Higher Fidelity Surrogate Models for Gyrokinetic Simulations

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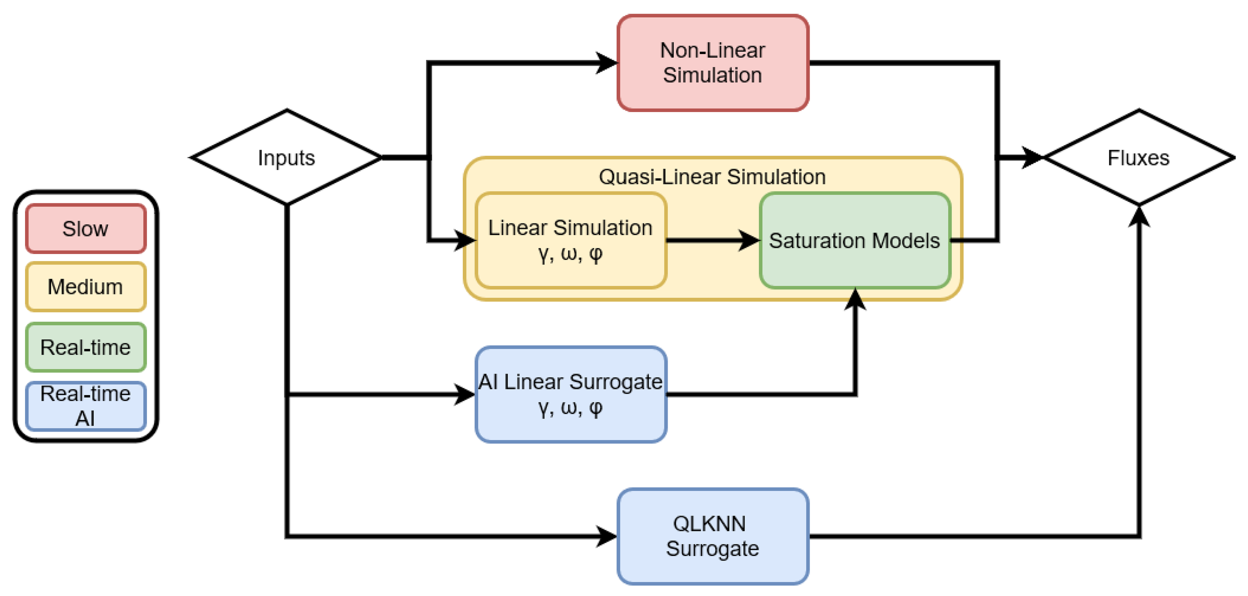
Introduction

Integrated Modelling

- Simulates plasma profile evolution and resulting transport on confinement timescales.
- Uses: Tokamak Design and ITER Scenario Simulations
  - Ideally need a high volume of accurate simulations.
- Bottlenecked by gyrokinetic simulations used to calculate fluxes which need to run ~10^4 times per second of plasma for integrated modelling

