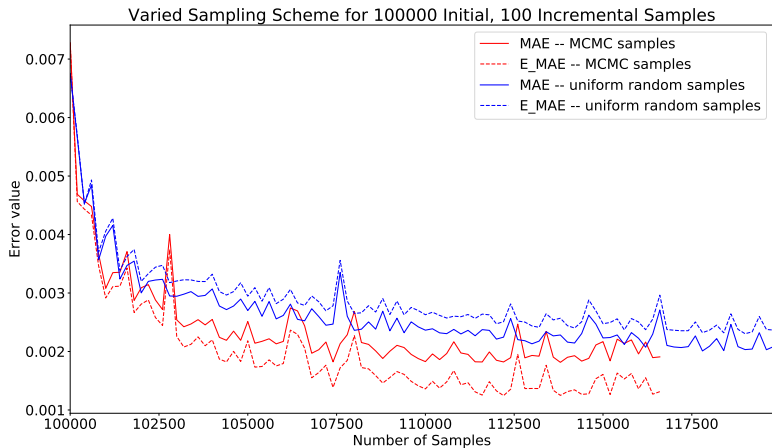
Evaluation set:

- Adaptive samples
- Generated during runtime

Validation set:

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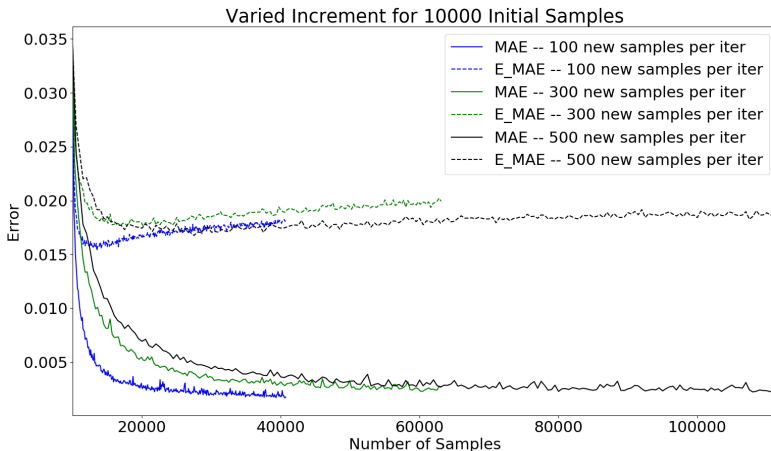
Placebo comparison – incremental uniform-random samples, no MCMC.

Adaptive Sampling: Results

Varied Sampling Scheme for 100000 Initial, 100 Incremental Samples

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

Varied Increment for 10000 Initial Samples

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.

- All methods portable $\rightarrow$ 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`