Progress towards high fidelity collisional-radiative model surrogates for rapid in-situ evaluation

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Motivation

Modeling the impact of injected atomic impurities in fusion plasmas is critical to the future success of ITER. Collisional-radiative (CR) modeling can be used to find desired quantities like ion populations, $\boldsymbol{n}$, and radiation power for use alongside plasma simulation codes. However, this often finds us handling a large and stiff problem. If we must solve the rate matrix problem in the steady-state

$$\frac{d\mathbf{n}}{dt} = \mathrm{R}(\mathbf{n})\mathbf{n} = 0$$

at each time-step of a plasma code, we create an undesired computational bottleneck for the primary plasma transport code.

A potential solution

In lieu of solving the expensive rate matrix problem, we propose using artificial neural networks (ANNs) to develop a surrogate model for a given gas species, such as neon, to be evaluated with given plasma properties: electron temperature, T_e, neon density, n_{Ne}, and deuterium density in the background plasma, n_D.

One issue with this proposal is the large time it would take to generate suitable training data sets for accurate but expensive CR models one would like to emulate, where one solve may take on the order of an hour.

Adaptively sampling the parameter space

To more purposefully and efficiently generate training data, rather than amassing many thousands of random training data sets over a very long time, we propose using an adaptive sampling method. Our hope is that by sampling a minimal, but representative, training data set in areas of high variance we may train an accurate surrogate in a shorter time.

We employ a low fidelity (LF) random forest regressor (RFR) surrogate to serve as a guide to where further parameter space samples should be taken to aide training the high fidelity (HF) ANN surrogate. The program flow of this method is summarized below:

Algorithm 1: Adaptive CR surrogate training sampling

```
Generate N_init initial samples of forward CR model evaluation;
Train HF surrogate;
while N_samples < N_budget do
    Train LF surrogate to map input field to scalar metric;
    Evaluate fine sample space grid using LF surrogate. Sort by variance;
    for i = 1 : N_samples/10 do
        Take input field of highest variance LF prediction. Generate new sample;
    end
    Train HF surrogate on expanded sample set. Evaluate surrogate metrics.;
    if R^2 > R^2_goal then
        Stop.
    end
end
```

Trialing the method

In this work we employed a compact CR model, that executes on the order of seconds, in order to aide rapid development of our methods. As a baseline, an ANN surrogate was trained on a data set of 3375 samples, with an R^2 of 0.99 on an unseen test set. Employing the adaptive sampling routine to train an ANN surrogate, using either average ion charge or total radiation power as scalar metrics for the RFR surrogate, we observe that the validation performance of the ANN surrogate does improve as the training set of initially 25 samples is augmented by samples from regions in which the RFR surrogate indicates very poor performance, see Fig. 1. In the end, considerably less samples are required for comparable performance on the unseen test data set. The best performing scalar metric produced an R^2 of 0.98 with only 1719 samples required, opposed to 3375.

Ultimately, we believe great time savings will be made in employing such an adaptive sampling method to training an ANN surrogate for CR models, which will provide a rapidly executable option of obtaining the necessary properties of ions and radiation power needed as input to flagship plasma transport codes.

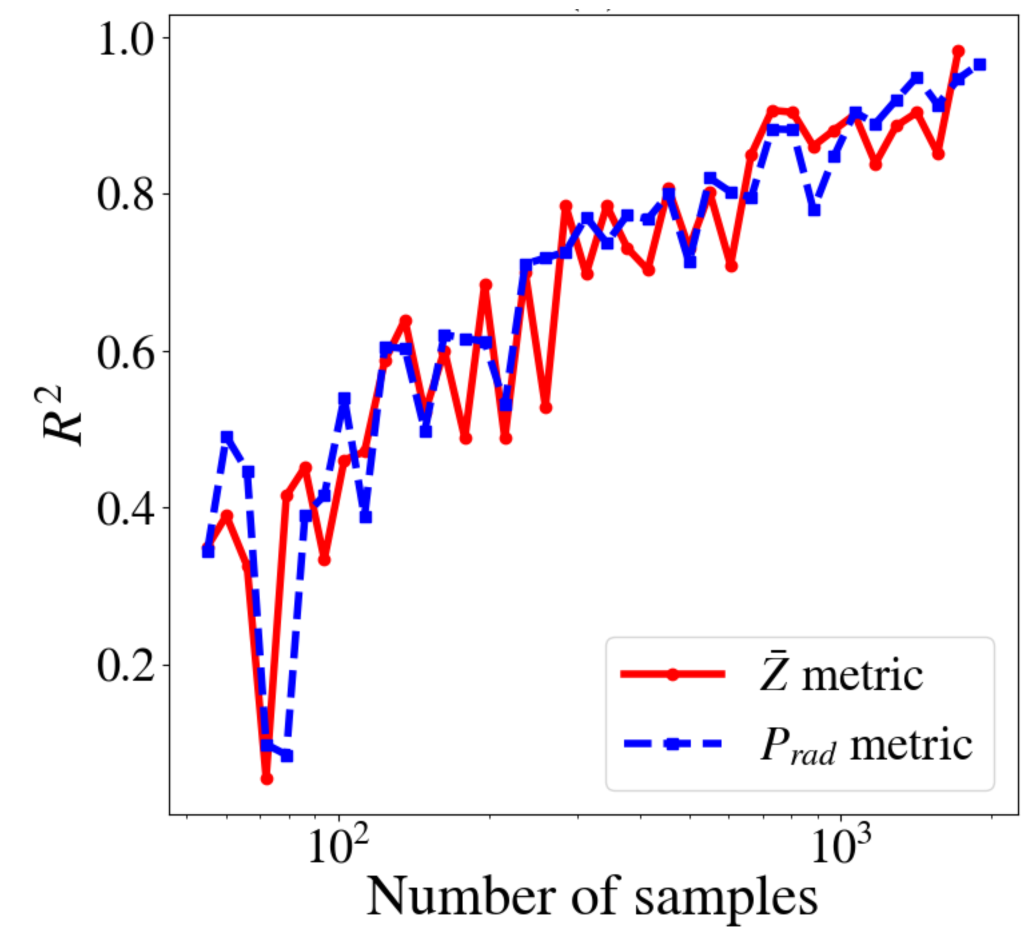

Figure 1. Validation R^2 improvement with acquired samples. The two curves are for separately trained surrogates using either average ion charge, or total radiation power as scalar metrics of the RFR surrogate.

Conclusions

With encouraging performance of a simple adaptively trained ANN surrogate, we are motivated to employ further enhancements to our method, and deploy it to train surrogates for multiple atomic species and then implement said surrogates within plasma transport codes in order to improve the physics descriptions of our simulations, without adding a prohibitive bottleneck to the computation.

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