Gyrokinetic Models – Flux Tube δf

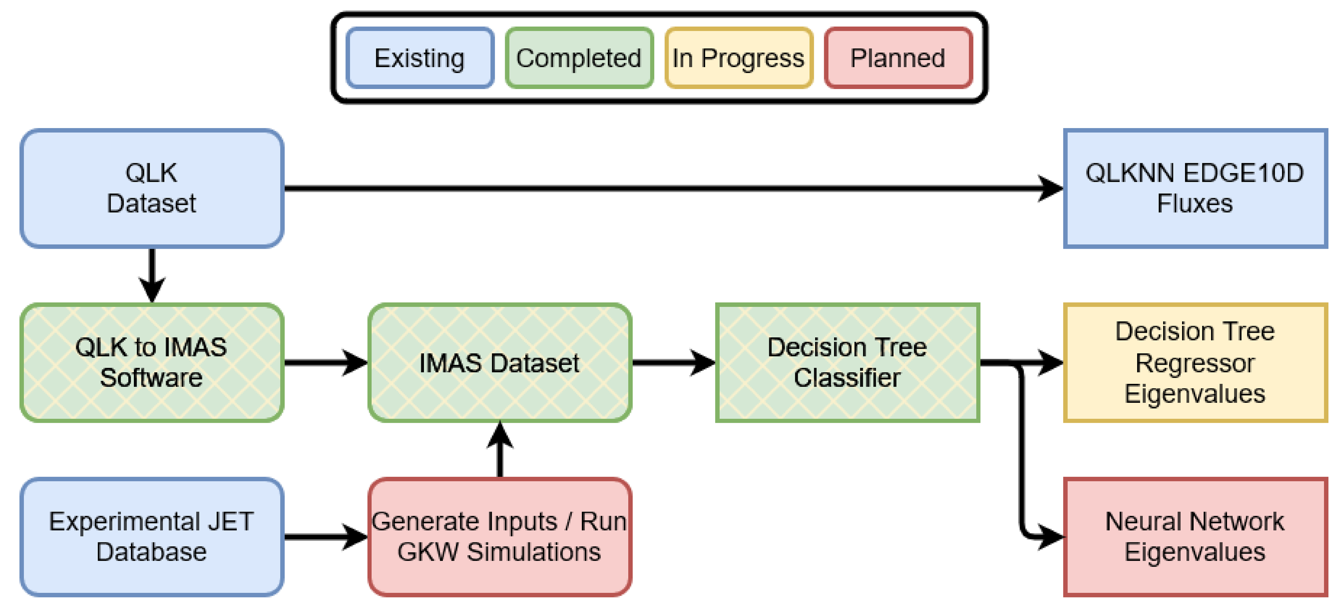
- Solve Fokker-Planck and Maxwell equations, integrating over the gyro-motion of particles to reduce dimensionality
- Inputs: gradients (Temperature, Density, Pressure, etc)
- Outputs: fluxes (particle, heat, momentum, etc)
- Even the fastest reduced models (quasi-linear) are too slow for real-time integrated modelling
- Can AI surrogate models trained on existing simulation results act as a reliable substitute for running new simulations?



FASTER Project

Improve on existing Gyrokinetic AI Surrogates [1,2]

- Train on higher fidelity Linear GKW [3] simulations instead of QuaLiKiz (QLK) [4]
  - GKW is electromagnetic as opposed to electrostatic
  - GKW uses arbitrary magnetic geometry as opposed to circular flux surfaces
  - However significantly increased runtime per simulation
  - Smaller training set (~100,000 vs 256M) with limited computation time
- Train on linear simulations to allow for experimentation of saturation models
- Train on Integrated Modelling and Analysis Suite (IMAS) [5] normalised data
- Test and compare different kinds of machine learning processes for stability classification and linear response regression
  - Decision Trees (XGBoost [6], this poster)
  - Neural Networks (NNs)
  - Gaussian Processes



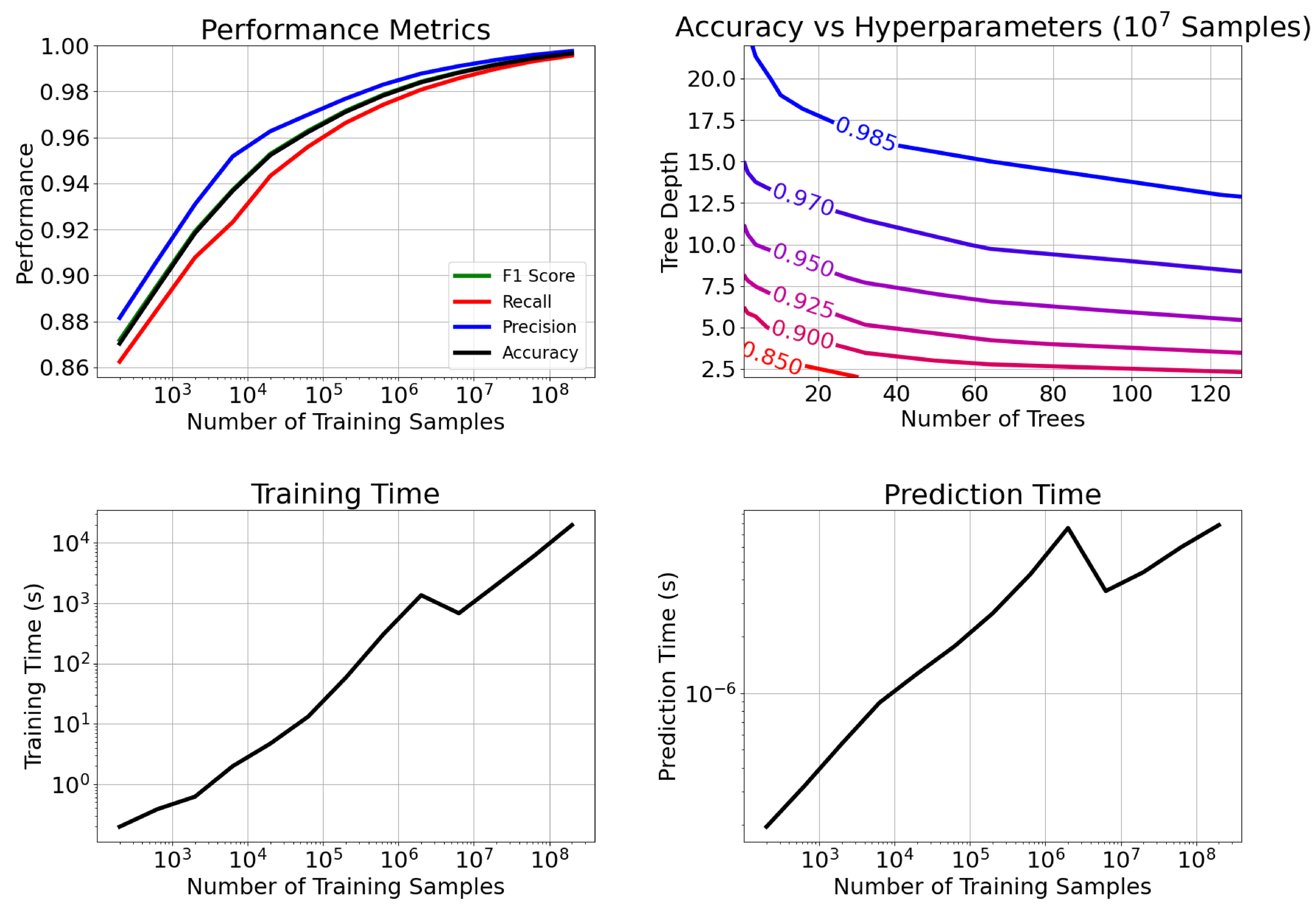
XGBoost Stability Classifier

- Training Dataset: 8D Hyper-rectangle (before conversion to IMAS) of 256M QLK Linear Simulations covering a wide domain of the parameter space to reduce interpolation.
- Trained using XGBoost Decision Tree ensembles (up to 25 depth and 512 trees)
- How does our model accuracy scale with number of training samples?

GKW simulations will be generated with more inputs available than were used for the existing QLK dataset

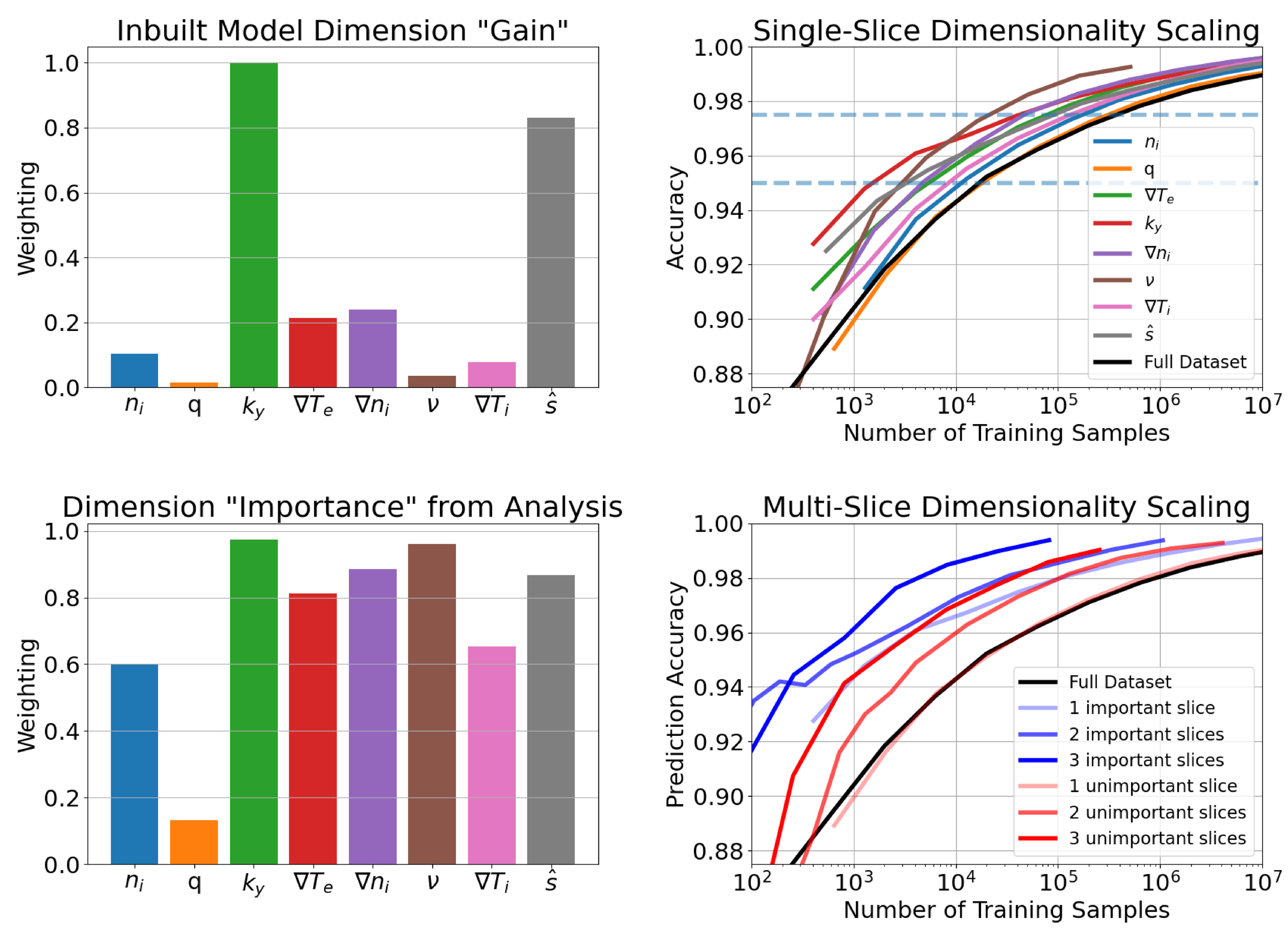
- How is the model scaling affected when an input is fixed?
- Which inputs are the most relevant for the stability decision tree?

Stabiltiy Decision Tree Classifier Scaling



- High baseline accuracy at low amounts of training points (90% with only 1000 points).
- Excellent scaling to almost 100% accuracy when training with 80% of the dataset (200M points).
- Good accuracy even with lower numbers of trees and reduced depth.
- Roughly linear increase in training time and prediction time with number of samples.
- Extremely fast prediction time on the order of 10^{-6} s

Dimensionality Scaling



- Top left: built-in average "information gain" when using a given input to split the data
- Top right: precision gain from fixing a given variable and training new models on subsets of the resulting data slice
- Bottom left: the resulting quantified "importance" of the variables from these results averaged at the 0.95 and 0.975 accuracy thresholds (dashed lines from top right plot)
- Built-in methods of XGBoost to classify variable importance not sufficient
- Bottom right: scaling of fixing multiple slices to further reduce dimensions

Conclusion and Further Work

Conclusion

- Conversion software to link QLK simulations to IMAS format developed and used to convert existing dataset on which to perform training.
- Highly accurate implementation of XGBoost Classifier to quickly predict stability
- Exploration of scaling with number of training points and number of dimensions in preparation for using smaller amounts of higher dimensional data (GKW)

Further Work

- Utilise XGBoost Regressors to predict growth rate and frequencies of dominant mode
- Train NN to predict growth rates and frequencies based on IMAS normalised QLK data
- Generate database of GKW simulations and apply XGBoost and NN pipelines
- Compare performance of different AI models trained on the same data

References

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